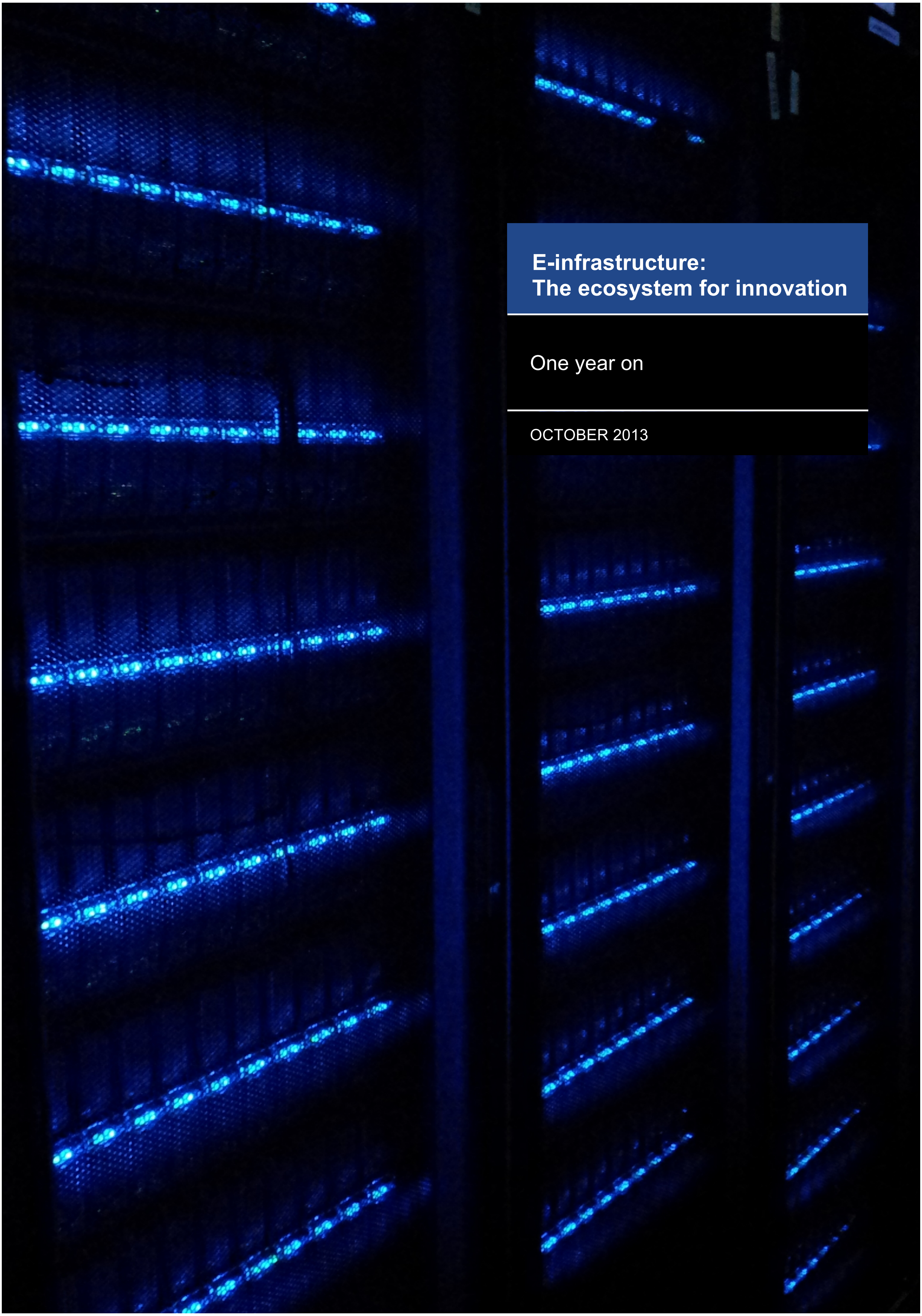

E-infrastructure: The ecosystem for innovation

One year on

OCTOBER 2013

Contents

Foreword

On 13th July 2011 I hosted a seminar to discuss the rapidly emerging importance to science and business of big data, high performance computing (HPC) and the associated e-infrastructure. That meeting convinced me that we are experiencing a fundamental change in the way that research and development are being undertaken. The use of modelling and simulation, and the manipulation of massive and dynamic data sets from experiment, is now central to discovery and innovation. Having access to the necessary e-infrastructure is therefore essential for academic and business excellence.

I commissioned Dominic Tildesley, then Vice President Discovery Platforms for Unilever Research and Development, to produce a report on how we could create the right e-infrastructure in the UK to ensure that we remained competitive in science and innovation. Dominic's Report, "A Strategic Vision for UK e-Infrastructure" was published in January 2012. Amongst other things, it recommended that I establish an E-infrastructure Leadership Council (ELC), with membership drawn from industry, academe and the public sector to advise me on the necessary course of action. This I did.

Using the analysis in the Report I was also able to secure £160 million in 2011 for investment in the UK e-infrastructure – software development, HPC, data storage and networks. I was able to supplement this in the 2012 Autumn Statement when the Chancellor provided an additional £189 million.

These investments and the work of the work of the ELC have helped to transform the profile of big data and e-infrastructure in the UK. From being an esoteric scientific tool in academe, it is now recognised as an essential element of UK national infrastructure to underpin our knowledge economy.

This document summarises what we have achieved over the past year or so. Whilst I am very pleased with our progress, the ELC has highlighted areas where there is more to do. Looking forward therefore, I will continue to work for the development of the UK e-infrastructure, in partnership with academe and industry, to ensure that our researchers have access to the best tools available.

I will also be working with the ELC to take forward the agenda set out in the Information Economy Strategy for a Data Capability Strategy in October 2013. This is further recognition by Government that big data and the enabling e-infrastructure underpins the delivery of virtually every aspect of our Industrial Strategy.

I look forward to being able to report further progress in another year's time.

Rt Hon David Willetts MP, Minister for Science and Universities

This document is dedicated to Professor Michael Wilson, Secretary to the E-infrastructure Leadership Council, who passed away suddenly and unexpectedly on 30th April 2013.

Executive summary

The 2012 *Strategic vision for the UK e-infrastructure* was a response to the paradigm shift that we are experiencing, in which the scientific process and innovation are beginning in the virtual world of modelling and simulation before moving to the real world of the laboratory. This is a shift in which sophisticated analysis and visualisation software are being used to mine massive amounts of experimental data from the life and environmental sciences to uncover new hypotheses and trends. The *Strategic Vision* set out a clear view of elements of the advanced computational capacity of the UK as a system – an e-infrastructure. It presented a ten-year strategy for the development and management of the UK's e-infrastructure. To implement the strategy it proposed a series of recommendations around software, hardware, networks, data services, cyber security and skills that will help to develop the e-infrastructure.

The Government has made significant progress towards achieving this vision:

- by establishing the E-infrastructure Leadership Council as a single coordinating body that owns this strategy and can advise BIS Ministers on its implementation and development;
- by investing £160 million in high performance computing and networks in 2011;
- by announcing a further £189 million of funding for big data and energy efficient computing in 2012.

The e-infrastructure in the UK today is a complex interaction of software, computer hardware, networks, data services, cyber security and the skills of the people who make the e-infrastructure work. It is a vital part of the "… science infrastructure that can give UK industry the edge over our competitors. 21st century infrastructure needed for a 21st century Britain."[1]

But there are still outstanding challenges to be faced in the years ahead to reap the benefits of these capital investments:

- The E-infrastructure Leadership Council has proposed the creation of Software and Data On-ramp Centres where academia will work with UK industry to exploit the e-infrastructure collaboratively by raising awareness in industry, especially in SMEs, providing support for the use of these capabilities, and making available cutting edge HPC facilities.
- A significant gap is developing between the available engineers in the workforce skilled in computational science and big data analytics, and the number demanded by industry and commerce, both now and, increasingly, in the future. To provide the workforce required, training in these skills is required within undergraduate degrees in many disciplines, at Masters level, and to refresh skills throughout the professional life of engineers.
- The hardware resources of the e-infrastructure will need updating as computer, data services and networking technologies continue to advance. The e-infrastructure requires sustained capital investment and especially recurrent support in order to maintain its effectiveness, and to provide the cutting edge facilities and expertise that academic and industrial researchers require.

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[1] Investing in Britain's future, Cm 8669, June 2013 at www.gov.uk/government/publications/investing-in-britains-future

Introduction

"It costs £500,000 to do each physical test of a car crash, and it's not repeatable. It costs £12 to run a virtual simulation of a car crash, and it's fully repeatable, so it can be used to optimise the design of a vehicle." Andy Searle, Head of Computer Aided Engineering, Jaguar Land Rover.

There has been a revolution in research and innovation. The ability to generate, collect and process almost unthinkable quantities of data for exploitation by industry, academia, and Government provides a real opportunity to enhance UK competitiveness and grow the UK economy.

The 2012 report *Strategic vision for the UK e-infrastructure* was a response to the paradigm shift that we are experiencing, in which the scientific process and innovation are beginning in the virtual world of modelling and simulation before moving to the real world of the laboratory. This is a shift in which sophisticated analysis and visualisation software are being used to mine massive amounts of experimental data to uncover new hypotheses and trends. The *Strategic Vision* sets out a clear view of the advanced computational capacity of the UK as a system – an e-infrastructure. It presented a ten-year strategy for the development and management of the UK's e-infrastructure. To implement the strategy it proposed a series of recommendations around software, hardware, networks, data services, cyber security, and skills to help develop an e-infrastructure ecosystem.

Recommendations from the *Strategic vision for the UK e-infrastructure:*

- Implement an agreed and costed strategy that recognises a balanced need for both capital and pre-determined recurrent resources, using the established baseline and additional Government funding to build the partnership. Increase private sector funding over a ten-year period.
- Create specialist centres to develop robust software of value to academy, industry and Government. Although this is only one element of the infrastructure, it is critical to its success.
- Embed training in e-science in all postgraduate training, including in successful Doctoral Training Centres. Use these modules to offer training to industry where appropriate. Support the publication of reports, technical workshops and conferences for the community funded by this programme.
- Set up a single coordinating body that owns this strategy and can advise BIS Ministers on its implementation and development. This E-infrastructure Leadership Council should be co-Chaired by the BIS Minister for Universities and Science and an industry representative.
- Support the Council with an independent E-infrastructure Secretariat providing the Council with information and costed proposals based on a wide consultation with academic, industrial and Government partners.

In response to these recommendations (thus far)

- In 2011 the Government provided £160 million of capital funding for high performance computing and network infrastructure. In the 2012 autumn statement they provided a further £189 million of funding to address Big Data and energy efficient computing.
- A number of specific investments are in the process of being, or have been realised, such as: the Hartree Centre at the STFC Daresbury Laboratory to create a state-of-the-art supercomputing environment with respect to both hardware and HPC skills, ARCHER to provide a national-level HPC service, and The Genome Analysis Centre to develop and enable computational and genomics data-driven approaches in the bio/life sciences, to name a few.
- In March 2012 Government created the E-infrastructure Leadership Council (ELC) to make recommendations to Government on all aspects of e-infrastructure. Members of the ELC come from the academic community, industry, the research and funding councils, Government departments, and the charitable sector.
- The Department of Business Innovation and Skills has provided a secretariat to the E-infrastructure Leadership Council to provide it with information and costed proposals based on a wide consultation with academic, industrial and Government partners.

This document provides an overview of the UK's e-infrastructure strategy as of 2013. The focus is on the initial steps, taken in the first year, towards developing an e-Infrastructure ecosystem. The document begins by outlining the motivation for an evolving e-infrastructure strategy, given the emerging technological changes and the opportunities that these present for the UK. The current e-infrastructure landscape is then described, accounting for the Government's recent investments in the area (since 2011). This is followed by a brief description of the considerations and next steps for continuing the development the UK's e-infrastructure ecosystem.

Technological developments

E-infrastructure must adapt to the often rapid changes in information and technology. Here, the three prominent developments concern **big data**, **evolving scientific models,** and **new computing architectures.** The UK must provide the infrastructure to leverage these technologies, in order to drive innovation and growth.

It is important that an information-based economy, like that of the UK, takes full advantage of changes in the information and technological landscape. The ELC has identified three technological developments that e-infrastructure investments must aim to support.

1) Big data

"The right use of big data allows analysts to spot trends and gives niche insights that help create value and innovation much faster than traditional methods" WIPRO Technologies[2]

Since the development of the original e-Infrastructure strategy, a new trend has emerged that will be of great importance for the evolution of the UK's future e-Infrastructure – Big Data. *Big data* refers to the fact that more data is being produced, consumed, and stored than ever before, resulting in datasets that are too large, complex, and/or dynamic to be managed and analysed by traditional methods. The big data problem is often described with reference to the 3Vs (*Gartner*): *volume* – the amount of data; *velocity* –the speed in which data is created, processed and transferred; and *variety* – the range of data sources. All of these are rapidly increasing, resulting in ever-greater complexity.

The goal is to be able to extract meaning, and therefore value, from big data. In the context of e-infrastructure, data includes both newly generated and existing publicly-funded data (i.e. from research projects and Government). The issue concerns managing the complexity; that is, considering how to store, manage and curate such data, and the software, analytical models, visualisations, and skills/expertise required to extract useful results.

In an information-based economy, issues of big data affect *all* sectors.[3] Infrastructure supporting big data enables value creation, by facilitating analysis, insight and innovation. This is explicitly identified by Government, who considers big data one of the "eight great technologies" to drive future growth in the UK.[4] The integration of big data with their analyses often requires novel computer architectures.

2) New computing architectures

There are disruptive changes taking place with respect to computer architectures. Massively multi-core technologies promise greatly increased computational power, reduced power consumption and are of a smaller (physical) size. Cloud technologies, in conjunction with improved networking capabilities, are enabling remote access to

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[2] http://visual.ly/big-data

[3] "Big data: The next frontier for innovation, competition, and productivity", McKinsey Global

[4] "Eight Great Technologies", David Willetts MP, Policy Exchange (Jan 2013), http://www.policyexchange.org.uk/publications/category/item/eight-great-technologies

increasingly rich set of computing resources. Given the trends in technological adoption, it is likely that increasingly powerful computational resources will become more accessible and widespread. In many cases they will need close integration with the data(bases) that they use.

Clearly, such advancements pave the way to tackling harder, more complex problems, and thus enable innovation and the development of new markets. However, different problems require different architectures - e.g. shared memory with many CPUs, many CPUs with distributed memory, data intensive computing, many GPUs pipelines, etc. In many instances, the applications of such technology cannot be used ‘out of the box’. New software and programming models, along with the appropriate training, promotion and support, are required to realise fully the potential of the opportunities that these new architectures present.

3) Model evolution

Mathematical and scientific models are developed to explain particular phenomena, forming the basis for technological innovation. An evolving paradigm is *multiscale modelling,* which involves combining models of different scales (size, granularity and/or time), and perhaps integrating those across scientific and engineering disciplines, to facilitate the understanding of large and complex systems. Figure 1 illustrates a multiscale model from the materials domain for bitumen. A multiscale approach drives innovation, as it provides the basis for tackling large-scale, challenging problems that were previously infeasible or too difficult to manage as a whole.

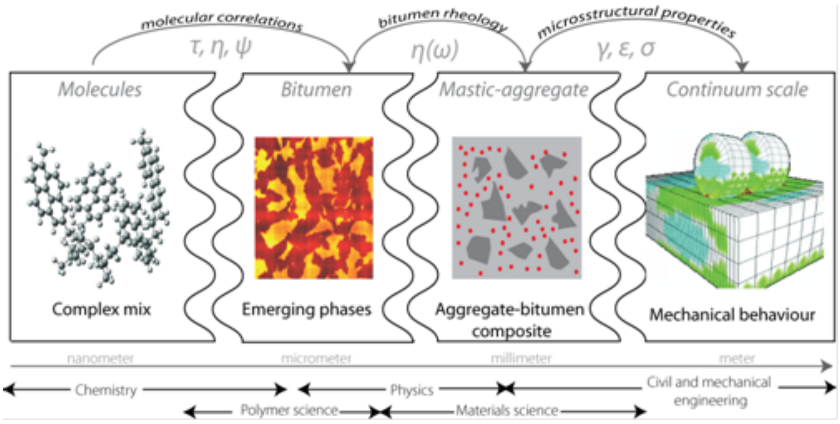

Figure 1: Multiscale modelling of the properties of bitumen, illustrating integration between models of different sizes and disciplines. (Image courtesy Capa-3d.org)

Such modelling has a strong computational basis: changes in models lead to changes in algorithms, which lead to changes in software. Sometimes these analyses can be done in a coarse-grained parallel manner, with clusters of cheap commodity computers providing the necessary hardware. In other cases, high-end computing resources are required to deal with the complexity of the approach. In general, the current generation of modelling systems are not readily adaptable to exploiting next-generation architectures (and *vice versa*). It follows that in addition to hardware resources, specific software and design expertise is required to support model development.

The opportunity for the UK

"We have some of the best scientists, excellent facilities and cutting edge technology, and it is our determination that we do all we can to ensure that the UK remains one of the world leaders in this field for many years to come" *David Cameron, Prime Minister, February 2011*

In a global context, these technological developments provide opportunities for nations that are suitably prepared to take advantage of the benefits. The UK is particularly well placed because:

1. The UK boasts a **strong research base** across a wide range of disciplines. UK academe is highly regarded, operating at the forefront of scientific research. UK scientists have a strong track record of using e-infrastructure resources to tackle advanced problems effectively; for example, in fields such as climate modelling, computational fluid dynamics, molecular modelling, cosmological simulation, genomics and the digital humanities.

2. It has **responsive funding bodies** that:
    a. Have strategic programmes that support innovation at various stages – from basic research in computer science through to commercialisation of ideas developed using e-science approaches.
    b. Have flexible mechanisms that are able to respond to emerging e-infrastructure technologies and enable their uptake by the research base.

3. It has a **world-class computing and network infrastructure** dedicated to meeting the needs of leading-edge and data-intensive research. This is being further enhanced by current investments to exploit the unparalleled opportunities opened up by new technologies and paradigms associated with "big data" in life sciences, health care, environmental monitoring, advanced manufacturing and the information economy.

4. It fosters an environment of **close academic-industrial** cooperation that promotes open access to facilities, cross-fertilization of expertise in e-infrastructure and translation of research outputs to the commercial sector.

5. The UK has an **established international network,** maintaining strong academic and industrial links with key global players. The UK is an active partner in international coordinating initiatives in e-science, such as the LHC computing GRID, European Social Survey and ELIXIR, and home to major industries attracted by the UK's outward-facing philosophy.

6. Its established knowledge-based economy means **existing infrastructure and skills** can be leveraged, and further developed, e.g. the UK's strength in software development. The UK holds unique and world-leading datasets of international importance; for example, longitudinal studies in the health and social sciences. Combined with skilled human resources, these can be employed to derive new knowledge and promote innovation.

7. There exists **strong Governmental support** for fostering innovation driven by computational approaches, as evidenced by recent capital investments in e-infrastructure and strategic leadership from BIS.

It is clear that by capitalizing on its existing strengths the UK has the potential to be a world leader. It is therefore necessary to ensure that both industry and the research communities are adequately prepared, equipped and supported to exploit these technology-driven opportunities, and thus drive jobs and growth.

UK Industrial Strategy

Changes in the international economy mean both an increase in competition and opportunities from global markets. The Government has developed an industrial strategy which is about setting out a long-term, whole of Government approach to growth working in partnership with business. This will give confidence now for investment and growth. The Business Secretary Vince Cable set out the Government's approach to industrial strategy in September 2012 [5]

Government has identified several areas where industry-government action can have a real and early impact namely in **sectors**; **technologies**; **access to finance**; **skills**; and **procurement.** In sectors industrial strategy is developing strategic partnerships with eleven sectors which could make the greatest contribution to future economic growth and employment in the UK and where Government can have the greatest impact. By summer 2013 Government working in partnership with business will publish 11 sector strategies.

Namely, these are:

Advanced manufacturing, including aerospace, automotive, life sciences and agri-tech

Knowledge intensive traded services, including professional and business services, the information economy and traded aspects of higher and further education.

Enabling sectors, such as energy (nuclear, offshore wind and Oil and Gas) and construction.

Horizontal policies, such as setting the legal and regulatory frameworks in which businesses across the economy operate are clearly crucial but action on access to finance, skills, technologies and procurement are often required too. Economic conditions vary across sectors and horizontal considerations give key insights into how to design and deliver policy.

The sectors addressed by the industrial strategy are all ones where societal drivers indicate there is likely to be significant increasing domestic and global demand; where UK business has the potential knowledge and skills to exploit new market opportunities (i.e. the UK has a comparative advantage in global markets in virtually all these areas); and where a sector-based approach has a clear role.

The sectors where innovation-based growth is predicted – namely the life sciences, agri-tech, construction, energy, manufacturing, information economy and professional services sectors – are also those which can exploit the e-infrastructure to accelerate that growth. It is therefore crucial that the e-Infrastructure is leveraged to reduce the time and expenditure associated with the process of innovation. Businesses that fail to do so will not only forgo new opportunities, but also lose any competitive advantage to rival firms, local or international.

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[5] *BIS Economic Paper No 18: Industrial Strategy: UK Sector Analysis*. http://www.bis.gov.uk/assets/BISCore/economics-and-statistics/docs/I/12-1140-industrial-strategy-uk-sector-analysis.pdf. (2012)

The role of e-infrastructure

E-infrastructure refers to the ecosystem of resources that allows distributed collaboration and computation, large-scale simulation and analysis, and fast access to (large) data collections (well organized according to accepted standards and with rich metadata), analytical and visualization services and facilities. This also includes the development and leveraging of leading-edge skills, methods and tools to exploit the potential of the available data and resources.

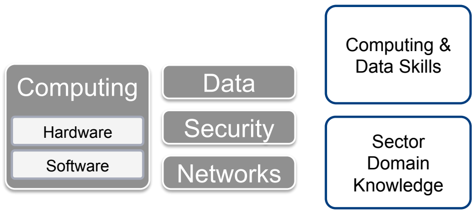

Figure 2: A vision of the integrated e-infrastructure ecosystem

E-infrastructure is crucial to innovation across a range of industries. An appropriate e-infrastructure is essential to ensuring that the UK is in a position to take full advantage of the opportunities that the technological developments bring. The result is to enhance UK competitiveness and grow the UK economy. Such readiness requires development of the e-infrastructure ecosystem, through investments into the:

- Appropriate **technical infrastructure**
- **Training and skills** necessary to leverage such infrastructure
- **Awareness and support** mechanisms for ensuring exploitation of the capability

The role of Government is to coordinate, encourage and foster the development of a national e-infrastructure strategy, implemented in collaboration with industry to ensure relevance and widespread usage and adoption for a full realisation of the benefits.

The e-infrastructure landscape

E-infrastructure is an ecosystem. Its components not only concern technical (hardware) aspects, but also software capabilities, training and skills development, promotion, awareness and adoption, and the provision of the appropriate management/governance structures.

The UK has been investing in e-infrastructure for a number of years, though this was without an overall vision, and thus developments have tended to be fragmented. The Government has recently recognised the value of e-infrastructure, undertaking coordinated efforts to build a cohesive ecosystem. The investments of 2011 have focused on the development of technical computing capability, particularly that around advanced modeling and simulations using HPC. Future investments will focus on Big Data with data management and analytics as well as aspects such as awareness, training and skills.

We now outline the current state of the e-infrastructure landscape.

Resource infrastructure

Resource infrastructure, as it pertains to the hardware aspects of e-infrastructure, falls into three categories: high-end computing (or HPC), networks and data services.

High-end computing infrastructure (architecture)

"High-Performance Computing (HPC) is critical for industries that rely on precision and speed, such as automotive and aviation, and the health sector. Access to rapid simulations carried out by ever-improving supercomputers can be the difference between life and death; between new jobs and profits or bankruptcy." *Communication from the EC: 'High-Performance Computing: Europe's place in a Global Race' COM (2012) 45 Final. Brussels 15.02.2012*

High-end computing (or High Performance Computing [HPC]) infrastructure provides the means to tackle computational problems that are too large, complex or would take too long on standard machines. Traditionally, HPC infrastructure was ranked on its size and cost. However, such a categorisation is no longer appropriate, as different problems require different architectures, e.g. shared memory with many CPUs, many CPUs with distributed memory, data intensive computing, many GPU pipelines, etc. The appropriate scale and architecture will be driven by the problem area, using a range of facilities from the local research-group level, to facilities of universities, regional, national and (occasionally) international. There has been investment into HPC resources in the UK for some time. However, a coordinated approach was taken by the Government with its investments in 2011. These are described in Table 1.

Project	£M
ARCHER *(EPSRC):* The major national supercomputing facility (replacing HECToR) hosted in Edinburgh. Under procurement, for launch in 2013.	43
DiRAC 2 *(STFC)***:** Upgrade to the distributed national HPC facility, spanning various sites. The focus is on particle physics and astronomy research.	15
JASMIN & CEMS *(NERC/Space Agency):* Development of a joint data analysis facility and infrastructure to support data intensive computing for atmospheric research.	7.75
MonSooN *(Met Office/NERC):* Upgrading the weather forecasting computer to facilitate the incorporation of new science from NERC funded research.	1
The Genome Analysis Centre *(BBSRC)*: Upgrade to the cluster, tiered storage and bandwidth capability.	8
Five Regional HPC Centres *(EPSRC):* Investment into HPC infrastructures for collaborative work to serve demand at various regions. Projects: e-infrastructure South Innovation Centre, N8 Research Partnership, ARCHIE West, HPC Midlands and Mid-Plus.	6.5
TOTAL	**£81.25M**

Table 1: Government capital investment into HPC for 2011-2012

The distribution of the UK's high-end computing infrastructure is shown in Figure 3.

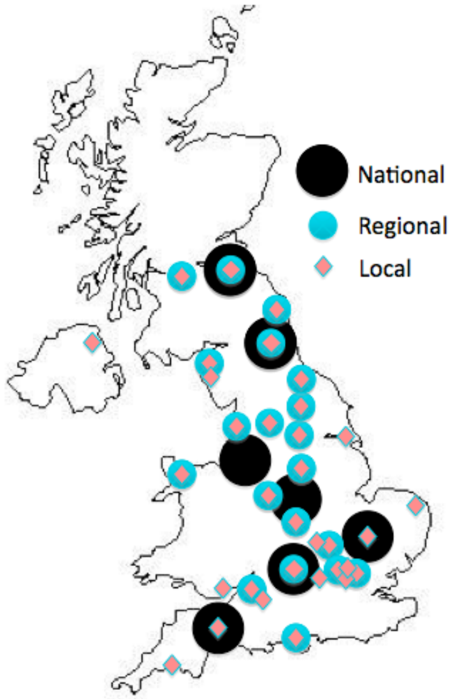

Figure 3: The distribution of high-end

Local infrastructure refers to that of Higher Education Institutes (HEIs)/Research Groups, typically involving new and evolving research themes. This leads to the creation of new computational models and processes, and computationally aware scientists and engineers for cutting-edge research in the UK.

Regional resources service a larger geographical domain and present in two distinct forms: (1) consortia of HEIs and research institutions (increasingly with shared resources), and (2) larger regional facilities generally dedicated to specific areas. Their geographical reach, range of expertise and existing resources equip them to offer these services to companies. However, the UK needs to do more to ensure the appropriate architectures are offered for the problems tackled in different sectors.

National resources provide high-powered, state of the art research computing facilities that typically cater to a wide range of academic disciplines. However, increasingly high technology business needs access to such infrastructure for innovation. The investments, as described in Table 1, refer to national level infrastructure, except for the Five Regional Centres. Resources also exist at the international level, such as the pan-European PRACE and the European Grid Initiative.

Networking infrastructure

To form an effective e-infrastructure ecosystem, individual components such as HPC need to be linked together via a high-performance (very high bandwidth) network tuned to the demands of those using e-infrastructure in leading-edge research and development. This is particularly important given the ever-increasing volumes of data involved.

Figure 4: The Janet6 Network Infrastructure

This network is provided by Janet, the UK's National Research and Education Network (NREN). Janet has been supporting research and education since its inception in 1984. To ensure that it remains able to support these communities it regularly undergoes major upgrade programmes. The latest of which is nearing completion and has been funded in part to ensure that Janet remains very highly scalable to the "data deluge" expected from the UK's research base over the rest of the decade.

The heart of Janet is a UK-wide backbone of 6,500 km of fibre which at its launch will provide some 2 Terabit/s of aggregated bandwidth. This is expected to increase four or five-fold over the next five years. This backbone is illustrated schematically in Figure 4 – it is no coincidence that the coverage of the backbone matches closely the distribution of HPC illustrated in Figure 3. It is an example of the coordination already being achieved within the ecosystem.

In recognition of the ever-increasing global nature of data-intensive research, Janet is seamlessly integrated into GÉANT, the pan-European interconnect of more than thirty NRENs, and from there to other NRENs and e-infrastructure across the world.

Although Janet's origins were in the university sector, it now supports a very wide range of users and uses, including collaborative research and technology transfer activities of universities with industry. As part of the e-infrastructure ecosystem, Janet will increasing support industry directly, to enable industrial research and development to benefit from access to the rich set of HPC and data already developed and exploited so effectively by academe and public funding.

Data infrastructure and services

The collection, storage, management and analysis of data are likely to be the most important source of wealth generation to be derived from the UK e-infrastructure. As this is recognised by Government, there are movements in developing the appropriate supporting infrastructure and services. For instance, in 2011 £24M was pledged for development of data infrastructure and the 2012 Autumn Statement announced the funding of a number of facilities for supporting big data.

It is important to note some data initiatives aim specifically at supporting HPC and simulation services, while others will support data provision, sharing, analytics, mining and visualisation. Regarding the former, each high-end computing service has some provision for storing data for making use of the service they offer, though none preserve data for the long term. However, a number of computational domains involve generating a large simulated data set, for repeated subsequent analysis; thus, there is a requirement for adequate post-generation storage and management facilities, which may be perhaps made available for other purposes. Regarding the latter, it tends to be the more recent investments that aim at analytics.

In 2011, RCUK published Common Principles on Data Policy,[6] to guide the Universities and Research Councils in developing their individual data policies. This enables a devolved approach, which is suitable given that management requirements (storage, security, etc.) will vary depending on the data concerned. The report states the importance of preserving data, developing and using standards for the structure of data and metadata, and encouraging its sharing to validate scientific results. The outcome would be rich datasets that can be used for a variety of purposes, to foster insight and innovation.

Regarding specifics, NERC and STFC have a different mandate, hosting data infrastructure for data related to their HPC services. The ESRC supports the UK Data Archive to host a wide-range of data from its grant holders, and the UK public sector. The RCs also rely on grant holders, or their institutions to provide appropriate data management facilities. The European Bioinformatics Institute at Hinxton (Cambridge), to which the Government recently committed £75M,[7] routinely stores biological data types (such as protein structures, biochemical network models, microarray data), while The Genome Analysis Centre at Norwich possesses a multi-PB data store for genomics data. To assist, the Digital Curation Centre (DCC) – dedicated to building capacity, capability and skills for research data management – also provides expert advice to those in UK education and research to manage their digital data.

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[6] http://www.rcuk.ac.uk/research/Pages/DataPolicy.aspx

[7] http://www.bbsrc.ac.uk/news/research-technologies/2011/111205-pr-investment-european-research-infrastructure.aspx

The Autumn Statement 2012 announced Government (capital) investment into a range of big data initiatives for the period 2012-2015. Table 2 presents a breakdown of those investments that relate specifically to data infrastructure, by research council and the particular focus. Some of these initiatives aim at particular research objectives for a discipline, while others are more general, such as the *Administrative Data Centres* that aim at linking, managing and analysing administrative data across Government departments and studies, and the *Business Datasafe* that aims at linking disparate (and sensitive) data sets across a wide-range of public and private sector organisations. Figure 5 represents the data infrastructure landscape in light of these investments.

Project	Implementer	Capital £M (2012-15)
Digital transformations in arts and humanities: Exploring historic artefacts, data and heritage and to support the development of new research-based creative outputs	AHRC	8
E-infrastructure for biosciences: Driving knowledge generation from genotype (simple 'big-data') to phenotype (massively complex 'big data')	BBSRC	13
Research data facility and software development: Extending capacity of the existing Research Data Facility, in providing data storage for the High Performance Computing services to foster collaborative and cross-disciplinary research	EPSRC	8
Administrative data centres: Providing a robust evidence-base to inform research, and policy development, implementation and evaluation	ESRC	36
Understanding populations: Capitalising on public data assets and extending the value of other publicly funded large-scale surveys, including vital events data, health records, welfare data, biomarkers and the genotyping of DNA samples	ESRC	12
Business datasafe: Aiding the management and analysis of organisational data, including store cards, client lists held by utility companies, banking transactions, mortgage details, communications data, and social scientific survey data	ESRC	14
Biomedical informatics: Creating a virtual UK-wide institute of medical bioinformatics, involving hubs of excellence across the UK, to enable large-scale analysis of complete biomedical, healthcare and social data.	MRC	55
Environmental virtual observatory: Providing improved access to environmental and catchment modelling information and prediction, and to make environmental data more visible/accessible to a wide range of potential users	NERC	13
TOTAL		**£159M**

Table 2: Government investment into a big data initiative, as announced in the Autumn Statement 2012

Other data infrastructure investments include the Open Data Institute,[8] a not-for-profit funded by the Technology Strategy Board (£10M over 5 years, subject to industry investment) and by industry is a big data undertaking dedicated to providing open access to data from across the public sector in order to enable industrial and academic exploitation. In 2012, the Clinical Practice Research Datalink,[9] a £60 million service funded by the MHRA and the National Institute for Health Research, was established to provide patient data for medical research. The Government has also earmarked £100 million for the NHS to sequence the DNA of up to 100,000 patients with cancer and rare diseases, which will include the development of appropriate data infrastructure (NHS).[10]

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[8] http://www.theodi.org/about

[9] http://www.cprd.com/

[10] https://www.gov.uk/Government/news/dna-tests-to-revolutionise-fight-against-cancer-and-help-100000-nhs-patients

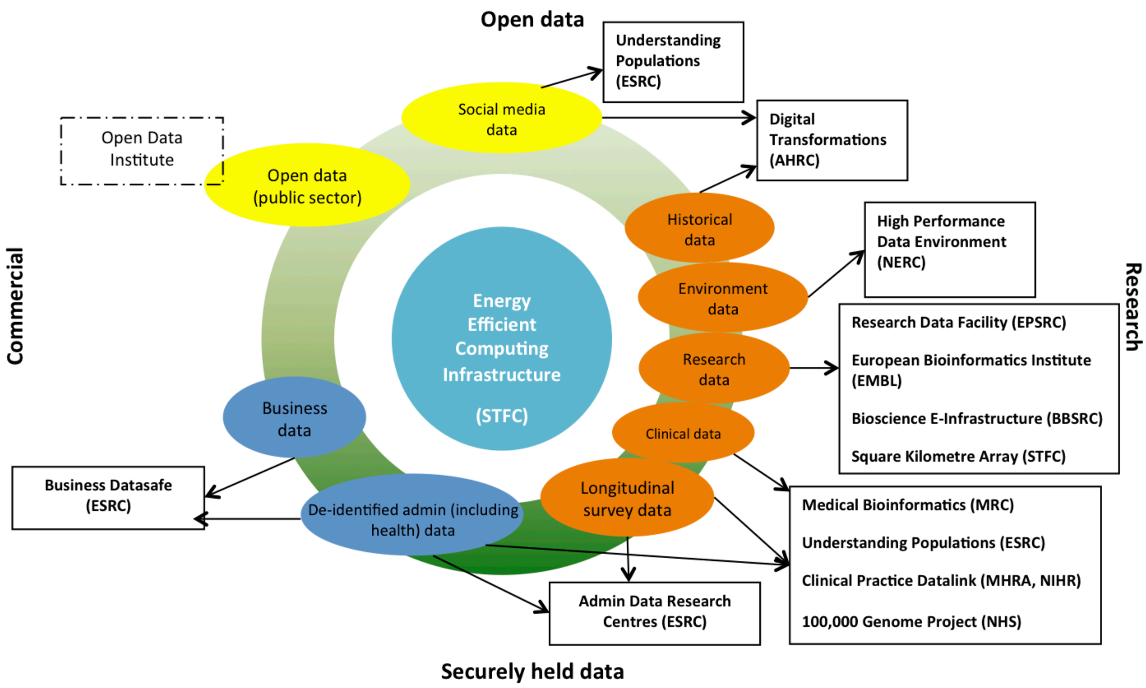

Figure 5: Recent investments into UK research & public data infrastructure

Software

Software is essential to a successful e-infrastructure programme, as it drives the scientific and technological innovation. It is critical to exploiting the e-infrastructure ecosystem, as it is software that enables the representation and processing of complex models, the ability to develop and run simulations, as well as the means to performing advanced data analytics. It is therefore crucial that UK invests in developing and maintaining a strong software capability.

The EPSRC has directly recognised the importance of software as e-infrastructure in its own right. Through their *Software as an Infrastructure* strategy, they have invested £45M over the previous five years into building software capability, developing software skills, maximising impact, and fostering long-term sustainability and support.[11] The BBSRC has long had funding streams (Strategic Tools and Resources Development Fund; Bioinformatics and Biological Resources Fund) dedicated to e-infrastructure including software development, purposely ring-fenced from hypothesis-dependent grant proposals. As presented in Table 3, the STFC manages a range of initiatives that include developing and promoting a software capability within the HPC space. Note that many of these initiatives relate to the high-end computing aspect. More is considered needed in software for data science and analytics.

Project	Investment Period	£M
Hartree Centre*:* National centre of software expertise for collaborative development of new models, algorithms and software (focusing on massively parallel and data intensive applications) to advantage HPC resources, and to encourage HPC adoption.	2011-2012	37.5
Energy efficient computing*:* Platform for the development of energy efficient computing, linking the facilities, operating systems, middleware and hardware for different classes of computing problems.	2012-2015	19

[11] http://www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/software/Pages/software.aspx

Project	Investment Period	£M
Square Kilometre Array computing platforms: Developing new algorithms and codes to exploit hardware technology and ensure proper scientific and technology transfer returns for the world's largest radio telescope project	2012-2015	11
TOTAL		**£67.5**

Table 3: Projects with a strong software component, as managed by the STFC

Software suffers from issues of sustainability concerning its on-going use, support, maintenance, promotion, availability and evolution. All too often the software capability developed as part of a project is lost when the project finishes and/or a staff member leaves. The Software Sustainability Institute, funded by RCUK and operated by a collaboration of Universities, also aims to address such concerns by actively promoting software-related issues. Specifically, the institute provides consulting services, advice on best practices, and drives collaboration and community engagement initiatives.

A related issue is software accessibility, which concerns the ability of software to be used by non-programmers or computational experts. The more people that are able to use software, the greater the possibility for analysis and insight. Improving accessibility involves providing suitable and familiar interfaces, and software hardening, making sure it is robust and that any failures occur in a soft and manageable manner. Further, it involves training software experts in the importance of such issues, and ensuring that projects with a software undertaking devote resources towards this aim.

Another challenge involves developing software in order to fully realise the benefits of innovations in hardware. For example, the Met Office has just embarked on a collaborative project to develop weather and climate models that aim to exploit the emerging Exascale technologies that are expected in the early 2020s. The size and duration of the project mean that development is a several hundred person-year effort.

It is important that software is considered a capital asset, because: a) it is crucial to operating and/or improving the efficiency of hardware infrastructure; b) it is possible for software to hold value over a longer period than hardware; and c) software can often be used for a range of different purposes – perhaps in addition to those for which it was designed. Software represents a significant investment that can provide a tangible ROI both in terms of the functionality it provides and by exploitation of the associated intellectual property rights. Even when freely licensed, the impact of software can result in significant returns, for example, through customisation and specialist consulting services.

Cyber security

"The risk is that many companies feel that when a cyber attack takes place their reputation is at risk and it could impact on share price" Francis Maude MP, Cabinet Office Minister, March 2013

Given the UK's information-based economy, and the increasingly online nature of UK society, issues of cyber security are of increasing importance. The Government is taking active steps in addressing such concerns. It has allocated £650M (2011-2015) to the delivery of its National Cyber Security Programme to strengthen the UK's cyber capacity.[12]

[12] *Securing Britain in an Age of Uncertainly: Strategic Defence and Security Review (SDSR),* HM Government, (2010)

The strategy aims to combat cyber threats/attacks, prevent cybercrime, protect UK infrastructure, promote/ensure the stability of the UK business environment, and develop the knowledge, skills and capability to address cyber issues. Some initiatives implemented so far include:[13]

- The establishment of two Cyber Research Institutes,[14] academic, industrial and Government (including GCHQ) collaborations for exploring cyber security issues. The first was launched in Sept 2012 (£3.8M) and the second in Mar 2013 (£4.8M).
- Recognising 11 Universities as Academic Centres of Excellence in Cyber Security Research,[15] aiming to enhance the quality and scale, as well as promote cyber research
- Investing £350M into Centres for Doctoral Training,[16] two of which will specialise in cyber security.
- Introducing the Cyber Security Information Sharing Partnership[17] (Mar 2013), to share security and threat information across Government and industrial sectors.

With respect to e-infrastructure, these initiatives will raise awareness and provide the capability to recognise and protect the value of the information contained. These will also promote related issues of compliance, such as with data protection legislation, to ensure, for example, proper anonymisation where personal data is involved.[18]

E-infrastructure access control

Given that an e-infrastructure ecosystem naturally entails shared resources, it is important that access is regulated in a manner that protects the value of information and meets any compliance requirements, while being compatible with business needs. Specifically, these concerns surround authentication, authorisation and accounting/audit (AAAI). JANET is in the process of trialling Moonshot, its unifying identity/access management infrastructure. UK e-science infrastructure also provides a single-sign on service, taking a Shibboleth and a certificate-based approach. Moving forward, the goal is to have shared AAAI mechanisms across e-infrastructure to reduce the overheads and risks of duplicate and/or redundant regimes.

Training and skills

A properly skilled workforce is crucial for an information-based economy. Currently, the UK ranks 5th in the world in IT industry competitiveness and in IT human capital (2011).[19] However, since 2003, the number of students taking Computing A-Levels has reduced by 63%, and ICT GCSE courses dropped 70% since 2005.[20] At the higher-education level, there has been a decline in the order of 50% for since 2001 in those completing computing

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[13] For a complete list, see https://www.gov.uk/Government/policies/keeping-the-uk-safe-in-cyberspace.

[14] http://www.gchq.gov.uk/Press/Pages/Second-Cyber-Research-Institute-launched.aspx

[15] http://www.epsrc.ac.uk/research/centres/Pages/acecybersecurity.aspx

[16] http://www.epsrc.ac.uk/skills/students/centres/Pages/centres.aspx

[17] https://www.gov.uk/Government/news/Government-launches-information-sharing-partnership-on-cyber-security

[18] The European Commission is currently reviewing issues of data protection. The UK Government is actively involved, to ensure that strong protection measures are balanced with the usefulness of information.

[19] *Benchmarking IT Industry Competitiveness 2011.* Economics Intelligence Unit, Business Software Alliance

[20] *Technology Insights 2012,* e-Skills UK.

subjects.[21] Given the increasing demand for those with STEM skills,[22] it follows there is a great risk of a skills shortage that could undermine UK's competitiveness.

Issues of training and skills underpin the success of any e-infrastructure undertaking. Skills must be developed, particularly in computational techniques and data science, to: 1) ensure the effective utilisation of e-infrastructure, and 2) be in a position to recognise and advantage new and potential opportunities. It is important that training initiatives aim at developing an appropriate mix of skills. For example, despite the demand for computational skills, computer science graduates have the highest rate of unemployment on leaving University of all subject areas.[23] This highlights the issue that those with a general computing background typically lack sector-specific expertise, while those trained for a particular sector often lack the relevant computational and data skills.

Developing computational skills should begin early. In line recommendations from the Royal Society,[24] Education minister Michael Gove MP announced in Jan 2012 that the existing ICT curriculum would be abolished in order to introduce new, more relevant computing courses. In line with this, the schools curriculum is currently being revised.[25]

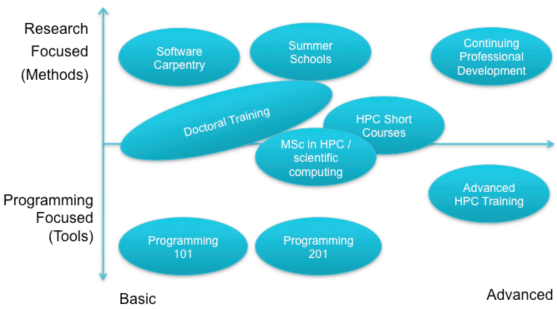

Figure 6: E-infrastructure training programmes, as supported by the Research Councils

There are a number of training initiatives at the higher-education level. These are operated and funded by a variety of different bodies. Universities and Research Councils support a number of academic programmes, from computational modules, and undergraduate and doctoral courses, to research projects, short courses, summer schools, etc. (see Figure 6). However, there remains an acute shortage of undergraduate summer schools and Masters'-level conversion courses. Institutions that deal in a particular capability or infrastructure will often provide the associated training programmes. The European Bioinformatics Institute (EMBL-EBI) provides a wide-range of courses, local, online and around the world, covering various levels and aspects of bioinformatics. Other, smaller-scale examples include the HPC courses by the Hartree Centre;[26] workshops in software by the Software Sustainability Institute;[27] and data management training by the Digital Curation Centre.[28]

Though the UK features world-class e-infrastructure training resources, several issues remain. First, many skills development programmes focus on HPC. Given the emerging opportunities that data present, there needs to be more in the way of data science training, addressing various aspects of the data life cycle including big data analytics and machine

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[21] *The Decline in Computing Graduates: A Threat to the Knowledge Economy and Global Competitiveness*, CPHC, eSkills UK, BCS, Intellect (2007)

[22] *The Demand for Science, Technology, Engineering and Mathematics* (STEM) Skills, Dept. Innovation Universities and Skills UK, URN 168-09-SC-on, (2009)

[23] http://www.hesa.ac.uk/index.php?option=com_content&task=view&id=1899&Itemid=239

[24] *Shutdown or restart: The way forward for computing in UK schools*. Royal Society (2012).

[25] https://www.education.gov.uk/consultations/downloadableDocs/040713%20NC%20in%20England%20consultation%20-%20govt%20response%20FINAL.pdf

[26] http://www.stfc.ac.uk/Hartree/Solutions/Training+and+education/39992.aspx

[27] http://www.software.ac.uk/what-do-we-do/training

[28] http://www.dcc.ac.uk/training

learning technologies. More generally, there is the issue of **fragmentation**; many different institutions provide a number of different training resources, varying in goals, material covered, duration, specialisation, levels of awareness, visibility, and exposure. While there is power in diversity, a lack of coordination can lead to skills shortages in particular areas. Related is **continuity**, which concerns how skills are further developed, perhaps across training institutions, and ensuring that skills are not 'lost', for example, as often occurs on completion of a project or as a member of staff leaves.

Awareness and adoption

A successful e-infrastructure ecosystem encourages technology adoption. Mechanisms must be available to raise awareness of the available resources and their possible uses, to communicate the potential of emerging technologies, and support collaboration.

Institutions will promote the services they offer, such as a University advertising their HPC capability. However, a coordinated approach is important to reach beyond a local and/or highly specialised audience. The Technology Strategy Board (TSB), the main UK body promoting technology-based innovation, maintains various initiatives towards this aim, across many sectors that stand to benefit from e-Infrastructure. These include Collaborative Research & Development programmes, innovation platforms to promote solutions in areas of emerging societal importance, and programmes targeting knowledge exchange, such as:

1) **Knowledge Transfer Networks (KTNs)** form communities of diverse organisations to stimulate innovation, and drive the flow of knowledge within, in and out of these communities. There are currently 15 active KTNs[29] servicing a range of industrial sectors, all of which collaborate to form a 'network of networks'.

2) **Knowledge Transfer Partnerships (KTPs)** assist UK business in accessing the knowledge and expertise of Universities and Colleges. This typically involves someone from academia undertaking a placement with an industrial organisation. As of Mar 2013, there are 903 active partnerships.[30]

3) **Catapult Centres** provide support for the transition of technology from basic University research towards prototypes that can be further developed into products in a purely industrial environment. There are currently 7 established sectors,[31] funded through £200M committed by the Government in 2010 for developing technology and innovation centres.

However, apart from general awareness, more is required to specifically promote the uptake and usage of e-Infrastructure resources. Towards this aim, the ELC has begun consulting with various industrial sectors to investigate the potential uses, benefits and strategies for improving e-Infrastructure awareness in industries best-placed to benefit. This detailed later in the discussion of Capability Awareness.

Management and governance

An effective ecosystem requires guidance, management and governance. At present, there are various groups responsible for the management of UK e-infrastructure at each particular level (Figure 7).

[29] https://www.innovateuk.org/-/knowledge-transfer-networks

[30] Quarterly Statistical Report on Current Knowledge Transfer Partnerships, Technology Strategy Board, 31 Mar 2013

[31] https://www.innovateuk.org/-/catapult-centres

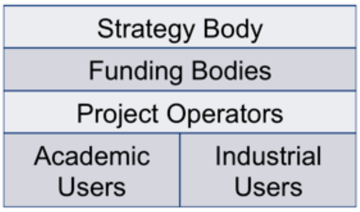

Figure 7: Levels of management for UK e-infrastructure.

The *E-infrastructure Leadership Council (ELC)* is responsible for the overall UK strategy, advising Government and creating action plans to address the nation's e-infrastructure requirements. E-infrastructure funding is managed and distributed by the *RCUK e-Infrastructure Group*, comprising the Research Councils and other managers of funding for programmes of delivery, such as the Higher Education Funding Councils (acting through Jisc), the Technology Strategy Board, and the Meteorological Office.

The *e-Infrastructure Project Directors Group* is a self-organised group of e-infrastructure project leaders that meet to coordinate their operational activities. Representing users, the *UK E-infrastructure Academic User Community Forum*, which evolved from the e-science programme, operates to further engage and promote the use of computers in research, while the newly formed *TSB E-infrastructure Research Special Interest Group* brings together industrial users from across the TSB Knowledge Transfer Networks. Each of the groups interacts with those at levels directly above and below, and generally share some representation.

Figure 8 represents some of the bodies working together in a coordinated manner to support a "pipeline", starting with the setting of policy and strategy, through funding and delivery, to exploitation of the UK's national e-infrastructure.

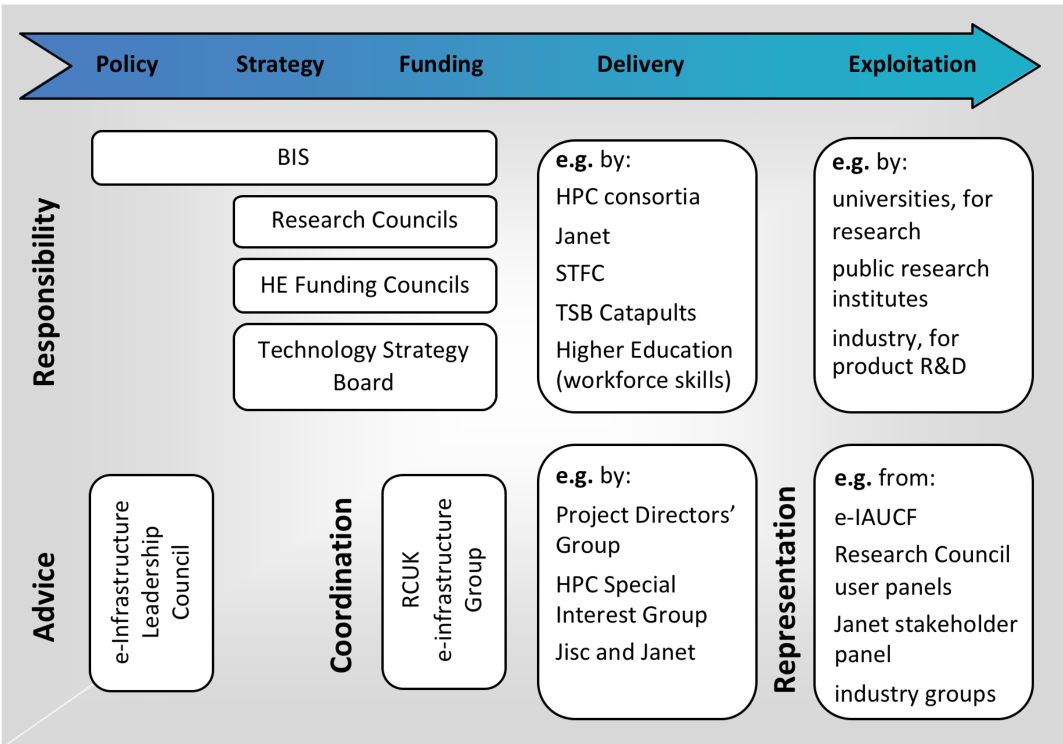

Figure 8: The e-infrastructure pipeline

Summary as of Jan 2013:

- E-infrastructure has been recognised as a driver for growth and innovation
- This was confirmed in the Tildseley Report (2012), which provided recommendations by way of a ten-year strategy to ensure the UK is in a position to take full advantage of changes in technology.
- The e-Infrastructure vision has since evolved to include issues of big data, data science and data analytics. It follows that data infrastructure and services become core components of the e-Infrastructure landscape.
- The Government has been active in their response, with the first round of investment focusing on capital investment into the UK's technical capability – particularly concerning high-end computing, networking and data services.
- Investment into e-infrastructure is in line with, and underpins, other Government initiatives. Examples include:
    - *100,000 Genome Project:* Sequencing patient genomes to improve treatment and provide data for research
    - *Square Kilometer Array:* Data management and analysis from the world's most sensitive radio instrument
    - *Research Partnership Investment Fund:* funding partnerships between HEIs and industry, such as Warwick's National Automotive Innovation Campus

Moving forward

"Business will invest more as they see us invest more in computational infrastructure to capture and analyse data flows released by the open data revolution." David Willetts MP, Minister for Science and Universities, Jan 24th 2013

The Government's 2011 investments have concerned building the foundations of an e-infrastructure ecosystem, by focusing on hardware (capital) resources. The next steps involve developing other aspects of the ecosystem, by ensuring that the technical aspects are actively and effectively exploited. In particular, this involves raising awareness of the industrial benefits of using the e-infrastructure, development of a software capability for industry to exploit, training the workforce with the skills that industry requires, and ensuring that the e-infrastructure provides security that industry can trust.

Capability awareness

It is important that awareness of the potential benefits of e-infrastructure is actively promoted to the business communities that can best exploit them. There is a need for national e-infrastructure "on-ramps" to assist UK business, particularly SMEs, to exploit academic knowledge and industrial domain expertise. This collective expertise will collaboratively build awareness whilst also creating solutions for real industrial problems.

Software and data on-ramp centres will help those companies that do not yet use the e-infrastructure to become aware of the support available and the benefits that it can bring them. For users who are aware of the benefits of modelling and simulation, and of big data analytics, the on-ramp centres will provide support for collaborative development of new models, algorithms and software, using the national e-infrastructure services to develop them to the point where they can be used for business as usual in commercial environments.

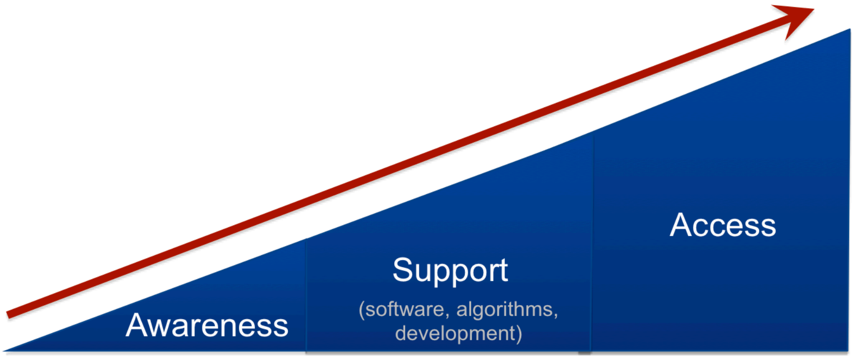

Figure 9: Software and Data On-ramp Centres will assist UK industry to exploit the e-infrastructure

Based on the developing UK industrial strategy, the ELC has identified six key industrial sectors in the UK economy best poised to advantage from e-Infrastructure (Table 3), and commissioned working groups for each sector to investigate the potential of these emerging technologies, and the level of infrastructure and support required to fully realise the expected benefits. Currently, the groups are working on proposals for *Software and Data On-ramp Centres*, to promote the benefits, use and re-use of the e-infrastructure, and to provide the support that each individual industry requires. It is envisaged that these centres will, at least initially, be coupled to TSB Catapult Centres.

Sector	Potential benefits of e-infrastructure
Life Sciences	Computational early-stage drug discovery (molecular simulation), gene-diseases mappings (humans, agriculture), epidemiology, biotechnology (including industrial biotechnological processes)
Construction	Designing new construction materials, and architectural models; simulating interactions within a smart city
Energy	Improving combustion techniques, fuel storage capabilities, extracting more from renewables
Engineering & Manufacturing	Development of new materials, design approaches, computational simulation of durability
Information Economy	New software, software customisation, network and data management infrastructure, more efficient digital media techniques.
Professional Services	Big data analysis, improved predictive technologies

Table 3: Industrial sectors targeted for e-infrastructure engagement support

The On-ramp Centres are intended to assist industry in developing and improving their software and data capability. Assistance covers data management concerns, such as collection, storage, protection, as well the development of software, models and skills for analytics, mining, and visualisation. As mentioned, software represents a capital asset that is crucial to the development of an e-infrastructure capability. The on-ramps should aim at developing capabilities as relevant to the sector, and promote maturation/sustainability and accessibility processes such that software is properly maintained, used, reused and can be leveraged by non-experts (where appropriate).

Initial interactions highlight the need for any initiatives to be specific rather than general, to be tangible with respect to targeting the needs of the particular sector. It the importance of ensuring the engagement of the whole supply chain within an industrial sector to fully realise the potential. A proposed approach, relevant for some sectors, is to build upon the established capability provided by the TSB Catapult Centres, which already offer a sector- (and location-) specific support for commercialising R&D.

Skills

132,000 jobs will be created in the big data field within the UK economy between 2012 and 2017.[32] The staff to fill these will require training in data analytics skills.

A strong e-infrastructure capability requires a community of highly skilled computational and data scientists (e-infrastructure specialists), as well as a more general pool of those skilled in software, and data analytics. The development of mathematical, computational skills is an issue of general concern being tackled by Government. An explicit objective of the UK Industrial Strategy is to develop the necessary mathematical, computational and scientific skills required for a 21st century information-based economy. The Department of Education is working towards increasing and improving the computational training provided in primary and secondary schools. Universities are being encouraged, where appropriate, to include computational training/methodologies as part of their undergraduate courses; and there is a desire to have professional bodies certify particular undergraduate courses to address industrial skills requirements. There remains an important and unmet requirement for specialist training courses in summer schools and for Master’s level conversion courses. Concerning data analytics, big-data initiatives, such as the Public Data Transparency Board that aims at making Government and research data (funded by the Research Councils) publicly available, involve a training/skills component so that data can be properly formatted, analysed, managed and preserved. It is envisaged that the Software and Data On-ramp Centers, as previously described, will also offer targeted training and skills development programmes, in the form of short and/or mid-career development courses, as relevant for the particular sector. These represent only initial steps – much more is required to develop the data analytics skills-base required to take advantage of the opportunities brought by big-data.

There remains the need for Universities to provide computational/data science training as part of their postgraduate courses in disciplines that e-infrastructure support. It is felt that this is best implemented through Masters’ level conversion courses, including as part of Research Council funded Doctoral Training schemes. Also required are more short and/or targeted courses, to enable skills development without a University-level commitment.

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[32] *Big Data Analytics Report*, e-Skills UK (2013).

Resource sustainability

The Government has invested in the initial procurement of hardware-related (HPC, data and network) e-infrastructure resources. However, technology rapidly evolves – Moore's law indicates that processing power doubles approximately every two years. In line with this, it is expected that hardware has a life of approximately three years. It is therefore important that investment is ongoing to sustain a level of performance and efficiency to maintain a competitive edge. The capital upgrade costs are expected to average about £50M/year over the ten-year period. In addition to capital investment, there is also the need for recurrent expenditure, to ensure that resources are well-maintained, and continue to operate at full productive capacity.

Conclusion

This document has introduced the e-infrastructure, its role in supporting UK industry and the economy, and the initial steps undertaken. There have been some positive developments in establishing the UK's e-Infrastructure capability. However, this document has also suggested that more needs to be done. The immediate focus is on:

a) establishing software and data on-ramps to support industrial exploitation of the e-infrastructure;

b) developing skills so the workforce is trained to exploit the e-infrastructure; and

c) cyber security, so that industry will trust the e-infrastructure.

The sustainability of the capital resources, and their operational funding, must be continually addressed over the next ten years to ensure that the e-infrastructure remains at the cutting edge. A strong industrial-public sector strategic collaboration is crucial to ensuring that the UK is best able to advantage the opportunities brought by developing technologies.

In identifying future needs, ELC Members have consulted informally with academe, industry and the public sector. However, given the resource available and the rapidly developing big data and e-infrastructure landscape, there are many potential stakeholders who have not been approached. The purpose of this document is therefore to provide an opening for further dialogue and engagement, especially with potential industrial users and their representative bodies.

The ELC is particularly interested in collaboration mechanisms that could leverage resources from the private sector to derive the maximum benefit from the public sector investments over the past year or so.

Such leverage is important as it demonstrates that industry recognizes that only by working in partnership with Government can the appropriate e-infrastructure be developed in the UK for both future scientific excellence in academe and for future globally competitive innovation in industry.

The ELC invites feedback on the propositions in this document to elc.secretariat@bis.gsi.gov.uk

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