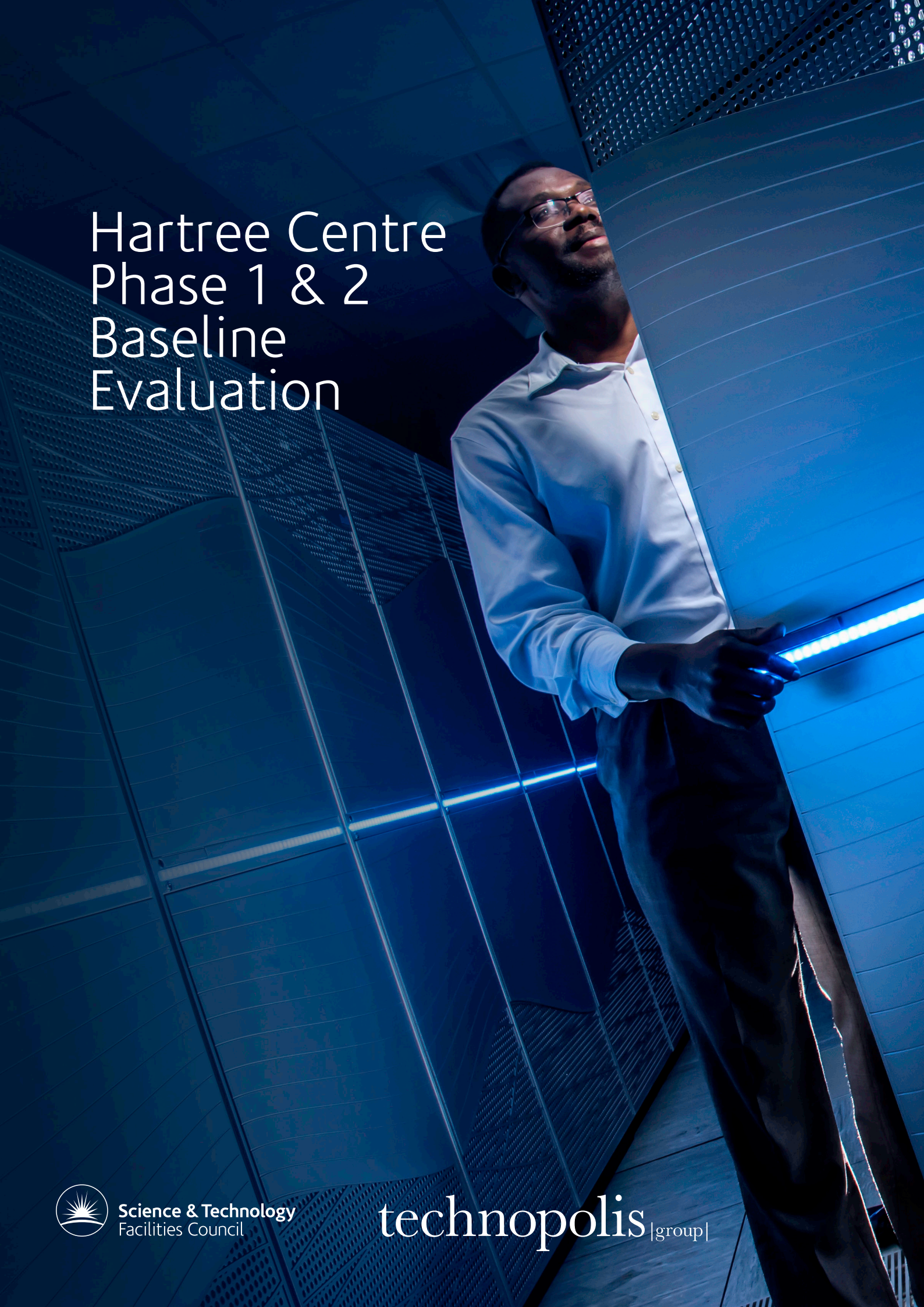
Hartree Centre Phase 1 & 2 Baseline Evaluation



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Hartree Centre
Science & Technology Facilities Council

Hartree Centre Phase 1&2 Baseline Evaluation

Final Report

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Executive Summary

This document presents the findings of a **baseline evaluation of the Hartree Centre**; a high performance computing (HPC) and data analytics research centre that is working to transform the competitiveness of UK industry by accelerating the adoption of HPC, big data and cognitive technologies. It provides an early view of the benefits the centre is delivering to its industry partners and the wider economy through an assessment of its first years of operation (phase 1 and 2 investments).

Key findings from the baseline evaluation

A unique service to industry

- The Hartree Centre combines world-class HPC and analytics facilities with a critical mass of high-level technical expertise, which is highly relevant to businesses in all sectors of the UK economy
- It is the only supercomputing centre in the UK with industrial engagement as its primary role and it can provide a quality and breadth of service that goes beyond anything the market will provide
- While the centre enhances its clients' internal skills and capabilities, most businesses continue to return, because of the combination of specialist skills and state-of-the-art facilities available

Supporting innovation, competitiveness and productivity

- In its first four years of operation, the Hartree Centre delivered more than 100 collaborative projects, working with many of the largest and most dynamic UK companies (such as Rolls-Royce and Dyson) and SMEs (such as Wavereach and Zenotech), across most sectors (from fast-moving consumer goods and high-value manufacturing, to transport, energy and healthcare)
  - Half of those consulted have seen or expect to see an increase in their sales income as a result of working with the centre
  - The centre is also making strong positive contributions to the innovative capacity, visibility, reputation and international competitiveness of its clients and users
- The centre has helped many clients develop innovative products and services and/or bring these to market earlier, from healthcare apps to monitoring systems for road and rail bridges
- The centre has led many software development projects, where newly-optimised codes provide faster processing and improved functionality that will deliver productivity benefits to businesses

Producing economic impact

- We estimate that the Hartree Centre's direct work with industry during the early phases will generate a total net economic impact (GVA[1]) of up to £27.5M in *commercial benefits* to these users. This is in addition to a £7.1M net impact from the *operational expenditure* of the centre in phase 1 and 2.
- These are already strong results for what is a young and relatively small centre of excellence, with total economic impact already close to the £37.5M initial capital investment in the centre for phase 1[2]
- We expect these benefits to intensify in the future. This study launched just four years after the opening of the centre, when the full benefits of early activities are still working their way through the system. As interactions with businesses mature – more joint projects, more time elapsed – we expect an even greater proportion of clients to report positive commercial results

[1] Gross Value Added. The HM Treasury Green Book recommends the use of GVA (instead of turnover) as a measure of impact because it discounts the added value generated along the supply chain and avoids double counting

[2] The additional £19M investment for phase 2 was focused on novel R&D rather than short-term industrial engagement and support. Significant commercial benefits from phase 2 investments were therefore not anticipated in the timeframe of this study

Creating wider social and economic benefits

- The Hartree Centre's focus on industrial competitiveness has not precluded it from carrying out important work with the public sector, which looks set to deliver wider social benefits. For example, it collaborated with the Met Office and NERC in the design and build of a next-generation weather and climate prediction model, which will aid advanced preparation and contingency planning in the UK
- The centre has also run projects to optimise several scientific codes such that they run efficiently on massively parallel, multi-core machines. The newly-optimised codes have been shared with the STFC's Scientific Computing Department for inclusion within a wider portfolio of scientific codes that are widely used by academics in the UK and internationally. The new codes will have had positive effects on the speed and robustness of various computational science activities
- The centre is one of the key assets on the Sci-Tech Daresbury Campus and has been influential in attracting several important new tenants to the growing cluster of high-tech businesses on site
- The Hartree Centre has organised, hosted or contributed expertise to more than 130 training courses and events, as part of a wider commitment to raise awareness of the potential of HPC and to help train the next generation of data-centric computing specialists. These events are mostly provided free of charge, but might normally cost attendees ~£1M per year

Looking to the future

- The combination of world-class HPC infrastructure and leading computational scientists and engineers means that the Hartree Centre will continue to address the needs of a wide array of UK businesses and other users. Its broad service offer provides opportunities for businesses of all sizes and sophistication, with clients possibly progressing from an initial training course, through to buying technical consultancy, all the way to collaborating on ambitious research projects
- As the centre continues to expand and extend its services through phase 3 – cognitive computing and big data (not the focus of this study), we expect it to have a more substantial impact on the wider economy, and both its strategic partnership with IBM Research and the delivery of cognitive computing will help to realise this
- The centre has a vital role to play in delivering the Industrial Strategy's ambitions to support firms in seizing the opportunities of enabling technologies such as artificial intelligence and big data. However, while the centre has the potential to make a difference nationally, it needs to overcome resourcing issues and achieve a sufficient scale of activity if it is to exploit this opportunity

Monitoring and evaluation

- The centre has been increasingly successful at generating industrial (and other) income, but it is likely to continue to need government investment given the high capital costs involved. Evidence of the impact generated from past investment is essential for maintaining this support
- The current baseline study offers an early view of the benefits emerging from the first years of the centre. It should form the start of a longer-term evaluation programme, with ongoing monitoring and evaluation, as well as a more substantive socio-economic study in several years' time
- This report includes a benefits assessment framework that we recommend centre management adopt as the basis for future performance assessment. This includes a series of suggested metrics, designed to allow the centre to more clearly understand (and demonstrate) the extent to which it is making good progress against objectives, as well as proposals for additional data collection activities that will help to provide the necessary evidence of the Hartree Centre's achievements

The following infographic summarises the main activities and benefits of the Hartree Centre:

Hartree Centre Key Benefits from its first four years of operations

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A high performance computing and data analytics research centre, with a strong industrial focus

Phase 1 - Industrial engagement

£37.5M investment from national e-infrastructure fund

To provide state-of-the-art equipment and facilities for commercial use, delivering competitive advantage to the UK

Phase 2 - Energy efficiency & data exploitation

£19M of further capital investment from Government

To address a growing need for large-scale data and analytics competence, and pursue advances in energy efficiency

BROAD SERVICE OFFERING

Platform as a Service
Software development and code optimisation
Collaborative R&D
Consultancy

SPECIALIST SUPPORT & EXPERTISE

100+ People

40 FTEs 2017

Internationally recognised software developers, computational scientists, engineers & data specialists

STATE OF THE ART FACILITIES

Petascale HPC
Hyperscale storage
IBM Watson data analytics
Energy efficient platforms
3D visualisation suite

Home to some of the most technically advanced high performance computing, data analytics, machine learning technologies and experts in the UK

55 UK-BASED CLIENTS

25 High-tech SMEs
12 Multi-nationals
13 Universities
5 Other public bodies

INDUSTRY PROJECTS

167 Projects developing new tools & data for application in key sectors across the economy

60% with commercial companies

70 projects with repeat clients

BROAD SPREAD OF SECTORS INVOLVED

32% consumer goods
14% ICT
14% manufacturing
6% transport
6% energy
7% chemicals

plus transport, health, pharma, defence, finance, oil & gas

Skills and Awareness

80%
Of users report improvements to modelling and simulation capabilities

93%
Of users report increased understanding of the potential value of HPC to their organisation

OVERALL ECONOMIC IMPACT

£7.1M from centre's operational expenditure

GVA *net* impact

£27.5M in commercial benefits to phase 1&2 users (upper bound estimate)

INCOME 2013/14 - 2016/17

£3.5M industry sales from 37 customers

£1M in grant and other income
including Horizon 2020 & Innovate UK grants

TRAINING & EVENTS

Organising, hosting or contributing expertise to 30 (2016)

950+ people training
3,760 days

£1M/yr (equivalent market price)

RESEARCH

Pre-competitive research

Internal R&D

Energy Efficient Computing research programme

DARESBURY CAMPUS

HPC collaborations with **5** tenant companies

"The Hartree Centre was recognised consistently as being the key asset in terms of securing the Campus' future success"
(Campus Impact Study, 2017)

The next stage: Phase 3 - Big data & Cognitive computing

£115.5M
£200M

Government investment – Grand Challenge Capital projects (2014)
Package of in-kind support from IBM Research

2 new programmes:
Hartree-IBM research programme
Cognitive accelerator

The Hartree Centre is a **high performance computing and data analytics research centre with a strong industrial focus**. It was set up in 2013 and has evolved over three phases to address increasingly complex user-led applications, and in response to four 'forces of change' shaping the future of supercomputing: industrial engagement; power usage; big data; and democratisation.

Three phases of funding and development

The centre has received three rounds of government funding. An initial £37.5M was provided for state-of-the-art equipment and facilities for commercial use **(phase 1 - industrial engagement)**. A further £19M was then provided in 2013 to address a growing need for large-scale data and analytics competence and pursue advances in efficiency **(phase 2 – energy efficiency / data exploitation)**. This second phase focused more on novel R&D (e.g. through an Energy Efficient Computing research programme), rather than industrial engagement and support. Significant commercial benefits were therefore not anticipated from phase 2 in the short term (i.e. not within the timeframe of this study). It is the first period of the centre's operation (phase 1 and 2) that are the focus of this baseline evaluation.

In June 2015, the UK Government then awarded the Hartree Centre a further £115.5M with which to expand over the next five years and to establish itself as the UK centre of excellence in Cognitive Computing and Big Data **(phase 3 – big data and cognitive computing)**. This phase adds two new programmes to the work of the centre; Innovation Return on Research (IROR) and the Cognitive Accelerator. In recognition of the centre's national standing, and further to considerable joint working in the first two phases, **IBM Research** signed a strategic partnership agreement with the Hartree Centre. The company is actively supporting phase 3 through a package of IBM technology, IP access and onsite expertise (up to 30 IBM Research staff), which has been valued at over £200M. Phase 3 is not the focus of this baseline evaluation, although the report does outline key features of this latest evolution, which are then integrated within the design of a future benefits realisation framework.

Facilities and expertise

The centre's **state-of-the-art facilities** offer access to one of the world's most powerful supercomputing and data analysis infrastructures dedicated to industrial R&D. Currently this includes the UK's first Atos Bull Sequana X1000 supercomputer system, alongside other Intel® platforms, large scale GPFS storage, an IBM data analytics cluster, 3D visualisation suites and a new data-centric architecture from IBM. These are complemented by a growing team of internationally recognised software developers, computational scientists and engineers, who provide support and **specialist expertise**.

Activities and usage

The Hartree Centre occupies a unique position in the market place, **offering a combination of hardware and specialist people-related services**, including Platform as a Service (PaaS), software development and code optimisation, collaborative R&D and consultancy. It is also engaged in a variety of pre-competitive research, as well as the delivery of various training, workshops and events.

In the first four years that the centre was fully operational, it completed **over 100 collaborative projects with industrial partners** including some of the largest UK-based companies like Dyson, GlaxoSmithKline, Rolls-Royce and Unilever. The centre has also worked closely with many smaller software developers and other high-growth potential digital SMEs, such as Global-365 and Zenotech. The evaluation has developed case studies to illustrate the working relationship between the centre and some of its clients, as well as the kinds of benefits being realised at this early stage.

The Hartree Centre is also developing next-generation HPC tools and has created an in-house **research programme** working with many of the UK's leading academic research groups, as well as public research organisations. Its Energy Efficient Computing (EEC) research programme has been exploring various aspects of power use in HPC, as well as devising ways of achieving step changes in efficiency, which will be essential for delivering high-performance – low-power computing capability.

Industrial engagement

Much of the initial investment in the Hartree Centre was to establish HPC facilities for commercial and business use and to support industrial engagement, with the aim of transforming competitiveness.

The evaluation findings in this regard are positive, with users confirming the relevance of the centre's approach to **working with UK industry**. Several of the country's largest technology firms have signed collaborative agreements with the centre, underlining its importance to business development efforts. Others explain that its combination of world-class facilities and specialist computational scientists places clear blue water between its support and other HPC services available commercially.

The centre's infrastructure and its development programmes are far beyond the reach of the very great majority of individual businesses, in terms of both affordability and capability, and the codification of these experiences in new tools supports the centre's outreach ambitions and the diffusion of HPC advice and capability development to the wider UK business community across all sectors.

It is also clear that the Hartree Centre is helping to **change views** as to the business-critical nature of HPC-related services. We found a marked increase in the numbers of users that changed their view of the importance of HPC before and after their involvement with the centre. It also appears that increased interest in (and understanding of) HPC capabilities then translates into increased usage.

Innovation and competitiveness

The centre is clearly helping firms to innovate, with a majority of survey respondents and interviewees reporting a positive outcome as regards to their **innovative capacity and competitiveness**. Our research also suggests that the centre's work has the potential to help develop very innovative products and services, with several clients already reporting significant contributions to innovations. For example, it has supported the development of tools to model power outputs for different layouts of wind turbines, or to combine various data sources to more accurately predict the likelihood of floods.

We found examples of **new products** being supported, including new consumer products brought to market earlier because of work at the Hartree Centre. There are other examples too, such as an iPad user interface for non-specialists to use HPC systems for ad hoc analytical support, plus newly-optimised versions of modelling and simulation codes that will deliver productivity benefits to client businesses, or are in several cases being sold on to third parties.

The Platform as a Service offering (pay-as-you-go access to HPC) was also widely reported to have allowed companies to carry out scientific and engineering analyses in a fraction of the time and at a fraction of the cost of a more conventional approach (using less powerful computers). These **process improvements** (e.g. in Rolls-Royce's engineering designs or BAE Systems' simulations), have tended to translate into more and better analyses and ultimately better designs.

The centre is also delivering wide-ranging **commercial benefits** to its clients. Half of industrial users have either seen an increase in sales income already or expect to do so in the near future, following their collaboration with the centre during the first two phases, and a smaller number also report an improvement in profitability. While most organisations were not yet able to quantify these impacts, several did give some indication of the scale of benefits.

As the centre's interactions with client businesses develop – more joint projects, more time elapsed – we expect to see a greater number and proportion of clients reporting positive commercial results.

Many clients also derive **reputational benefits** from working with the Hartree Centre, reflecting its status as a national centre of excellence and the exacting nature of the collaborative work that is being undertaken. We identified a number of specific instances (particularly amongst small software and technology firms such as Renuda, 3DSIM and Embecosm) where clients reported an improvement in the reputation and market position of their companies as a result of working with the centre.

Skills and capability development

The centre has delivered skills outcomes through a range of events. It has organised, hosted or contributed technical expertise to over **130 training courses and skills-development activities** since it was launched. This is part of its wider commitment to raise awareness about the potential of HPC and to build HPC technical competencies by training the next generation of computing specialists. These events have usually been offered to industry and academia free of charge, but the **equivalent market price** of the training provided is likely to be **more than £1M per year.**

The Hartree Centre's mainstream HPC and big data activities are also delivering substantial knowledge transfer and skills development outputs; skills do not flow exclusively from training activities. The centre is **enhancing its clients' internal skills**, including through one-to-one training. For instance, over 80% of users reported that their work with the centre had helped to improve their modelling and simulation capabilities, while 78% reported improved knowledge of data science techniques.

Despite this, most **client organisations continue to collaborate with the Hartree Centre** as the means by which to access the necessary specialist skills, returning to work with the centre rather than trying to transfer or recruit such people within their own organisations. This conscious division of labour holds for both smaller and larger clients.

Contributions to research

The Hartree Centre participates in a **wide range of research projects** as a means by which to develop its internal capabilities and tools, as well as its cutting-edge technical support to clients. Some of these activities are internally financed, but most are funded by Horizon 2020, EPSRC and other national and international grant providers. For example, the centre participated in a £700K Innovate UK project (TSERO) to apply newly developed techniques to compiling energy efficient code for HPC systems and data centres. The resulting integrated monitoring system, which can significantly reduce the energy use of computing operations, has also been demonstrated at the Hartree Centre.

Much of the research work undertaken relates to the phase 2 **Energy Efficient Computing programme**, through which the Hartree Centre – in collaboration with others – has sought to explore different aspects of power use in computing, as well as ways to achieve step changes in energy efficiency. This is a long-term area of work, and more time will be needed for wider impacts to be realised. However, there are already a number of research projects completed, with various outputs that provide good learning and that can serve as useful showcases to a wider client base.

The centre has also provided support to the STFC Scientific Computing Department's (SCD) work on **code optimisation** of various scientific software tools that are widely used by academics. This will have had a positive effect on the confidence, speed and robustness of various computational sciences.

The centre has also worked with various **academic groups at universities** across the UK. For example, University College London has collaborated with the centre in implementing a high-throughput molecular simulation system, utilising the power of HPC to accurately determine biochemical properties within clinically relevant timescales. While work with universities has not been the centre's primary mission, it has also played an important role in several computer science studies, and this has helped improve researchers' visibility, reputation and income in a number of cases.

The centre is also participating in several **international research networks** (such as the Partnership for Advanced Computing in Europe, PRACE), which enable its staff to monitor developments in HPC technology among global research and industry players. In some cases, this watching brief will also allow the centre to influence strategic research agendas and allow staff to identify potential new strategic partners and funding opportunities, both here in the UK and abroad.

It is also worth noting that the centre has strengthened its **links with several major global players** through its research activities, including with IBM, ARM and Atos Bull. For example, a major new collaboration with Atos UK&I includes plans for new HPC as a Service and 'Deep Learning' as a Service offerings, plus co-design and development of next generation hardware and software solutions.

Wider benefits

The Hartree Centre has demonstrated that its offer is relevant to businesses across many sectors, but at this stage in its history it has only engaged substantively with a few tens of firms. As such, its wider **contributions to the competitiveness of UK plc** will only materialise in the future, as it expands its footprint, deepens its relationships with existing clients and builds up its digital assets.

Our economic analyses estimate the local economic impact of the Hartree Centre, but there is also a more qualitative aspect to local effects, with the Hartree Centre forming an integral part of the Sci-Tech Daresbury science and innovation campus. The centre is regarded as one of the key assets of the Campus and is likely to have been influential in attracting some of the **growing cluster** of high-tech tenant companies to this site, contributing to a growing community of researchers and industrialists.

The importance of the centre to the wider **Liverpool City Region** (LCR) has also been recognised as part of the recent Science and Innovation Audit (SIA) process, which highlighted the significant role of the Hartree Centre in enhancing the region's world-leading HPC and cognitive computing capabilities.

While the Hartree Centre has focused mainly on industrial engagement, it has also done important work with public agencies and institutions that look set to deliver **wider social benefits**. For example, it collaborated with the Met Office and NERC in the design and build of a next-generation weather and climate prediction model for the UK. Specifically, it worked on the computational framework to support the efficient operation of the new model on the latest HPC architectures, which will bring benefits to the UK by enabling better advance preparation and contingency planning.

Overall economic impact

We estimate that the Hartree Centre will generate a **net economic impact** of up to £27.5M in commercial benefits among its phase 1 and 2 users. This is in addition to £7.1M in net economic impact that the centre has generated as a result of its operational expenditure during these first two phases.

These are **already strong results** for what is a young and relatively small centre of excellence, with an estimated economic impact already close to the £37.5M initial capital investment in the centre (the additional £19M phase 2 investment was focused on novel R&D, so significant commercial benefits were not expected in the timeframe of this study). We would also expect the benefits to intensify in the future.

The study launched just four years after the opening of the centre, when the **full benefits of earlier activities are still working their way through the system**. As interactions with client businesses develop – more joint projects, more time elapsed – we expect to see a greater proportion reporting positive commercial results. Similarly, as the centre expands and extends its services through phase 3, we expect it to have a more substantial impact on the wider economy. Its strategic partnership with IBM Research and the delivery of cognitive computing will help to realise this.

Future monitoring and evaluation

If the costs of maintaining facilities were fully reflected in fees charged to clients it would likely push prices above the level many would tolerate. Therefore, whilst the centre is increasingly successful at generating income, it is likely to continue to need public investment to support its work. Evidence of past impacts will be essential and a **longer-term evaluation programme** should be put in place, with ongoing monitoring and a more substantive socio-economic study in several years' time.

We have developed a **proposed benefits assessment framework** as part of the study, which we recommend that the senior management of the centre adopt as the basis for future performance assessment. This includes a series of **suggested metrics**, designed to allow the centre to more clearly understand and demonstrate the extent to which it is making good progress against goals.

We have also recommended five **additional data collection activities** to enable the centre to better track and value its contributions to client businesses, possibly as the basis for a more substantive socio-economic impact study several years hence. This suggested new Evidence Programme would include an annual client survey, an annual business survey, an inventory (and valuation) of digital assets, ad hoc case studies of client business transformation, and a rolling programme of sector studies. We have costed these various measurement activities at around £125K a year, at the lower bound, with suggestions for how affordability might be increased through co-financing.

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1 Introduction

This report presents the findings from a **baseline evaluation** of the Hartree Centre. Such evaluations are undertaken early in the life of an intervention, to serve as a tool for future monitoring and evaluation effort and provide a benchmark against which subsequent progress can be assessed. It therefore focuses on activities and achievements during the first two phases of the Hartree Centre, providing an early view of the benefits delivered to industry and the wider UK economy through its first years of operation.

1.1 The Hartree Centre

The Hartree Centre is a high performance computing (HPC) and data analytics research centre, opened in 2013 and based at the Sci-Tech Daresbury Campus in the borough of Halton, Cheshire. Its mission is to help transform the competitiveness of UK industry by accelerating the adoption of HPC, big data and cognitive technologies, thereby helping to keep the UK at the forefront of industrial innovation.

The centre has evolved over three phases of funding and development to address increasingly complex user-led applications, in response to four 'forces of change' shaping supercomputing (industrial engagement, power usage, data exploitation and cognitive computing / democratisation)[3]. It has been the recipient of £172M of Government funding, including most recently a £115.5M investment as part of BEIS' Grand Challenge Capital projects (for phase 3). This latest investment has been matched by IBM Research with a package of technology, IP and expertise valued at more than £200M.

At the time of the study, the centre employed ~40 FTE staff (software developers, computational scientists, engineers, data specialists and business development managers), while the facilities themselves offer a range of infrastructure and capabilities (including petascale HPC, high throughput computing, hyperscale storage; the Watson IBM data analytics platform, accelerated and energy efficient platforms, software, and immersive 3D-enabled visualisation suites). The centre offers various external services (Platform as a Service, software development and optimisation, collaborative research), in addition to internal R&D work. Phase 3 adds two further programmes; Innovation Return on Research (IROR) and the Cognitive Accelerator.

In 2017, Technopolis was commissioned by STFC to undertake a baseline evaluation of the Hartree Centre, to provide an early view of the benefits it is delivering to its industry partners and the wider UK economy. The study was asked to measure and demonstrate the benefits and impacts of the centre and its activities, providing an evidence-based understanding of the value generated from public and private investment during the first two phases. It was also to include the development of a suggested benefits realisation framework and plan for the centre, which would help drive and capture benefits in the future.

The evaluation builds on the earlier Sci-Tech Daresbury Campus Impact Study (SQW, January 2017) for STFC, which included consideration of the contributions of the Hartree Centre within the wider activities on the Campus (the Hartree Centre is one of the main tenant organisations, at the centre of an expanding community of technology businesses). That Study made a number of recommendations, one of which was to take full advantage of the Hartree Centre's capabilities to drive future growth.

1.2 Approach and Methodology

This study included three distinct, but inter-related stages:

- **Stage 1: Scoping** – Preliminary activities to prepare for the impact assessment. This included reviewing information on the centre (its income, expenditure, projects, users and suppliers); the development of a project database and basic characterisation of the project portfolio; the development of logic models for the centre's activities; and the finalisation of the approach.

[3] For more detail see Figure 1 in the next section.

- **Stage 2: Evaluation** – The main data collection and evaluation phase of the impact assessment. Activities included: a programme of in-depth interviews with ~15 key staff and stakeholders; a series of online surveys of academic / industrial users and suppliers, and interviews with a sub-set of these to obtain more in-depth detailed, evidence and testimony; and the development of case studies of selected users and projects. Appendix B lists the user/supplier organisations consulted.
- **Stage 3: Future Framework** – The development of a proposed framework and plan for future benefits. This included the development of an updated performance evaluation framework for the Hartree Centre to adapt for use in the future. This entailed the development of: new logic models, which track backwards from the Hartree Centre's mission and overarching objectives to define a series of impacts, outcomes, outputs and inputs; a set of performance metrics that derive from these; and a proposal for future data collection, based on the data requirements of the KPIs.

1.3 Data challenges

The study has had to contend with several data challenges, which together have led to the evaluation being a little more qualitative in its approach and findings than we had anticipated at the outset:

- There is a **timing issue** inherent with an early stage (baseline) evaluation. With the study launched just four years after the opening of the centre, the full economic benefits of earlier activities are still working their way through the system.
- The Hartree Centre's **administrative systems** were not initially set up to provide the range of data on finances, activities, projects and outputs necessary to feed into an impact assessment. That said, the centre has made substantial improvements to project tracking recently and is working on several additional reporting systems, including one to catalogue its 'digital assets'
- With a business model that involves staff working intensively with individual clients, the Hartree Centre had amassed a relatively **small pool of clients** by early 2017 and we had to work hard to secure responses to our consultation requests. Response rates are good, but with a small population the number of replies is inevitably small and caution is needed in drawing conclusions
- Another challenge was **commercial confidentiality**, with several clients keen to protect their business advantage and declining to give a full account of their interactions or share information relating to business and financial improvements, or not consenting to information being shared more widely
- Finally, there was a widespread challenge related to **the valuation of benefits**. Many clients signalled a high degree of satisfaction with their Hartree Centre collaborations and were ready to articulate the kinds of benefits derived in narrative terms. However, these were often rather intangible and mixed in with multiple other activities. Few organisations were yet able to quantify these impacts

We expect the situation to improve in the future, as the centre's data collection and reporting continues to improve, its client pool expands and the body of work carried out with individual clients flows through to the bottom line. There are several data issues remaining, however, that affect the ability to judge the overall effectiveness of the Hartree Centre. For instance, there is a need for more and better information about trends in the use of HPC-related services in the wider economy. In the final chapter we offer some suggestions for additional data collection activities that would help the centre to better monitor the changing HPC landscape and track its own contributions.

2 The Hartree Centre

The Hartree Centre is a high performance computing (HPC) and data analytics research centre, based at the Sci-Tech Daresbury Campus in the borough of Halton, Cheshire. The centre's mission is to transform the competitiveness of UK industry by accelerating the adoption of HPC, big data and cognitive technologies. Through this, the Hartree Centre seeks to: (i) keep the UK at the forefront of industrial innovation; (ii) enable businesses and research partners to produce better outcomes, products and services, and to take better decisions, more quickly and cheaply; and (iii) create skilled jobs and train people to excel in these, and help to grow the UK economy.

2.1 The history and evolution of the centre

In 2011, Lord David Willetts, as Minister of State for Universities and Science, invited a group of academics, industrialists, hardware and software suppliers and experts from the Research Councils to discuss the establishment of an e-infrastructure for the UK. This culminated in the Strategy for the UK Research Computing Ecosystem, which recommended addressing the fragmented landscape for funding and access to HPC resources, and earmarked funding for its development. This was a turning point for UK computing infrastructure, which was followed by the creation of the UK e-Infrastructure Leadership Council, an investment of £165M to improve the UK's HPC landscape, and further commitments in 2012 and 2014 to supporting Tier-1 and Tier-2 facilities. The UK academic network (JANET) and high-capacity data storage across the Research Councils were also enhanced at this time.

UK scientists can access Tier-0 HPC facilities through the European PRACE Research Infrastructure.[4] Access to Tier-1 HPC resources in the UK is then coordinated by EPSRC on behalf of all the Research Councils, providing access to the National ARCHER system. In 2012, EPSRC also led the development of a strategy to ensure a diverse and competitive Tier-2 and 3 HPC ecosystem in the UK to facilitate improved access to HPC resources at all levels, international, national and regional. There was also a commitment to make these facilities more commercially relevant, with the encouragement of greater industrial engagement and improved access. These facilities were established with matched funding from host institutions and with industry collaborators in several cases. Notwithstanding these improvements, the overall HPC ecosystem was still mainly configured to the needs of academics.

The Hartree Centre was opened in 2013[5], as the government's response to a growing need in industry for access to HPC-related infrastructure and services. HPC is quickly moving from the realm of science and compute-heavy commercial uses (e.g. engineering simulations or oil exploration) to a more widespread application by businesses, as they increasingly employ data analytics to make decisions based on big data and find ways to integrate AI capabilities into their technology infrastructure.

The Hartree Centre has since evolved over three phases of funding and development to address increasingly complex user-led applications, in response to four 'forces of change' shaping the future of supercomputing. It has been the recipient of three rounds of funding, totalling more than £170M:

- **Industrial engagement (phase 1).** The centre was supported initially by a Government capital investment of £7.5M and a £30M national e-infrastructure investment. This was to provide state-of-the-art equipment and facilities for commercial use, with the aim of delivering competitive advantage to UK clients through a range of software development and advanced modelling.

[4] The PRACE infrastructure is explained in some detail in The Scientific Case for High Performance Computing in Europe, 2012-2020: from petascale to exascale, Partnership for Advanced Computing in Europe (PRACE), 2014.

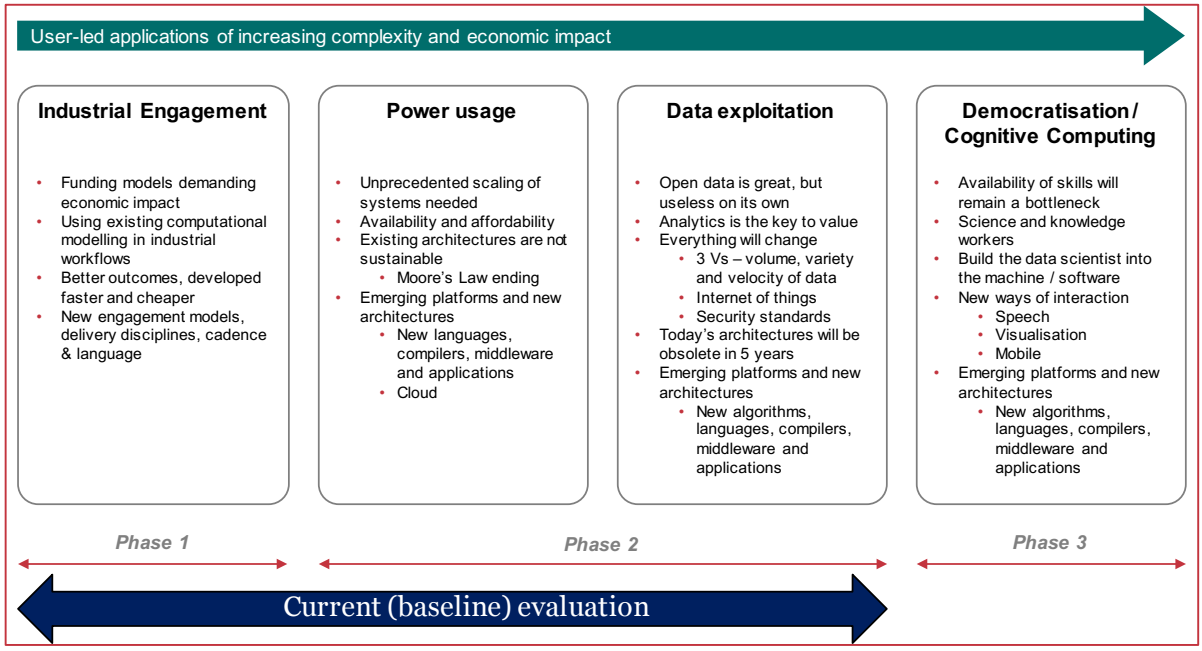
[5] Its origins go further, with its basic mission and business-facing activities having been created first within STFC's Scientific Computing Department (SCD) at Daresbury several years earlier. Moreover, Daresbury has been at the forefront of computer science in the UK for 50 years, and installed the UK's first Cray-1 supercomputer in 1978. The Hartree Centre also inherited the SCD's pre-existing links with IBM and the early work on a simplified user interface to allow non-HPC experts to use HPC systems. The Hartree Centre has also benefited from earlier regional development initiatives including an important collaborative project involving Unilever, Infineum and Syngenta working together on computer aided formulation (CAF) and simulation of chemicals. The CAF project was originally match-funded by the Knowledge Centre for Materials Chemistry (KCMC), but was taken over by the Hartree Centre, to strengthen its business focus, and this has emerged as a major strand of the Hartree Centre activity.

- **Data exploitation / energy efficiency (phase 2).** A further £19M of capital investment was provided in 2013 for next-generation, power-efficient technologies, with the intention of addressing the need for large-scale data and analytics competence and achieve energy efficiency in HPC. This investment was focused on novel R&D, rather than short-term industrial engagement and support.
- **Big data, cognitive computing and democratisation (phase 3).** In 2014, the Government announced a further £115.5M investment to expand the centre over next 5 years. This investment – part of BEIS' Grand Challenge Capital projects – was intended to establish the Hartree Centre as the UK centre of excellence in cognitive computing and big data, and to improve the competitiveness of industry through accelerated adoption of computing and associated technologies. This phase adds two new programmes to the work of the centre; Innovation Return on Research (IROR) and the Cognitive Accelerator.

The expansion of IBM's collaboration with STFC was crucial to the Government's 2014 commitment, and the investment was subsequently matched by IBM Research, with the agreement of a package of technology, IP access and onsite expertise valued at £200M. This includes the establishment of an embedded team of IBM Research staff at Sci-Tech Daresbury, which had grown to a headcount of 23 staff as of December 2017 (with a commitment to get to 30). This presence is important for building the critical mass of expertise that will be important for the next stage of the Hartree Centre's development. Working alongside colleagues from the Hartree Centre and elsewhere in STFC, the IBM Research team works directly with businesses using cutting-edge data science tools to solve, specific and complex commercial challenges that may have a wider applicability across UK industry. Initial areas of collaboration have included projects on molecular modelling, genomics, the Internet of Things and uncertainty quantification.

Figure 1 presents a schematic overview of the evolution of the centre across its first two phases and through to phase 3. In practical terms, this amounts to an extension in the scope of the centre, with the activities launched in the first phases continuing to be delivered in phase 3. The mission in phase 3 is largely unaltered, focusing on strengthening the global competitiveness of UK business by facilitating and accelerating the adoption of HPC, big data and cognitive technologies.

Figure 1 Evolution of the Hartree Centre (based on four 'forces of change' in supercomputing)



Source: The Hartree Centre, October 2016

2.2 The Hartree Centre's finances and staffing

Operational **expenditure data** for the Hartree Centre over the last four financial years (2013/14 to 2016/17) shows annual costs of around £4M (£17M in total). There were up to 100 different expenditure items each year, however, the majority (59%) was accounted for by staff costs (internal and external). Other significant expenditure included equipment and supplies (e.g. computer hardware/software) other than the major capital items, professional services (legal, consultancy) and utilities (electricity).

Table 1 Hartree Centre Operational Expenditure by area, 2013/14 – 2016/17

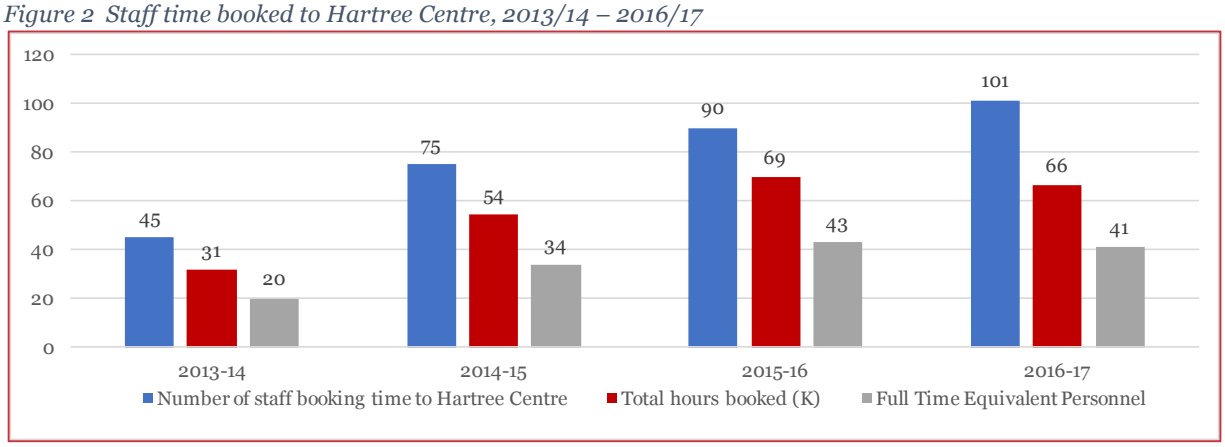
Expenditure Category	2013/14	2014/15	2015/16	2016/17	4-yr Total
Staff (+ secondments, agency, T&S)	£1,410,359	£2,372,639	£3,196,100	£3,240,724	**£10,219,822**
Equipment and supplies	£769,406	£508,194	£1,126,479	£639,436	**£3,043,515**
Services	£696,512	£616,896	£584,286	£390,695	**£2,288,389**
Utilities	£418,915	£592,643	£233,930	£387,180	**£1,632,669**
Total operational expenditure	**£3,295,193**	**£4,090,372**	**£5,140,795**	**£4,658,035**	**£17,184,395**

Source: STFC Finance Directorate

The centre employs around 15 people directly (2017 data), but many more individuals have booked time to Hartree Centre job codes over recent years (mostly staff who are employed by the Scientific Computing Department (SCD), but working on Hartree Centre projects), amounting to an equivalent staff complement of around **40 FTE personnel**[6]. This includes computing specialists (software developers, computational scientists, engineers, data specialists), centre management and support staff. Data on hours booked also shows that the number of staff booking time has increased from 45 to 101 over the past four years. The number of full time equivalent (FTE) staff that this equates to has increased from 20 (in 2013/14) to 41 (in 2016/17).

Having noted that the centre is focusing on industrial engagement, its timesheets over the first four years underline the commitment made to the establishment of the centre and its wider business development activities. For the period since 2013, 80% of staff time (22,200 days) was booked to six broad categories: applications, systems, operations, business development, technology support and user support.

Figure 2 Staff time booked to Hartree Centre, 2013/14 – 2016/17



Source: STFC Finance Department

[6] Note that as of 31 March 2018 the number of Hartree Centre personnel had grown to 60 FTEs. The centre is actively recruiting further additional expertise and SCD staff will no longer be transferred.

STFC data on the Hartree Centre's **capital expenditure** shows £56.1M of phase 1 and 2 funding was spent between April 2011 and March 2016. Phase 3 capital expenditure also began in the latter part of this period, with £57.0M spent in the FY15/16 - 16/17 period (the remaining £58.5M of phase 3 funding is forecast to be spent relatively evenly over the three years 2017/18 to 2019/20).

Table 2 presents an overview of the Hartree Centre's '**Fixed Asset Register'** (as of January 2018), covering only those items purchased through phase 1 and 2 funding. The register includes 47 items of hardware, software and other infrastructure, with a total value of £30.7M (revalued cost, as of January 2018). A further £27.8m[7] of phase 1 and 2 assets no longer appear in the register because they have been 'retired' (mostly repurposed for use elsewhere in the public sector – see Section 6.4).

Table 2 Hartree Centre Fixed Asset Register (phase 1 and 2 only), January 2018

Type	Revalued Cost (Jan '18)
Server	£16,627,994
Supercomputer (IBM iDataPlex system + BGAS Rack)	£3,611,399
Ventilation	£2,264,620
Electronic (visualisation system)	£2,920,493
Electrical (power system)	£1,602,901
Buildings	£406,264
Dell Cluster (training suite)	£79,800
Network	£25,052
Other IT	£3,180,306
	£30,718,829

Source: STFC Finance Department. Excludes retired assets.

2.3 The Hartree Centre's facilities

The Hartree Centre's state-of-the-art **facilities and equipment** have evolved over the period covered by the study. They currently (2017) include various Intel® and IBM data centric platforms, alongside large scale GPFS storage, an IBM data analytics cluster, Maxeler FPGA system, an immersive 3D-enabled visualisation suite and other amenities. The table below provides an overview.

Table 3 Current (2017) equipment / facilities overview (excluding retired assets)

Intel® Platforms
Atos Bull Sequana X1000 - Supercomputer capable of performing 3.4 quadrillion calculations per second. Its innovative liquid cooling technology and build density make it one of the most energy efficient HPC systems available, ranked within the TOP20 of Green500 list of the most energy efficient supercomputers in the world.
Lenovo NeXtScale - A conventional high performance system featuring 8,192 cores. Uses water-cooled rear door heat exchangers.
Lenovo System x iDataPlex system - A conventional high performance system featuring 2,016 cores which hosts the Intel® Xeon Phi accelerators. Uses water-cooled rear door heat exchangers.
Intel® Xeon Phi - Accelerator co-processor using a many core architecture; it has greater parallelism and a much larger number of cores than an ordinary CPU (central processing unit).
IBM big data analytics cluster – A mix of NeXtScale and Idataplex products used to support a wide range of open source and commercial data analytics software.
IBM data centric platforms – heterogeneous systems offering a new approach to HPC
IBM Power8 Firestone (Panther) – System includes 512 POWER8 cores, 64 nVidia Kepler K80 GPUs, IBM ESS GS4 storage and Mellanox Infiniband. Also IBM FlashStorage in IBand and CAPI-attached options.
IBM POWER8 Minsky – System includes 656 POWER8 cores, 82 nVidia Pascal GPUs, IBM ESS GS4 storage, Mellanox Infiniband and NVMe

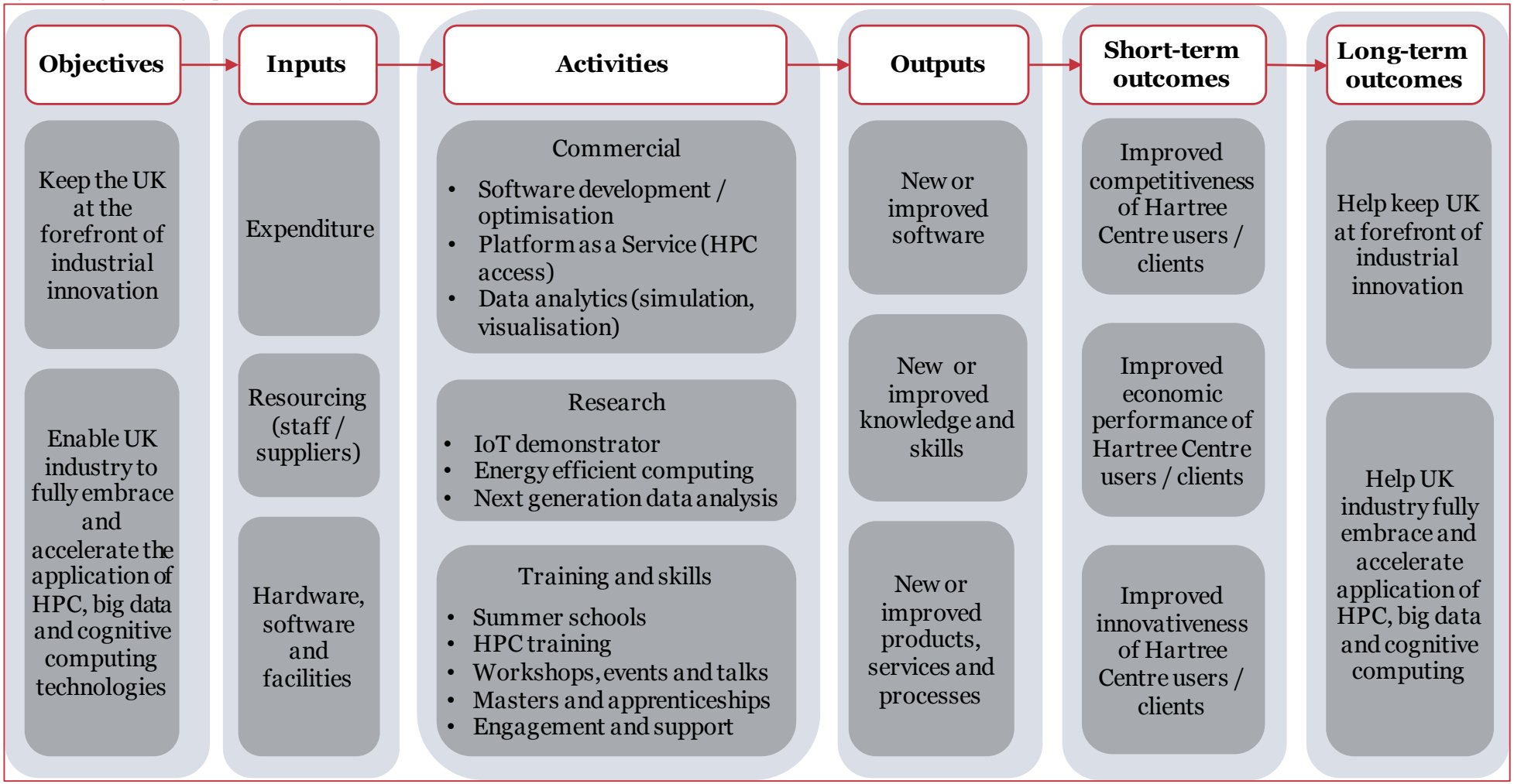
[7] The difference between current and retired phase 1 and 2 assets (£30.7M + £27.7M = £58.5M) and total phase 1 and 2 capital expenditure (£56.1M) is accounted for by the revaluation of assets within the fixed asset register.

Accelerated platforms and emerging technologies
Maxeler field-programmable gate array (FPGA) system - Five Maxeler MPC-X2000 nodes (containing in total 40 Maia dataflow engines) each node has 8 DFEs and 48GB RAM per DFE, giving an aggregate performance of 160,000 parallel multiply-adds and 3.1TB/s memory bandwidth for the entire dataflow sub-system
Clustervision novel cooling demonstrator - A novel cooling demonstrator, with nodes immersed in mineral oil to remove heat and transfer this to a building water loop via a heat exchanger. 120 nodes, each node is 2 x8 core Intel® Xeon (Ivy Bridge E5-2650v2. 2.6GHz), 64GB RAM, a total of 1,920 Cores.
ARM 64-bit platform - – 48 Cavium Thunder-X 1 ARM64-compatible processors, each with 96 cores, housed in Lenovo NeXtScale chassis. Used to investigate the energy efficiency of ARM processors when compared with Intel®.
Other Facilities
3D visualisation suite - helps users to analyse how highly complex systems affect our lives. Through computational modelling and simulation, the outputs of these methods are visualised in to immersive and interactive models. These models can be interacted with and modified by engineers, designers and scientists to create the optimum product or service. In simulation, the products act in exactly the same way as they do in real life. So, it is very quick (minutes) and easy to change the formulation of a detergent for example in simulation, whereas a real formulation prototype (actually mixing liquids) may take many weeks. Users have been able to study DNA molecules by moving them around the state of the art, eight-projector, 120-degree surround visualisation system using motion sensor technology.
Training suite - Several rows of desks with workstations. There are two presenters' areas with separate workstations and projectors onto wall mounted screens. There are separate facilities for seminars, lectures and workshops.

2.4 Logic model for phase 1 and 2 of the Hartree Centre

Figure 3 presents a logic model for the Hartree Centre's first two phases, which are the main focus of this baseline evaluation. It sets out in simple terms the logical sequence and causal relationships among: the aims and objectives for the centre; the resources (inputs) used and the activities undertaken; and the results (outputs) and changes (outcomes and impacts) that it was hoped would be realised – which should in turn contribute towards addressing the initial objectives identified. It therefore captures the core intentions and expectations for the centre and has served as the basis for the evaluation. We return to the logic of the centre in Section 12 (future benefits realisation framework), where the models are extended to include activities and intentions introduced in phase 3.

Figure 3 Logic model for phase 1 and 2 of the Hartree Centre



3 The Hartree Centre's activities and usage

3.1 Introduction

This chapter of the report presents an overview of the Hartree Centre's principal activities. It is a descriptive piece to help the reader follow the discussion in the subsequent, evaluative chapters.

3.2 Portfolio of activities

The Hartree Centre's portfolio of activities and services (during the first two phases) includes:

- **Collaborative / contract R&D.** The centre provides a research and development (and consultancy) service to help industry develop better products, services, processes and software. Using HPC, big data analytics, simulation and modelling, it works with businesses in short- or long-term collaborations to help find solutions to challenges that they face (speeding up R&D, improving processes, reducing costs), or to demonstrate proof of technology. As well as commercial access, the centre also works with researchers as partners in UK/EU-funded projects
- **Software development and optimisation.** The centre helps businesses to optimise existing codes, or write new ones, to utilise multi-core, many-core systems. It is also an Intel® Parallel Computing Centre, allowing Intel® to work with the centre on designing and testing software for the most advanced microprocessors, the building blocks of the supercomputers of the future
- **Platform as a Service (PaaS).** The centre offers access to computing power through a range of platforms. In particular, in partnership with OCF[8], it has offered clients on-demand access to its HPC facilities on a pay-as-you-go basis (pence per core hour), allowing companies to access advanced supercomputing infrastructure flexibly and at an affordable price (most clients do not have the workload to justify buying and running their own HPC cluster). For example, an annual subscription of £350 has been charged for the OCF enCORE service for up to five registered users, with additional users added at a small fee. Compute usage is then charged by core hour used[9]
- **In-house R&D.** The centre carries out internal projects and participates in pre-competitive research to build in-house capabilities, tools and international networks. These are essential for the centre, help its clients indirectly and ensure developments are driven by industry need
- **Energy Efficient Computing (EEC).** Internally, and in collaboration with partners, the centre is exploring aspects of power use in computing, and looking to devise ways of achieving incremental improvements, as well as step changes in energy efficiency. Activities include: the development of tools and approaches to support the optimisation of scientific applications for both performance and energy; collaboration with hardware/software vendors to support co-design and delivery of integrated solutions; rewriting of scientific applications to enable portability to new low power architectures; understanding the total cost of ownership of HPC system through better measurement and monitoring; and sharing best practices across UK industry and academia
- **Training and skills.** The Hartree Centre runs a range of training programmes, workshops and events, helping to address the widely reported[10] shortages of digital skills among new and existing workers, by preparing a next generation of specialists, and opening-up the power of computing

3.2.1 Phase 3 activities

While this evaluation focuses on the impacts of investments and activities in phase 1 and 2, the study team has also interviewed various Hartree Centre staff to understand plans for the current third phase. This has also informed our suggested Benefits Framework, presented later in this report.

[8] OCF will stop its enCORE service in 2018, but the centre will continue offering PaaS through different systems and organisations.

[9] For example, a job running on a compute node for one hour = 1 core hour and the minimum charge per compute job is one node (24 cores) for one hour, therefore 24 core hours. Compute charges start at less than £0.075 per core hour, with discounted rates for high use customers. http://www.ocf.co.uk/hpc-on-demand

[10] e.g. Digital Skills Crisis, House of Commons Science and Technology Committee, Second Report of Session, 2016/17, 7th June.

In simple terms, phase 3 added **two new programmes** to the work of the Hartree Centre:

- Innovation Return on Research (IROR). Run in collaboration with IBM Research, this is looking to develop a series of inter-related cognitive computing research programmes (TRL3-5) in four areas, with a view to developing new insights and software tools for use across industry, based on pre-competitive collaborative projects. Work has begun, with several projects underway
- Cognitive Accelerator. This is a business-facing consultancy programme, which makes use of IBM's 'Watson' cognitive computing (machine learning) tools. The services are being delivered by the Hartree Centre and IBM Watson staff, tackling client-defined challenges (or opportunities). For example, a collaboration with Alder Hey Children's Hospital has led to the development of a new app that can anticipate and answer questions from patients before they come to hospital.

The following paragraphs explain these new elements of phase 3 of the Hartree Centre in more detail.

The majority of phase 3 funding goes towards **Innovation Return on Research (IROR)**. This collaborative research programme with industry is a longer-term undertaking, focused on three areas - Chemistry & Materials, Life Sciences and Science, Engineering & Manufacturing - plus a fourth cross-cutting area called Enabling Technology. The latter will create new tools, software, models and methods needed to underpin the other three, as well as transfer these to other sectors and problems.

Each area has developed its own broad research strategy, or Statement of Work (SOW), which was developed initially by IBM Research and STFC and provided a general view of possible priorities and actions. These have been developed further through a series of workshops, with typically 10-15 companies attending each event. This follows a process (InCEPT™) developed by Hartree and Cambium LLP[11]. The output is a list of priority areas and possible projects where companies have signalled an interest in using data centric technologies in a specific research project related to an industry challenge. From this, actions to define a research programme and work packages addressing this challenge are identified, as well as the process and potential routes to commercialising the research in future.

For each work package, those involved will share their know-how and their data over a period of many months. Models and software will be generated and tested. The outputs will go to the companies involved, while the models and software created (the IP or "assets") are intended to belong to IBM Research and/or the Hartree Centre / STFC to be used again and hopefully be commercialised. This is not clear cut however, as there is a general wariness amongst prospective business participants about the risks of helping the centre – or IBM Research – develop solutions of general utility to all players in a sector (organisations do not want their competitors to take advantage of the insight and IP created during a project based on their data). The Hartree Centre has therefore tried to negotiate agreeable terms with company partners, which place some restrictions on how Hartree and/or IBM (the owners) can use software developed during a project (e.g. to prohibit use with direct competitors). Protracted discussions around these issues, while mostly now resolved, have delayed the launch of projects within the work programme. They may continue to limit the types of project that can be launched.

Chemistry is currently the most advanced area of activity and has launched several projects. These include projects to enable rapid development of accurate models and efficient deployment of simulations to HPC resource, to apply cognitive accelerators to simulation methodologies, to develop efficient computational work-flows and to provide non-expert users of HPC systems with platforms to access the power of HPC without the need for extensive training. This last project enables a boost in the uptake of modelling, simulation and HPC use in industry. The research projects under discussion will be longer term, however, potentially with very substantial (economic) impacts.

[11] Working in collaboration with Cambium, the Hartree Centre developed a structured process called InCEPT™, which uses direct insights from businesses to guide the translation of pioneering research, incorporating data-intensive technologies into commercial benefits. Following internal development of potential research ideas, a series of workshops are hosted with a cohort of relevant businesses, to review and refine the concept to enhance its applicability to challenges faced by those businesses. The process ensures a strong link between the creation of digital assets to real business problems. It also enables access to real company data that strengthens and validates the projects.

Specific results from these industry application projects will go to the companies involved, while the models and software created (the IP or **digital assets**) are intended to belong to IBM Research and/or the Hartree Centre / STFC to be used again and hopefully commercialised (including through research consultancy). STFC are currently exploring the commercialisation of software from Chemistry and have supported this via a £300k proof of concept fund award.

The Hartree Centre will place particular emphasis on the creation and exploitation of digital assets[12] in phase 3, as a means by which to help to sustain the centre in the longer term, while also facilitating wider dissemination and use of the insights and IP produced through its consultancy and research programmes. IROR digital assets have been defined as "outputs of joint research and development collaboration consuming capital funding to create digital content that has residual asset value". Four clear categories have been identified to aid the classification of project outputs, identify how these improve on the state of the art, and pinpoint anticipated exploitation routes. These are:

- Software: Software created or extended from STFC or IBM background IP in the Hartree GitLab which meets a documented use case and passes quality standard for code (robust, tested, documented, maintained). This could include the realisation of libraries into specific solutions
- Workflow: Encoding a method or process into a digital workflow to reduce the time to answer (via novel methodologies or automation of current processes [pre & post processing]), explore greater part of the problem space or enable re-use in other areas/domains
- Patent: licence conferring a monopoly position in exchange for discloser of the inventive step
- Cognitive or Data Analytics asset: includes a configured machine-learning model against industry use case, and a probabilistic or statistical algorithm model derived from background IP, foreground IP or open source software and that derives actionable insight

There are then three 'pillars' within the new **Cognitive Accelerator** consulting service:

1.Business engagement (business development and fast-track cognitive consulting): In this commercial pillar, the centre looks to identify a company's 'pain points' where it may be possible to exploit large amounts of unstructured information / data (pattern identification, machine learning, etc.) and to develop solutions using Watson tools. The main example of a cognitive solution so far is the collaboration with Alder Hey Children's Hospital, which has led to the development of a new software app that is able to anticipate and answer questions from patients before they come to hospital.

There is an expanding pipeline of 20-30 opportunities, where the Hartree Centre Business Development and IBM teams are discussing potential projects with prospective clients, mainly in the private sector. There is commercial sensitivity around these, but the following are examples from the public sector:

- The Advanced Propulsion Centre (APC), which represents a range of automotive companies with high-level technology readiness level (TRL) projects, are discussing looking at (terabytes of) data on engine efficiency and trying to find patterns that would be of more general interest to industry
- The Henry Royce Institute for materials science has been discussing how to use cognitive computing for discovery of advanced materials from intelligently mining existing literature

The Hartree Centre is also developing some "use cases" to show companies what is possible. The intention here is to show something powerful, but with wide applicability, as well as something relating to real world issues, but not necessarily company specific (e.g. relating to wing shape).

2. Skills and ecosystem development (Hartree Centre staff skills development): The aim is for Hartree Centre staff to take over the running and delivery of the Cognitive Accelerator consultancy activities within 2-3 years, by developing internal skills base and staffing levels. However, there are continuing

[12] The centre is already developing digital assets through its mainstream consulting work (e.g. revised software codes that are designed to run on next generation computer architectures), but those are typically developed for paying clients using their existing proprietary software as a starting point and delivering a new algorithm for the client's exclusive use. While the Hartree Centre has created a new digital asset in these cases, the new software belongs to the client and there are often restrictions on re-use of these assets (or intermediate building blocks) with other organisations (sometimes just within the same market).

challenges with recruitment that mean the centre may have to continue to rely on IBM staff to a degree that was not foreseen. There may also need to be a rethink of business models to find a more sustainable basis for project execution; for example, when operating at its most intense, the Alder Hey project required eight people on site, which is not practicable across multiple projects.

3. Grand challenges (more fundamental, client-defined cognitive projects involving research): The Hartree Centre is looking to build a new 'Watson-based' service that helps to address a major challenge for industry or society. It is too early for this to be defined, however it could be something (for example) in advanced manufacturing, in health or in education (e.g. IBM Watson has done some groundwork on what might become a region-wide or national Autism service, which would be developed to support schools and families, and would draw on inputs from parents / clinicians / researchers). The Grand challenge work will probably involve an industry client and IBM Watson.

3.3 Project portfolio

In the first four years of operations, the centre completed **167 projects** with around 60 different organisations. Within this portfolio, around 100 projects (60%) were carried out with **commercial businesses**. There were ~40 *unique* business users in total, including some of the largest UK-based companies, such as GSK, Rolls-Royce and Unilever. The balance of the project portfolio includes a mix of in-house projects and collaborations with academic research groups and other public bodies.

Larger businesses account for around 80% of commercial projects. Many are household names in the UK, from aerospace firms (BAE Systems) through to pharmaceuticals (GSK) and consumer products (Unilever). The centre also works with the UK subsidiaries of other multinationals (e.g. DNV GL, Siemens and Waters). In addition, the centre works with several smaller, software developers and other high-growth-potential digital **SMEs**, such as Global-365 and Zenotech.

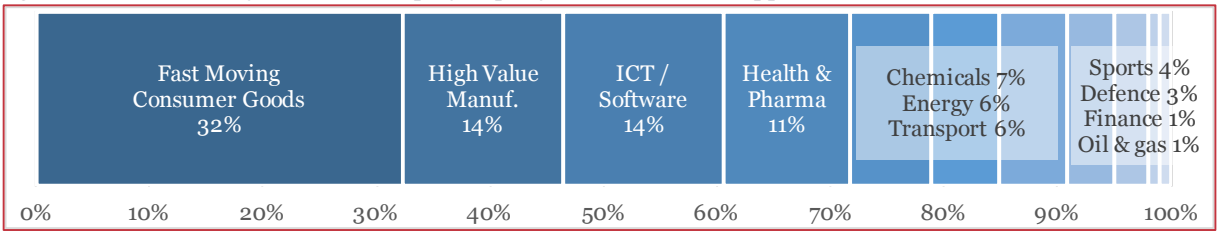
Table 4 List of users / partners in phase 1 and 2 projects

Commercial User Multiple projects	Commercial User One-off		Academic User	Other Public User
• BAE Systems • Constelcom • GSK • IBM Research • Infineum • Johnson Matthey • Lenovo • Novidec • Optis • Renuda • Rolls-Royce • Unilever • Zenotech	• 3DSim • Atkins • Rail Delivery Group • DNV GL • Dstl / Marriot • Dyson • EDF • Global-365 • Intel® • PSE Ltd	• Royal Society of Chemistry • Siemens • Sun Chemical • Falcon Project • Tracsis • Trendalyze • TSC • Victrex • Waters • Micromass • WaveReach	• Cambridge University • Chester University • Durham University • EPCC (Edinburgh) • ErasmusMC • Imperial College London • Liverpool University • Manchester University • Stirling University • Strathclyde University • UCL • University of Essex	• Met Office • National Physical Laboratory • Wider STFC

The Hartree Centre Programme Directory includes basic information on each project: reference number, title, PI name, start/end date and customer name (with various gaps[13]). Additional information is recorded in Project Detail forms, but these are only available for ~70 projects (mostly **commercial/ external projects**, which require more extensive approval processes). Extracting additional information from these forms has allowed us to expand the details held on these 70 projects and provide a basic characterisation of the portfolio. For instance, the following figure presents an overview of the portfolio (~70 projects) by application area. It shows that over half of these projects (60%) fall into three main areas: fast moving consumer goods; high-value manufacturing; and ICT / software.

[13] Mainly relating to the academic or internal projects.

Figure 4 Distribution of (commercial) project portfolio across broad application areas



Proportion of all phase 1 and 2 projects, where known (n=70)

Commercial work is split between charged-access to HPC facilities and more involved collaborations with Hartree staff. Much of the collaborative work involves the creative use of the facilities and computational scientists in supporting a given business' product development. There is also a steady flow of code optimisation, reconfiguring existing software packages to work more quickly with new, more powerful computing architectures. Applications range from new improved formulations for a variety of consumer products, to working with the Rail Delivery Group on a range of models and tools.

3.4 User communities

Industrial engagement is central to the Hartree Centre and its objectives. The centre sits between academia and industry, keeping a foot in both camps and providing a link between the two. Other UK HPC centres (e.g. the Edinburgh Parallel Computing Centre or EPCC) do industrial engagement, but this tends to be one amongst several main functions. The Hartree Centre is essentially an industrial engagement centre, with academic projects, rather than the other way around. Companies may come in the first instance with a relatively simple question (in search of a quick result), but after a couple of smaller projects will understand the potential and overlap with their commercial interests, and become interested in longer-term questions, leading to further research.

In the past four years, the Hartree Centre has also worked with many of the UK's leading **academic research groups**, as well as various public-sector research organisations, including the Met Office. Academic research constitutes a smaller part of the Hartree Centre project portfolio (~10% of projects) than the EPCC based at the University of Edinburgh.

3.5 Commercial income

Financial data for the Hartree Centre over the last four years shows **total income** of around £4.5M for the period, with annual figures varying between £750K and £1.4M. Much of this income (78%) is accounted for by 'industry sales,' with the value of commercial income growing slightly over the period. Grant income (from UK and EU sources) has increased significantly, from £0 in 2013/14 to £400K in 2016/17. The split between industry sales and grant income is around 70/30 currently.

Table 5 Hartree Centre Income by area, 2013/14 – 2016/17

Income	2013/14	2014/15	2015/16	2016/17	4-Year Total
Industry Sales	£754,957	£992,805	£967,457	£824,118	**£3,539,336**
Grants (TSB/IUK, RCs, Unis)	£-	£77,600	£408,091	£391,554	**£877,245**
EU projects (H2020)	£-	£-	£3,036	£24,381	**£27,417**
Fees and travel reimbursements	£19,550	£22,585	£17,271	£34,078	**£93,485**
Total	**£774,507**	**£1,092,990**	**£1,395,855**	**£1,274,131**	**£4,537,483**

Source: STFC Finance Department

There are 37 organisations listed against the £3.5M of **industry sales**, mostly private companies, but not all. However, the income is skewed, with more than 80% of all commercial income (83%, £2.9M) derived from just eight of the 37 named organisations. These are mostly organisations that have worked with the centre for several years and have developed their interactions over multiple projects.

4 Innovation and competitiveness

4.1 Introduction

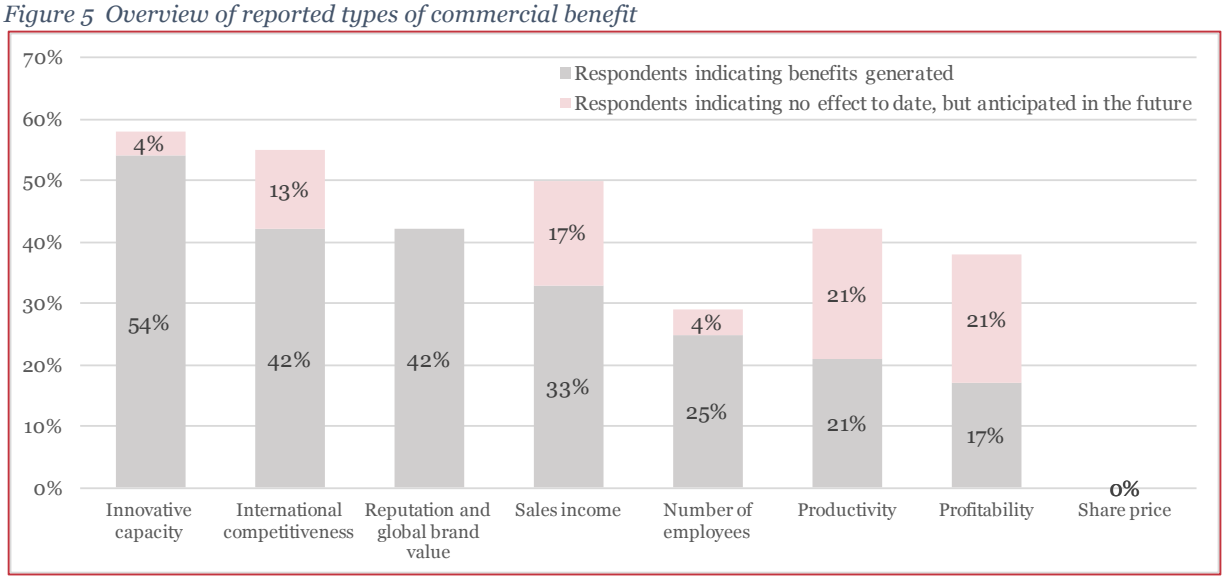
This chapter presents an overview of the contributions of the Hartree Centre to innovation and industry competitiveness, which are the principal objectives for the centre.

Figure 5 presents the results of our industry survey wherein we asked respondents to indicate which of eight types of commercial benefit they had realised as a result of their work with the Hartree Centre. The 15 survey responses have been augmented with feedback from our interviews with nine businesses that preferred to give an interview rather than complete the survey. While the absolute numbers (24) are small, this does amount to 55% of the centre's industry clients, which is a good response rate. The figure is sorted by number of respondents reporting each benefit being generated. In recognition of the fact that benefits may not have materialised yet, we also invited people to indicate which if any of the benefits they expected to realise at some point in the future (shown separately in the figure).

The responses suggest the Hartree Centre is delivering wide-ranging benefits to its clients, with a majority of respondents reporting two or more types of commercial improvement each, including many that judge their relationship with the centre to have improved their **global competitiveness** and a majority saying that it had increased their **innovative capacity.** Other widely reported benefits – already realised – related to **users' reputation** (42%) and **sales income** (33%). In addition, a significant minority reported **improvements in employment, productivity and profitability**. An improved share price is the only category that failed to attract any responses from our sample of users.

As the Hartree Centre's interactions with client businesses develops – more joint projects, more time elapsed – we would expect to see an ever-greater proportion of its client portfolio reporting positive commercial results. The cognitive computing work also has the potential to transform client's business processes, and should have a more profound impact on even the largest client businesses.

Figure 5 Overview of reported types of commercial benefit



Source: Technopolis survey of Hartree Centre industry users. Proportion of respondents (n=24) indicating that the Hartree Centre had generated different types of commercial benefit (or these were anticipated in the future).

In the remainder of this section we look more closely at many of these areas of commercial benefit and provide specific examples to illustrate the contribution of the Hartree Centre to particular companies.

4.2 Reputation and brand value

Our survey and interviews suggested that many clients (42%) derive reputational benefits from working with the Hartree Centre, reflecting its status as a national centre of excellence and the exacting nature of the collaborative work that is being undertaken. We identified several specific instances where industry clients report an improvement in the reputation and market position of their companies, which appears to be particularly beneficial to small software and technology companies:

- **3DSIM** (acquired by Ansys) was able to select the most appropriate new product development strategy following proof of concept work and has seen reputational benefit from work with Hartree
- **Embecosm** is a firm working in compiler development and computer processor modelling. It has worked with the Hartree Centre on several occasions, including developing the first compilers that can optimise for energy consumption (traditionally compilers optimise for code speed). The company name-checks the Hartree Centre on its website, alongside its commitment to contribute to the development of next generation software and electronics: "We are very fortunate to work with world-class academic partners that include INRIA (France), Bristol University (UK) and The UK Science & Technology Facilities Council high performance computing centre at Daresbury." Embescom reported that there have been some indirect commercial benefits through their engagement with the centre. The company also expects that the reputational benefits of working with the Hartree Centre will allow it to access more customers in the HPC space
- **Peter Marriott** – an independent consultant – has been carrying out fluid dynamics work for the Defence Science and Technology Laboratory (Dstl) and running Direct Simulation Monte Carlo simulations with the Hartree Centre. He is clear that this is positively regarded by Dstl and allows him to compete with larger consulting engineers, running equally sophisticated modelling
- **Renuda** is able to run more sophisticated simulations and derives substantial reputational benefits, supporting its market position among blue-chip clients. Working with the centre has been good for its image, helping to demonstrate the level of analytical sophistication that it can deliver
- **WaveReach** is a small start-up based at Sci-Tech Daresbury that worked with the Hartree Centre to help develop a novel data security product (Lighthouse) for the Internet of Things. It trialled a network of sensors at Daresbury and worked with the Hartree Centre on a range of activities from data visualisation (e.g. geo-mapping) through to system integration (AI security agents). The ambition had been to cut time-to-market by an estimated 6 months for the new product. However, because of site network security issues, the project was less widespread than planned. Even so, the work has played out well in discussions with prospective clients and the company has benefited from the centre's extensive networks with businesses, government and academia

4.3 Productivity benefits

The cost of entry (money and people) is a major barrier restricting the more general deployment of HPC by industry, which will in turn act as a brake on the rate at which businesses are able to digitise more of their research and innovation activities. The Hartree Centre occupies a unique position in the market place, offering a combination of hardware and specialist people-related services of relevance to the large numbers of firms that cannot justify the costs involved in buying and operating their own cluster, or do not have the internal capabilities to make good use of cloud-based HPC services.

We identified several instances where clients reported improvements in productivity as a result of their work with the Hartree Centre, primarily concerning an **increase in the speed of their research and engineering processes** (time-to-market) and new product development. For instance:

- **Unilever** has seen improvements to its new product development (NPD) processes for new formulations (faster, more what-if-analyses, fewer physical tests)
- Historically, **Dyson** built physical models and put them into a testing chamber. With the advent of 3D printing this process has become much faster, but the Hartree Centre could not only offer speed,

but also greater insight and accuracy ("we can tell you where the noise is coming from"), allowing Dyson to solve problems more quickly

- **Rolls-Royce** has updated its in-house engineering design software with the support of the Hartree Centre, accelerating run times and bringing it a step closer to virtual 'whole-engine design'
- The Virtual Engineering Centre (VEC) at Sci-Tech Daresbury has worked with a number of large UK manufacturing organisations such as **BAE Systems**. Work has included the development and digital testing of systems that support the safe flight of unmanned aircraft and innovative software that has supported autonomous mission management software. The VEC has direct links with the Hartree Centre and, through its Virtual Engineering Simulation Laboratory, provided BAE Systems engineers (and its other clients) with direct access to the centre's HPC clusters.
- **University College London** has collaborated with the Hartree Centre in implementing a high-throughput molecular simulation system, utilising the power of HPC to accurately determine biochemical properties within clinically relevant timescales (see Figure 6).

Figure 6 Improvements in speed of biomedical research – University College London

The successful application of high throughput molecular simulations to determine biochemical properties is of great importance to the biomedical community, if these can be turned around in a clinically relevant timescale.

In order to be able to achieve such turnaround times, while maintaining accuracy, UCL have developed the Binding Affinity Calculator (BAC), which utilises the power provided by a high performance computing system to automate all of the stages required to compute free energies of binding: model preparation, equilibration, simulation, post-processing, and data marshalling between resource. Such automation enables a molecular dynamics methodology to be used in a high throughput manner not achievable by manual methods.

This work has been facilitated by UCL's collaboration with the Hartree Centre, through the hosting of a researcher from the University to work on implementing the system on Hartree resources, as well as an allocation of compute time to run large scale investigations. The centre also supported two SMEs (EnsembleMD Ltd and CBK SciCon Ltd) who were working with UCL to develop industrially relevant software associated with BAC. These various activities have in turn supported the work of a spin out company seeking to harden and deploy the workflow for customers in the pharmaceutical industry.

The Hartree Centre also offers '**Platform as a Service**' (HPC on demand), which gives cloud-based access to its various HPC facilities as users need them. This was widely reported to have allowed companies to carry out scientific and engineering analyses in a fraction of the time and at a fraction of the cost of a more conventional approach (using less powerful computers). These process improvements tend to translate into more and better analyses and ultimately better designs, rather than cheaper design, with clients reaping much of the benefit, while not necessarily paying a premium for the more sophisticated simulations.

Figure 7 presents a series of strikingly positive testimonials relating to the enCORE HPC on demand service (run by OCF plc, an IT services company)[14], which underline the importance for smaller technology companies in particular to access these state-of-the-art facilities on a pay-by-use basis, allowing them to compete on an equal footing with their larger, global counterparts.

The outsourcing arrangement with OCF plc has enabled the Hartree Centre to extend its industrial engagement and increase its system utilisation levels within the context of its internal staffing challenges. We understand that the Platform as a Service offering has also helped to attract businesses to trial HPC-based services, which can lead to clients moving on to work directly with the centre on development projects. Providing Platform as a Service does mean that the Hartree Centre is offering broadly similar services to those on offer in the market privately (though with bigger facilities and dedicated user support and expertise). However, given the relevance of HPC on-demand to businesses across the UK – and the centre's finite staff – such arrangements make good sense.

[14] The enCORE HPC on demand service was run through an outsourcing arrangement with OCF plc. This will stop in 2018, but the Hartree Centre will continue to offer PaaS through other systems and organisations.

Figure 7 Feedback relating to specifically to the enCORE service

"Access to enCORE services has allowed QED Naval to compete with corporate level capabilities and increase the size of models with the power to run projects faster and more efficiently, but with SME overheads which provides better value for money to our clients. In short, access to the enCORE services increases our speed of learning." Jeremy Smith, Director, QED Naval

"OCF were able to quickly step in with the enCORE service when our normal compute provider shut down for a month. We were quickly up and running with the enCORE service, which delivered excellent performance. This was vital for our business, and we continue to use the enCORE service to meet our growing HPC needs." Dr Mauro Arruda, Director, Digital Engineering Ltd

"OCF allowed us to rapidly upscale our CPU capacity. This makes it possible for specialist SMEs such as Simpact to meet the demand from large OEMs, where previously this was the domain of only a handful of international companies." Dirk Landheer, Director, Simpact Engineering Ltd

"Services like enCORE are excellent for our busy work periods and to lend support to our own 80 node in-house server cluster. It's useful to have temporary, extra compute resource. In peak periods, we can continue to take on new projects whilst maintaining or exceeding our customers' expectations. We would definitely use enCORE again. We used enCORE to process a 5 million cell test case for simulation of wind loads on solar panels. It was not a large case, which for us is typically 40-50 million cells, but it demonstrates the capabilities of enCORE. We possess expertise in a range of flow related design and engineering projects, for example aerodynamics, building physics such as flow inside and outside buildings and even medical apps, such as airflow inside an incubator. They are all very different projects, but could all easily be processed using enCORE. Eric Terry, Managing Director, Actiflow

"In 2012, as part of a pilot project we trialled enCORE to test an existing CFD case. Our own internal server cluster is smaller than enCORE's and we wanted to run a case on a larger, more powerful machine. The potential to run larger and faster CFD calculations using a cloud service was of interest. The pilot was successful and, in 2017 Renuda started using Constelcom Ltd's Constellation platform to access Hartree as HPC as a service. Constellation brings additional value as it makes it possible for Renuda to manage its users and projects and for its employees to very easily access their data and run simulations. This is now used for several industrial projects which would not be possible without the convenience of the service and the power of Hartree's systems. " Nicolas Tonello, Director, Renuda

"Using enCORE enables us to deliver very large HPC simulation projects at a fraction of the cost and time it would take to realise in-house. As a result, we can take on board new business with reduced scheduling concerns as enCORE provides the ideal platform for dealing with peak load demands. enCORE's state-of-the-art hardware, competitive pricing and simple setup procedure make it a much more attractive HPC platform than the typical Cloud offerings available today. OCF's excellent support services and flexible secure data delivery are further plus points. A lean business model, enabled by services like enCORE, has allowed our company to reduce infrastructure investment while increasing our growth rate in a global and highly competitive engineering services industry." Andrew Jackson, Head of Development, Engys Ltd

The Hartree Centre is also heavily involved with the enhancement of proprietary software (e.g. **code optimisation**), which allows clients to run more complex simulations faster using larger, multicore HPC systems. The centre has delivered newly-optimised versions of various modelling and simulation codes, mostly proprietary, which will deliver analytical and productivity benefits to its clients' own businesses. In several cases, the updated software is now being sold to third parties. Examples include:

- **Met Office, GungHo**. This was a project to design and build a next-generation weather and climate prediction model for the UK. It was a collaboration between the Met Office, NERC and STFC. The Met Office is developing a new model of atmospheric dynamics for weather prediction and climate simulations, and the Hartree Centre was working on the computational framework to support the efficient operation of the new model on the latest HPC architectures (the work continues with the Met Office through the follow-on LFRic project, which is implementing the recommendations from GungHo). The Business Case to Government for the new £100M HPC facility at the Met Office states "the supercomputer's sophisticated forecasts are anticipated to deliver £2 billion of social benefits to the UK by enabling better advance preparation and contingency plans to protect people's homes and businesses"

- AU3D and Precise projects are code modernisation and code optimisation projects that have been undertaken for **Rolls-Royce,** where the company wanted software to run faster so that its simulations could be completed significantly more quickly, thereby enabling them to explore more design options in a shorter space of time. They are a good example of the Hartree Centre's skillset and how this can help a business that 'has everything'. Interestingly, the AU3D project also came directly out of the Intel® Parallel Computing Centre (Intel® PCC) collaboration

- **Atkins'** road traffic simulation modelling software was optimised to run on multi-cores, such that scenario simulations could be run at much greater speeds. Highways England has invested in five new Regional Transport Models that use Atkins' SATURN (Simulation and Assignment of Traffic to Urban Road Networks) traffic modelling software to help predict the economic impact of the extensive road network investments up to 2020 and beyond. Performing simulations of the size and sophistication needed to better understand investment certainty can result in long runtimes – a major obstacle to the transport modelling industry. The Hartree Centre took part in a collaboration to port SATURN to GPUs, which run up to 30-times faster than the standard version, with potential to increase speeds still further. Atkins can now run simulations in a few minutes, rather than days, and can therefore provide clients (or internal decision makers) with results much more quickly. Atkins licences its software to various third parties, and expects to be able to encourage existing and new clients to invest in the new version.

4.4 Contributions to innovative products and services

There is a clear thread throughout most of our desk research, interviews and surveys that suggests the Hartree Centre's work has the potential to help develop very **innovative products and services**, and several clients have reported specific contributions in this regard:

- **DNV GL**, an international classification business, with a growing number of offshore engineering interests in the UK and internationally, launched a collaborative research project with several UK academics and industrialists, including the Hartree Centre. The project set out to improve the accuracy of designing offshore wind farms. This is a new 'real world' problem. DNV GL's engineers design wind farms and wanted to improve the accuracy of their modelling, and in particular the impact of one wind turbine on another: the blades of one machine will tend to change the airflow for the turbines downwind and can significantly affect efficiency levels across the farm and overall power outputs. The new dataset and model runs are expected to allow designers to develop a truer and more accurate estimate of power outputs for a given layout of the wind turbines across the 'farm'.
- **WaveReach** provides consultancy, integration support and expertise on Internet of Things (IoT) solutions, especially within a rural setting. Examples of research projects to date include road and rail bridge monitoring, real time tracking of individuals at hospitals, airports and other public areas, and electricity power distribution for condition monitoring systems. WaveReach's engagement with the Hartree Centre began in 2016 with the company being successful in an STFC funding competition. A further win via the Digital Catapult in early 2017 secured them rent free space on the Sci-Tech Daresbury Campus for 10 months. WaveReach is developing systems that collect data either real-time, or via devices connected to the global Sigfox IoT network and other backhaul communication systems. Data is sent to the Hartree Centre, processed, and then forwarded to the customer. In particular, they are developing solutions to ensure that the Hartree Centre receives only anomalous or important data from sensors. This will maximise the efficiency of data processing. WaveReach is currently working on prototypes and pilot projects, collaborating with the Hartree Centre and IBM Watson staff to develop software to generate valuable and meaningful results. Working with the centre has provided the company with several benefits. For instance, it has provided them with access to equipment that would otherwise have been unaffordable. This has helped quicken the development of prototype development, which is especially important because a lack of access to technology had previously been a barrier to growth.
- **KnowNow Information** developed a proof-of-concept for a flood management tool for local authorities and emergency services. (see figure below)

Figure 8 Future commercial potential – KnowNow Information

KnowNow Information (kn-i) looks to help organisations operate more efficiently through better understanding of data and subsequently improving the interoperability of their services. The firm has worked with the Hartree Centre and wider STFC on their 'Whether you do or Weather you don't' flood event model. This is a statistical model which combines static geographic data, variable weather condition data and historic emergency incident data, leading to a more accurate prediction of the likelihood of flood events. The model is formed of two distinct phases:

- The first phase looks to prove and validate that a correlation can be positively identified between a weather event, and then weather-induced events in a specific location within Hampshire
- Phase Two centres on working with experts in the emergency services, Environment Agency and local council response teams to determine whether some form of proactive response (e.g. evacuation of local residents) is the optimal way forward

KnowNow's engagement with the Hartree Centre began through the firm's attendance at an Open Data conference there in 2014. At the end of the event, KnowNow entered an innovation competition where it provided a concept paper on the model. KnowNow won the competition, providing them with c.£15K's worth of computing time and labour from the Hartree Centre. Since then, the company has not only utilised the centre's computing capacity (bringing data processing times from 1.5 days on a typical laptop to under 25 minutes), but used STFC staff knowledge to help with data cleaning and algorithm development.

Following their work with the Hartree Centre, KnowNow had developed a technical Proof of Concept for the model. The project is currently on hold however, as – for political reasons - government funding for the business Proof of Concept has been pulled. The company plans to re-visit the model again in another four to five years, by which time they hope the political, economic and funding climate will have changed. Once implemented, they believe that the model can generate a number of societal benefits:

- Enable more accurate local level predictions about flood risk
- Generate financial savings for users (e.g. local councils) by helping to direct emergency resources to where they are most likely to be needed. The company's own estimates suggest that users can save £10 for every £1 spent on the package
- Better flood prediction models will help save lives by helping install the more appropriate mitigation measures, and ensuring the better targeting of emergency services resources

The company also envisages substantial future commercial opportunities. The firm's own market analysis indicates that in the Hampshire area alone, the market for the model is worth approximately £10M. It is also hoped that the algorithms developed can be applied to environmental emergencies such as wildfires, tornadoes and earthquakes.

The Hartree Centre has played a pivotal role in the development of the technology. In the absence of the centre and the innovation competition it ran, the package would have remained a theoretical idea – the centre has provided the opportunity to turn the theory into something more concrete. As such, the firm felt that much of any future commercial benefits seen from selling the model will be attributable to the initial work with the Hartree Centre.

4.5 Sales income and profitability

Our survey and interviews identified several businesses that have seen an **increase in sales income** (8 to date, another 4 expect to see increased sales in the future) following their collaboration with the Hartree Centre, as well as a smaller number reporting an improvement in profitability. Most of these respondents were unable to quantify the scale of the increase in income or profitability, however, five companies were able to give some indication of the scale of benefits:

- One client was able to describe a meaningful improvement in the size and profitability of a part of their business, which they attributed in large part to the work that they had been doing with the Hartree Centre over the past five years
- An SME in the HPC services sector estimates that its work with the Hartree Centre has added around £150K to its bottom line
- We identified another instance where a client anticipated substantial future benefits, with cost savings of up to £2M and additional income of more than £1M
- IBM Research is a strategic partner with STFC in the Hartree Centre, with a particular focus on IROR, so it is perhaps not quite right to view the company as a client (or suppliers). Nevertheless,

IBM Research did complete a survey return and give several interviews and it reports a positive impact on its innovative capacity, international competitiveness and reputation

- Unilever estimated it can benefit by scaling processes to achieve faster time to market (see figure)

Figure 9 Unilever's strategic partnership with the Hartree Centre

Unilever is one of the world's leading producers of consumer goods and includes among its brands household names such as Persil, Dove and Hellman's. The company's products are sold in more than 190 countries and its market research suggests that on any given day two billion consumers worldwide are using its products. With this kind of market reach, any improvement in its products can result in substantial commercial improvements through better sales volumes or margins.

Digital R&D is vital to Unilever's ability to meet its strategic objectives, as the business aims to secure year-on-year growth globally. The company's €900M R&D spend (EU R&D Scoreboard) is still expected to help deliver around half of that additional annual increase. The discipline of lean has caused the company to think hard about where to focus and how to improve how they do things, including R&D.

Digital R&D is about the digitisation of the company's overall product development and deployment processes. This is not a short-term transformation; the rate at which one can transition to a fully digital set up, from idea to lab to manufacture, requires a number of important developments in enterprise-wide software systems on the one hand and the science of materials and manufacturing on the other. Unilever's links with the Hartree Centre are helping to contribute to both sides.

The work at the Hartree Centre on 'pour flow simulation' was pioneering and had enabled the company to design and manufacture a new liquid-detergent cap that pours without dripping. Unilever invested heavily in the new cap too, however, the Hartree Centre work was the breakthrough that "got us over the line." The Hartree Centre modelling delivered substantial savings in development costs – in terms of both lower staff time and very many fewer physical tests – and has also accelerated time to market. The design also includes some improvements in manufacturability, which also produced some savings.

The company's work with STFC on the development of computer-aided formulation (CAF) has been valuable, delivering productivity gains in product development on the one hand and accelerating innovations more quickly and more cost-effectively (in terms of the new product development process) than would have been the case otherwise. It is even possible new formulations would not have been identified at all had Unilever still been relying on more conventional experimental methods.

The impact of in-silico methods on the business will be significant and if one could estimate the likely volume of turnover that would have been lost by being slower to market, that would approximate to the additional income captured. Since household products sell in high volumes, being able to launch a new product relatively earlier can generate significant new sales revenues.

Unilever is also working with the Hartree Centre on several projects relating to its wider business, beyond New Product Development. The Hartree Centre project is analysing vast amounts of process control data in order to develop improved understanding of the factors associated with line stops. The results of the analysis can then be used to focus engineering resource to make targeted interventions. Improvements of 5-10% on the line's output would be seen as valued significantly within the business.

5 Skills and capability benefits

5.1 Training courses and events

The Hartree Centre has been running training courses and information events from the outset, as part of its wider commitment to raise awareness about the potential of HPC in industry and academia. It is also looking to build competence around HPC applications and has therefore been involved with the creation and delivery of a range of education and training courses, for students on the one hand and practitioners on the other. It has chosen to address both the public and the private sectors and has consciously involved the international HPC community in both the delivery and as participants, to enrich the learning experience for UK-based scientists and engineers. Benefits to participants include:

- Getting to grips with or expanding knowledge in relation to the latest tools and techniques
- Gaining new skills in areas demanded by employers
- Networking with like-minded individuals
- Meeting new partners and collaborators

The Hartree Centre provided an overview of **training and workshop activities** for the four years, from 2013. These data show that the Hartree Centre has organised, hosted or contributed technical expertise to over 130 training courses and skills development activities since it was launched, helping to train the next generation of computing specialists, upskill industry workforces to make the power of computing accessible, and inspire industry, students and the public. This training is often delivered in collaboration with the Scientific Computing Department (SCD) and industry partners (such as IBM Research, Intel®, Nvidia, Maxeler), as well as involving the Hartree Centre's own specialists in software development, data analytics and visualisation.

There were too many courses to present in full here. For legibility, therefore, Table 6 lists the workshops and training events held at Sci-Tech Daresbury and involving the Hartree Centre, for 2016, which (at the time of writing) was the last year when full data was available. We understand, however, that this mix and scale of activity is typical of the schedule seen in previous years.

It is important to note that a good proportion of these events have been led by SCD rather than the Hartree Centre (e.g. the Collaborative Computational Projects / CCP events), although these do use the Hartree Centre's facilities / resources. There is also substantial involvement from industry, including for example, hackathons organised by the Hartree Centre but delivered jointly with IBM Watson. Notwithstanding these caveats, it is clear that the Hartree Centre is involved with the hosting or delivery of a range of events for advanced users from academia and industry and for more general introductions again for public and private sectors. This includes software courses, subject-specific masterclasses and more public events such as the Daresbury open week, where the Hartree Centre was a major attraction.

Table 6 Training events hosted at the Hartree Centre in 2016

Course / workshop	Duration	Academic	Industry	Other	Total	Total days
MCC-UKCP-EPCC Workshop	5 days	38	0	0	38	190
Energy Materials / Computational Solutions	2 days	15	0	0	15	30
Watson Developer Training Course	2 days					
Particle Physics Masterclass	3 days					
UK Water Partnership	2 days	17	17	0	34	68
2nd CCPBioSim/CCP5	3 days	72	0	0	72	216
IBM Software (Familiarisation Workshop)	1 day	0	0	49	49	49
COSSAN Software Training	3 days	36	0	0	36	108
NERC Scientific Computing Forum	2 days	20	0	0	20	40
Hartree Centre / IBM Hackathon	3 days	10	30	0	40	120
Software Development for Xeon Phi	3 days	27	0	0	27	81
CCPBioSim / CCP5 Training Week	5 days	63	0	0	63	315

Course / workshop	Duration	Academic	Industry	Other	Total	Total days
Summer School, WK1 - Big Data	5 days	11	6	0	17	85
Summer School - Wk 2 - Eng. Sim.	5 days	18	3	0	21	105
Summer School - Wk 4 - HPC	5 days	15	2	0	17	85
Daresbury Open Week	5 days					
CCP5 Summer School 2016	9 days	65	0	0	65	585
GungHo Meeting (Met Office)	2 days	27	0	0	27	54
Designing Future X-Ray FELs	3 days					
CECAM / Psi-k / CCP9 Graduate Schl	5 days					
Hands-On Tutorial (Code_Saturne)	5 days					
Fortran Modernisation Workshop	2 days					
HPC101 Training Course	1 day					
KKR Hands-On Course	5 days					
Sim. for the Experimentalist & Industrialist	2 days					
NHS Design Group	1 day					
DREAM Big Data Winter School 2016	5 days					
DL_SOFTWARE Training Course	3 days					
AMOEBA advanced potential energies	1 day					
Computing Insight UK 2016	2 days					
Total	**100 days**	**434**	**58**	**49**	**541**	**2,131**

Source: Hartree Centre management team

According to the data provided for 2016, Hartree was involved with the planning and delivery of 30 events, lasting 100 days combined. The mean duration of these courses was just over three days however, the events range from a single day through to several weeks (for the Hartree Centre Summer School). Delegate numbers were available for 17 of the 30 events, which gives a total of 541 people and 2,131 'training' days. If we assume the 17 events amount to a typical cross-section of all courses and workshops, that would suggest around 955 people (541/17*30) attended events across the whole year for an estimated total of 3,760 training days. These courses and events are **mostly provided free of charge to delegates**, albeit several of the events do attract external funding.

As shown in Table 6, academics accounted for the great majority of delegates in 2016; some 434 people or 80% of the total (where delegate information was available). Indeed, nine of the 17 events where we have data, were for academics only, with 363 coming to these events. Industry delegates accounted for the next largest category (58; 11% of all delegates). STFC staff / IBM Research and other delegates represented 9% of all attendees. However, all of this last group come from one event, the IBM Software Familiarisation Workshop' which appears to have been an internal-only session. The heavy academic focus reflects in part the number of events that are delivered collaboratively with SCD, and this is likely to overstate the balance of industrial engagement seen in the Hartree Centre-only events. However, the Hartree Centre has also received feedback to suggest that the difficulty of releasing individuals from their day job for more than one day has also limited the level of industrial attendance at some events.

The following bullet points provide a fuller and more qualitative description of the range of the Hartree Centre's external events and training activities:

- **Ad-hoc training and events** – the Hartree Centre runs a number of bespoke hands-on training programmes, workshops and other events throughout the year, focused on subjects such as data analytics, cognitive computing, code optimisation, visualisation, modelling and HPC. For example, in 2017 it hosted a workshop to explore developments made through the Intel® Parallel Computing Centre (Intel® PCC) programme (see below). It was also involved in an outreach event (in partnership with IBM Research) aimed at promoting careers in STEM to female students

- **Hackathons** – the Hartree Centre hosts open and organisation-specific hackathons to equip individuals and organisations with the skills needed to exploit data and cognitive tools. The open hackathons are usually based around a sector or theme and are open to companies, entrepreneurs, coders and designers. The centre also looks to run these events in partnership with specific organisations that want to access a wider pool of people to tackle specific challenges. For example, EDF Energy (who monitor data coming off nuclear power plants) were interested in data analysis and what could be learned from looking at different monitoring systems together. A Hackathon was held, where EDF Energy's problem was introduced and then the Hartree Centre showed the tools that are available for data analysis, using EDF data. Conversations with EDF Energy are still ongoing, but it is hoped this will turn into a new client relationship and more substantive work
- **Intel® Parallel Computing Centre (Intel® PCC) Training Course** - an Intel®-funded 3-day course, which is run once each year and offers 40 people (mainly external academics and staff/academics from Diamond and ISIS) free access to, and training on the use of, Intel® Xeon Phi. The course is run with the assistance of Intel® staff, which is a draw for attendees. Course material covers the essentials of parallel software development, common mistakes and the correct implementation, Intel®'s suite of tools and finally its new many-core architecture. The course has proved popular and it has been necessary to remove internal applicants to make space for external attendees. The academics would not get access to this hardware otherwise – and the Hartree Centre can give them access to 42 nodes. This work gives the Centre a link to Intel® and is also a way to upskill internal staff about multi-core architecture; knowledge they can then apply in future projects. This course is now being scaled up, with two events to be held in 2018, rather than one
- **Hartree Centre Summer Schools** – Week-long training courses, run each year, with internationally renowned academics and industrial organisations delivering lectures and think pieces. Since 2013, some 170 attendees have participated and in 2016 four such weeks were hosted, each focused on a different topic (big data, engineering simulation, visualisation, HPC). There was not a Summer School in 2017, but there are plans to reintroduce this course in 2019.
- **Post-graduate HPC programme**[15] - The University of Liverpool runs an MSc in Big Data and HPC in conjunction with the Hartree Centre. It focuses on theory as well as the practical application of Big Data and HPC technologies and seeks to help develop new talent in computing. The Hartree Centre offers two bursaries per year and has also facilitated the sponsorship by industry of several scholarships covering the tuition fees for the MSc. Students are co-supervised by the Hartree Centre and get to work with industry partners

There is exit poll data for one or two events that have been run, however, it concerns satisfaction levels in the main, and does not provide the basis for estimating / quantifying the resulting benefits to participants. Under these circumstances, the simplest solution is to use a proxy indicator based on the equivalent market price for the cost of this kind of academic / technical training. A charged course for academics might cost around £250 a day; one might perhaps double that for private sector delegates. This would produce a figure of ~**£1.1M in training benefits to industry and academia**[16].

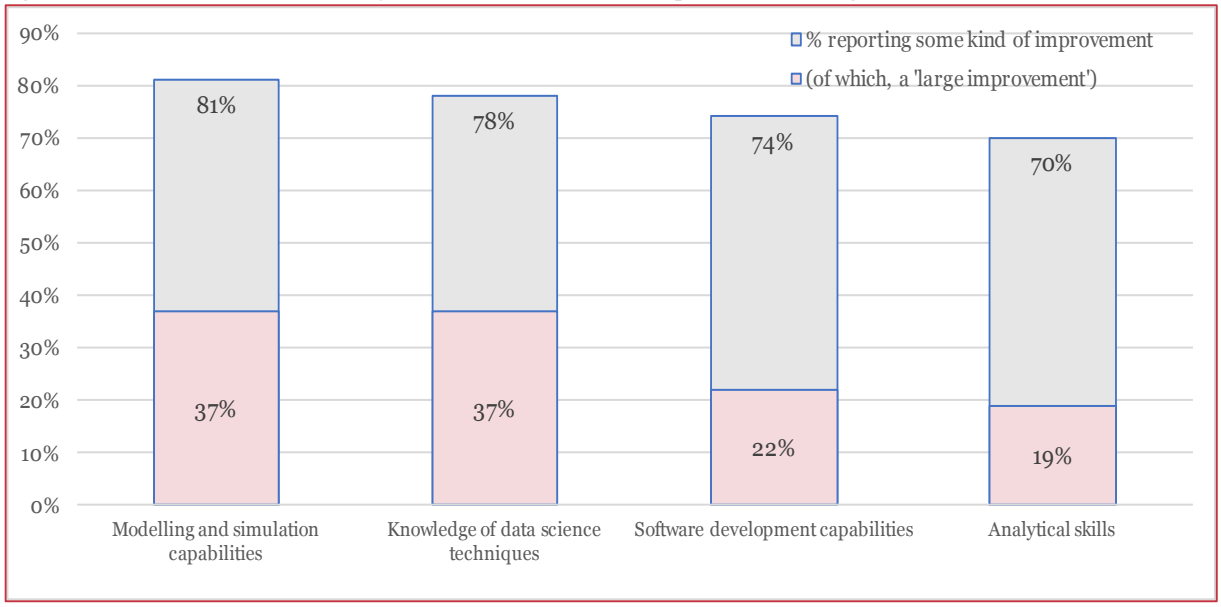
[15] https://www.liverpool.ac.uk/study/postgraduate-taught/taught/big-data-msc/overview/

[16] Academic-related training benefit: 3,760 x £250 x 0.8 = £750K. Industry-related training benefit: 3,760 x £500 x 0.2 = £375K

5.2 User benefits – skills and capabilities

The Hartree Centre's mainstream HPC activities are also delivering substantial knowledge transfer and skills development outputs; skills do not flow exclusively from training activities. Our academic and industry user surveys suggest that using the Hartree Centre has led to improvements in knowledge and skills. As shown in Figure 10, over 80% of respondents reported that their work with the Hartree Centre had helped to improve their 'modelling and simulation capabilities,' while 78% spoke about improvements in their knowledge of data science techniques. For both options, over one-third of respondents indicated that the Hartree Centre had enabled improvement by a 'large extent.'

Figure 10 The extent to which use of the Hartree Centre has improved knowledge and skills



Source: Technopolis academic and industry user surveys, 2017. Base = 27

Respondents had an opportunity to elaborate on their answer and describe the single most important benefit that the Hartree Centre had enabled. Response levels were poor amongst industry users, but amongst academic users a commonly identified factor was having access to state-of-the-art resources and equipment that helped take their research further, as well as making it much more efficient. Specific examples of up-skilling benefits reported include:

- **Infineum** have paid (market rate) for a post-doc in the Hartree Centre for 18 months. The company is keen to build its modelling capability and so they have paid for the post-doc in order to develop and internalise the expertise within their own company. Infineum have also now bought a small (25 core) cluster– and the Hartree Centre will provide them with free training to use it. Hopefully this will mean that Infineum can do more internally, but are still working with the Hartree Centre for bigger requirements and in future research areas. The company is already sending lots of people to the phase 3 workshops – so there may be potential for a good relationship moving forward
- **Unilever** has benefited substantially from its work with the Hartree Centre and IBM Research, with the development of an iPad-based user-interface to HPC that allows staff on its production lines to call-off analyses linked with evident operational issues. This simplified user interface is being developed for wider application in other sectors and by other companies

The Hartree Centre uses techniques that are burgeoning (e.g. HPC is faster and higher resolution), and is exposing companies to this, encouraging people to think about how these techniques could disrupt their sector or business. Some initially expected that the Hartree Centre would put HPC in to the hands of users, and that they would quickly become expert users and do a great deal more work independently. However, instead these organisations keep coming back to the centre. Therefore, while most clients learn enough to know how to exploit HPC in their organisations, fewer see a case for going further and recruiting or growing specialist internal teams. There are though a few examples where clients have gone on to invest in their own cluster and teams; **Dyson** bought their own cluster, as did **Infineum**. These two organisations started from a relatively low base, so they obviously benefited from their interaction with the centre and have gone through a process of upskilling.

Figure 11 Skills benefits – Embecosm

Embecosm is a firm working in hardware modelling and embedded software development. One of their core services is developing and integrating compilers. These are instruments that translate programming code into binary format which computers can then process. Much like language translation, code can be translated in a multitude of ways and using a wide variety of different approaches. One of Embecosm's current areas of activity is developing machine-based learning to help make compilers both as effective and efficient as possible.

Embecosm has worked with the Hartree Centre on the Total Software Energy Reporting and Optimisation (TSERO) project. This centres on developing compilers to improve the energy efficiency of computing operations. By making the code translation process as efficient as possible, it will reduce the amount of electricity and/or battery life required, thereby saving energy. Embecosm has previously conducted work looking at efficient code translation on nano-cards. TSERO's focus is taking the idea further and applying it to larger computers as well.

The organisation highlighted some important skills-benefits associated with their work with the Hartree Centre. As part of their funding proposal, Embecosm included a commitment to provide training to potential future high performance computing engineers. The firm therefore put some 17-year-old students on the Hartree Centre's high performance computing summer school. Traditionally, the Hartree Centre has run this programme for PhD students but Embecosm felt there was nothing content-wise that would preclude the involvement of much younger students. As such, the project has helped showcase high performance computing and engineering as a potential educational and career choice for young people. One of the students concerned got straight As at A-level and is now reading Engineering Mathematics at Bristol University. Another is studying Mining Engineering at the Camborne School of Mines. Embecosm itself has also experienced skills benefits, particularly a better understanding of the applicability of HPC in compiler research.

Embecosm also added that there have been some indirect commercial benefits through their engagement with the centre (becoming a supplier to one of the other partners involved in work with the centre). They also felt that there will have been reputational benefits associated with working on cutting-edge government backed research, and with a centre located on the very well-regarded Sci-Tech Daresbury campus. They anticipate future market opportunities too. Future apps for autonomous vehicles and artificial intelligence will require lots of processing power, and therefore efficient code translation. Its research will therefore become even more salient.

5.3 HPC awareness

Our survey data suggest that a majority of the Hartree Centre's clients were already aware of **the importance of HPC** before they had the opportunity to work together; however in several cases, the collaboration has demonstrated the potential of high performance modelling and simulation to a client's business. It is also clear from responses that the typical user organisation does change its view as regards to the business-critical nature of HPC-related services. While the number of responses is small in absolute terms (n=27), there is a marked increase in the proportion of these users that change their view of the importance of HPC, before and after their involvement with the Hartree Centre (half indicated that HPC was considered 'very important' before their involvement with the centre, while 70% indicated that HPC was considered 'very important' afterwards).

The majority of respondents across the two surveys (93%) said that they expected HPC capabilities to be of some importance to their future work, a figure that included all the academic respondents. It also appears that this added interest in HPC capabilities has translated into increased usage of HPC capabilities within the survey respondent group at least. Of the 27 respondents, 25 (93%) said using the centre had led to some increase in understanding of the value of HPC capabilities in their organisation while 23 (85%) also spoke of an **increased use of HPC**.

6 Research and technology benefits

6.1 Introduction

The Hartree Centre participates in a **wide range of research projects** as a means by which to develop its internal skills, capabilities and tools, and to improve its cutting-edge technical support to clients.

Where the centre's commercial work is producing digital assets[17], these belong to the clients and would not typically be re-usable by the Hartree Centre (except with the same client), and as such the value to the centre is essentially the commercial fee paid to the centre by the client. However, the tools produced as a result of non-commercial work (within the phase 3 IROR programme) are intended to be re-usable and added to a growing catalogue of digital assets.

The Hartree Centre is also participating in several **international research networks**, which enable its staff to monitor developments in HPC technology among global research and industry players. In some cases, this watching brief will allow the centre to influence strategic research agendas. Such networks also allow it to track policy developments, which are increasingly important in this space with, for example, rapidly growing interests in pervasive technologies like AI or its applications (cybersecurity). The centre has a vital role to play in delivering the Industrial Strategy's ambitions to support firms in seizing opportunities in these areas. Insights into national and international research priorities also helps the centre position itself to apply for grant funding. For example, its involvement with the UK Science and Innovation Audit (SIA) process may help to prepare to apply for funds through the recently announced £115M Strength in Places Fund. These networks also allow staff to identify potential new strategic partners and other R&D funding opportunities, both here in the UK and abroad.

It is also worth noting that the Hartree Centre has strengthened its **links with several major global players** through its research activities, including with ARM and Atos Bull. For example, a major new collaboration with Atos UK&I was announced in 2017, which included the purchase of the UK's first Bull Sequana X1000 supercomputer system, as well as plans for new HPC as a Service and 'Deep Learning' as a Service offerings, along with co-design and development of next generation hardware and software solutions and application optimisation services. Another key focus of the Hartree-Atos collaboration is energy efficient computing.

6.2 Scientific benefits

The Hartree Centre has **worked with several academic groups**, and while this has not been its primary mission, it has played an important role in a number of computer science studies.

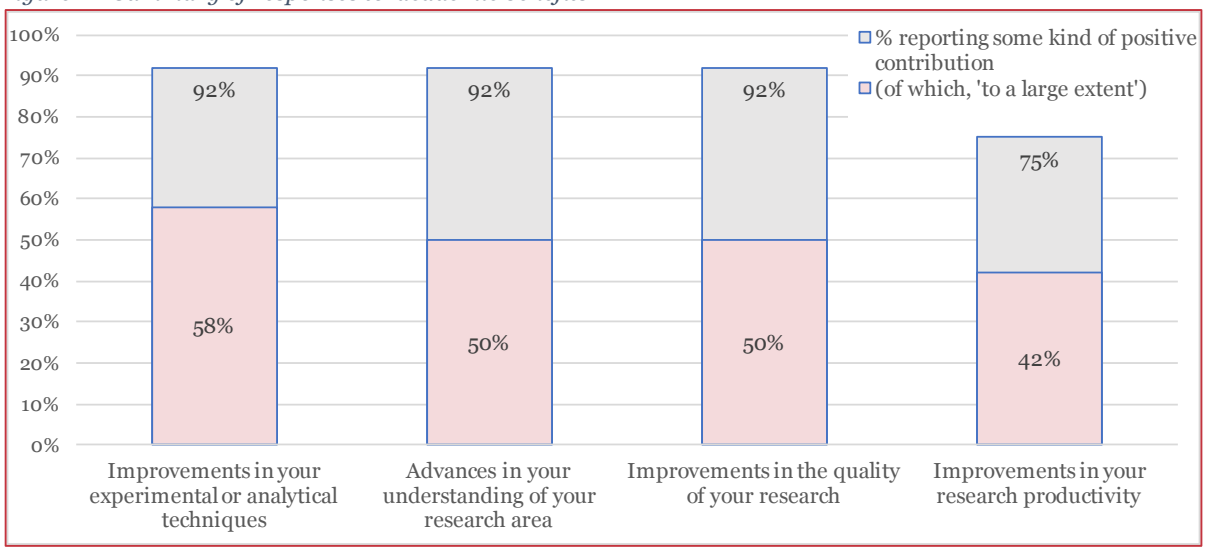
The academic user survey provides some evidence of the Hartree Centre **generating broader research benefits**. As shown in Figure 12, when asked to comment on whether the centre had contributed to improvements in different facets of their research, almost all respondents (11 of 12; 92%) indicated there had been some positive effect in terms of analytical techniques, domain knowledge and research quality. When invited to comment on the significance of those benefits, around half indicated there had been a substantial benefit, and particularly for analytical techniques.

In other cases, it seems that an association with the Hartree Centre has helped **improve researchers' credibility, visibility and reputation**. Of the 12 respondents answering the academic user survey, nine said that their use of the centre had helped to improve their scientific impact within their field, while nine also said that usage had led to an enhancement of their national or international reputation. A further eight spoke about the collaboration helping them to **secure additional funding**.

[17] A digital asset is similar to a physical asset inasmuch as it is a discernible entity (digital not physical) that has value to its owner, and possibly others, where they purchase / are granted access to use that asset. For a fuller discussion, see Section.

These improvements to research approaches and visibility have also led to more tangible impacts in the form of research publications. Eight respondents reported that their work with the centre had led to research publication in journals.

Figure 12 Summary of responses to 'academic benefits'



Source: Technopolis, academic user survey, November 2017 (n=12)

6.3 Optimisation of scientific software tools

The Hartree Centre has been involved in the optimisation of several scientific software tools, originally developed at the Daresbury Lab, so that the codes will run on the massively parallel computing architectures used by Hartree's industry clients.

The DL_MESO simulation code is a case in point.[18] As part of its ambition to improve the utility of this physical chemistry modelling tool for its industry users, Hartree worked with IBM Research to optimise it for parallel execution on its BlueGene/Q machines. Hartree also worked with the Intel® Parallel Computing Centre (Intel® PCC) to optimise the code to run on Intel® Xeon Phi co-processors. Hartree is continuing to carry out further work on DL_MESO, including a GPU port of one of its codes.

The software tools are widely used by Hartree's industry clients. Unilever, Infineum and Syngenta were granted royalty free licences by SCD to DL_MESO code as part of a Computer Aided Formulation project. Part of the agreement involved granting them commercial DL_MESO licences in exchange for experimental data to allow Hartree/SCD to improve the predictive modelling capabilities of the software. Generally, these tools are available on an open-source basis to support the work of academics. DL_MESO is available additionally as an internationally distributed software package, generating its own revenues (£10K one-off perpetual licence; £1.5K for an annual licence). SCD said that substantive data on (commercial) sales are not available.

[18] DL_MESO is a general-purpose mesoscale simulation package. It was created in 2003 and has been developed since 2009 by Dr Michael Seaton at the Daresbury Laboratory, with an EPSRC grant under the auspices of the Collaborative Computational Project for the Computer Simulation of Condensed Phases (CCP5). It allows modelling of fluids at a scale between molecular dynamics and computational fluid dynamics. DL_MESO continues to be supported by the SCD and CCP5, and its current version (2.6) is capable of both serial and parallel execution; it is used by Hartree in its industry projects.

While Hartree's development work has been focused on the needs of its industry users, the resulting optimisations have made it into the publicly released versions of DL_MESO, which is widely used by UK and international academic communities. The codes are more generally maintained, developed and distributed by the STFC Scientific Computing Department (SCD) through its Service Level Agreement[19] with the EPSRC.[20] The Hartree Centre contributions have facilitated useful improvements in software performance that should benefit many computational scientists nationally and internationally.

6.4 The Hartree Centre's R&D activities (and EEC programme)

The Hartree Centre carries out in-house research projects, in part as a means by which to improve its services to industry. Some of these activities are funded internally, however, many projects have benefited from external funding, including Horizon 2020 grants, Innovate UK and EPSRC funding. Some of the externally-funded projects (e.g. the Advanced Manufacturing Supply Chain Initiative funded ADDoPT project) also involve working with industry.

Much of the research work undertaken relates to the **Energy Efficient Computing programme** (EEC - one of the main activities of phase 2), through which the Hartree Centre – in collaboration with others – has sought to explore different aspects of power use in computing, as well as ways to achieve step changes in energy efficiency. This is a long-term area of work, and more time will be needed for wider impacts to be realised. However, there are already a number of research projects completed, with various outputs that provide good learning and that can serve as useful showcases to a wider client base.

The EEC has used external grant funding to work on developing energy-efficiency solutions that it can apply to its own clusters as well as those of its customers. This is partly motivated by a concern about cost and environmental impact – large computers are power hungry – but it is also a question of technical feasibility for next generation computing, where issues of power and heat generation are acting as a brake on development. More broadly, the programme is intended to give the UK a leadership position in the development of scalable energy efficient HPC hardware and software.

Initial investment in the EEC programme included the purchase of innovative energy efficient hardware and supporting infrastructure for accurate monitoring of power consumption. There was relatively little additional funding available for staff, and so potential income sources were sought. However, it became clear early on that there was not yet sufficient industrial interest in energy efficiency (businesses were still focused on buying new / better hardware to drive performance, and not yet ready to properly consider energy efficiency and its impact on their bottom line – although this is now starting to change). Instead, the Hartree Centre looked to external grant funding sources to support the EEC work, where it has been quite successful in generating income streams to support R&D activities.

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[19] The current 5-year Service Level Agreement between STFC and EPSRC began in 2016 and involves a team of around 23 FTES within the Computational Science and Engineering Division of SCD supporting 9 Collaborative Computational Projects (CCPs) and 8 High-End Computing (HEC) communities in areas ranging from NMR Crystallography to Mesoscale Engineering Sciences. The SCD team supports these various communities of EPSRC computational scientists with a range of services, from training, to code porting and optimisation, development, maintenance and distribution.

[20] During the 1970s, a major part of the growth in computational science capability at Daresbury was brought about by the establishment of Collaborative Computational Projects (CCPs), bringing together key academic groups in thematic areas to share code and computational methods, with support from Daresbury in code development, optimisation, maintenance, support, and training. Today, the SCD at the Daresbury and Rutherford Appleton Laboratories provides computational science support to 20 communities of researchers organised in CCPs and High End Computing Consortia. This programme of work is now known as the Computational Science Centre for Research Communities (CoSeC) - a partnership between STFC, EPSRC, BBSRC and MRC.

This programme remains a cornerstone of STFC's support for computational science in the UK. CoSeC supports a wide range of scientific research topics including biological and medical sciences, as well as the physical sciences and engineering. Examples of research aided by CoSeC include: drug design and delivery; catalysis and energy storage; and brain scanning technologies that identify and track the signs of dementia. CoSeC also provides training for highly-skilled researchers as well as professional development opportunities for people who are passionate about working both in science and software development.

Through close collaboration with other software and research initiatives such as, for instance, the Hartree Centre, the software and expertise supported by CoSeC continues to develop and evolve, by providing opportunities to extend partnerships and harness cooperation across more areas of science, thus supporting the advancement of interdisciplinary research. Research topics include: the study of viruses and proteins at the molecular level; the engineering of matter into new and useful materials; and fusion energy, one of the most promising options for generating large amounts of carbon-free energy in the future.

The grant funding obtained for EEC activities includes £151K of an Innovate UK project (TSERO), which was introduced above. This project has developed an integrated monitoring system, which has been put in place at the Hartree Centre and will serve as an exemplar for other HPC facilities.

Other externally-funded EEC projects include:

- ComPat - an ongoing Horizon 2020 project, where the Hartree Centre's role focuses on providing expertise in intelligent scheduling to support MultiScale Computing applications. The work is developing advanced energy driven scheduling across various computing architectures and compute centres including the unique range of architectures at the Hartree Centre
- Vineyard - another H2020 project, Whose aim is to create energy efficient data centres by building platforms that seamlessly integrate with programmable hardware accelerators. The Hartree Centre role is to provide an easy to use interface that accurately measures the energy use of applications on different hardware and intelligent middleware that distributes running applications to available hardware by minimising some objective functions such as time to completion or total energy used.
- EuroEXA - a large H2020 project which seeks to produce a demonstrator of a pre-exascale machine, based on ARM architecture and FPGA, that will be the first step in developing an exascale[21] solution within reasonable power budget. The intention is to deliver a 3.4 petaflop system in two racks (for comparison, the latest Atos machine was 6 petaflops in 24 racks – so the intention here is to produce something that is very much denser and therefore more energy efficient). If the project can prove that it is possible to increase scale, using middleware and software to make the system run efficiently, then this could be a game changer (or at least show that a game changer is possible) – as it will prove that you can scale a system, but still be able to afford to power it.

It is too early to demonstrate or quantify impacts from EEC work at this stage, however, based on initial tests, the Hartree Centre's view is that the programme's methods and technologies could deliver up to a 20% energy saving based on current levels of HPC use.

6.5 Re-purposing of equipment and equipment depreciation

Another type of benefit the study has reflected upon is the **re-purposing of equipment** for **greater return on Government investment**. For example, the IBM BlueGene/Q system, which cost £37.5M originally, was sent to support the DiRAC team as a source of spare parts for their BlueGene/Q[22]. Similarly, the Lenovo Intel® X86 system was sent to Durham University in 2016 to provide extra storage space for their work.[23] The systems are provided to the new (public sector) user with no charge being made (they are donated for free), with no ongoing liability for the Hartree Centre.

It is normal practice to include the costs of capital equipment in an organisation's balance sheet and then make a charge to the accounts each year in line with the rate of depreciation. That might typically be five years – at 20% a year – for most computing equipment, with the machine 'written off' afterwards. In practice, supercomputers may tend to get replaced or repurposed earlier than this – or at least the critical elements – and may have an 3-5 year working life. Ultimately, 5-8 years out, the remaining elements may be further deconstructed for reuse in other systems with some components starting to be recycled in a more fundamental sense. The final value of equipment is likely to be trivial in comparison with the original purchase price; at the time of writing, eBay US had several Cray supercomputers for sale – or their core elements at least – for a few hundred dollars.

[21] *Exascale* computing refers to computing systems capable of at least one exaFLOPS, or a billion billion calculations per second. Such capacity represents a thousandfold increase over the first petascale computer that came into operation in 2008.

[22] See https://www.hartree.stfc.ac.uk/Pages/DiRAC.aspx

[23] The Hartree Centre was one of several donors that enabled The Institute for Cosmological Computing at Durham University to build itself a supercomputer from recycled parts and increase its contribution to DiRAC (distributed research utilising advanced computing), the facility for theoretical modelling and HPC-based research in particle physics, astronomy and cosmology

The STFC Annual Report states that computing equipment is depreciated over five years and the 2016/17 accounts show a total figure for depreciation of around £95M; this accounts for depreciation across all asset types and for the whole of STFC and its £750M operating account (property, plant and equipment was valued at £1.5 billion, with IT equipment valued at around £100M at its current use value).

By contrast, the Hartree Centre's operating expenditure is quite small in comparison with its balance sheet; with the most generous assumptions about capital depreciation, its multiple HPC cluster and storage assets ought to be being depreciated at a rate of £5M a year. This cost is not currently picked up in the prices charged to clients for access to HPC clusters and staff, as it would likely push prices above the level that many would tolerate. This kind of financial analysis helps us to understand why even the largest companies with heavy computer-intensive science and engineering requirements (e.g. Unilever) still prefer to rent access to HPC systems rather than own them. It also highlights the costs involved in maintaining state-of-the-art facilities and the fact that a full-service facility is far beyond what the market will provide or can pay for. While the Centre is already generating substantial industrial (and other) income, it is likely that it will continue to need investment from government.

7 Wider benefits

We have discussed the Hartree Centre's contributions to the competitiveness of UK plc in general terms only, referring to its broad coverage of economic sectors, as well as to its new sector strategies and wider business engagement. At this stage in its history, the Hartree Centre has only engaged substantively with a few tens of firms and its wider impacts on UK competitiveness will only materialise in the future, as it expands its footprint and builds up its digital assets. It is worth highlighting, however, the role that the centre has played in the developing cluster of high-tech companies on the Sci-Tech Daresbury Campus, as well as the important work that it has done with public agencies and institutions.

7.1 Clustering effects

Our economic analyses in the next chapter estimate the local economic impact of the Hartree Centre through consideration of the territorial scope of its staff payroll and purchases. There is however a more qualitative aspect to this idea of local effects, with the Hartree Centre forming an integral part of the Sci-Tech Daresbury science and innovation campus (designated as an 'Enterprise Zone' in 2011), contributing to a large and growing community of researchers and industrialists.

The Sci-Tech Daresbury Campus Impact Study (SQW 2017) presents a comprehensive review of this geographical hotspot, with more than 100 tenant firms located alongside the STFC Daresbury Laboratory and Hartree Centre and 890 (FTEs) employees on site.[24] The report concluded that "The Hartree Centre was recognised consistently as being the key asset in terms of securing the Campus' future success and is seen increasingly as being of international significance." Examples include:

- **OPTIS**, a French company that specialises in lighting simulations, has opened a UK office on the campus. It utilises the Hartree Centre's HPC resources to help clients in the automotive industry to design interiors that perform better in varying lighting conditions. Modelling the effects of different light-sources on materials used in the interior is a highly complex computational task
- The **Virtual Engineering Centre (VEC),** which is also located on the campus. A University of Liverpool-led initiative, VEC is the UK's leading centre of virtual engineering technology integration for industrial and commercial applications. In partnership with the Hartree Centre, it combines in-house multi-disciplinary expertise in virtual engineering, with access to the latest technology infrastructure (including HPC) to address industry challenges. The two organisations have worked together to establish relationships with industry, large and small, including working on bespoke digital tools for firms (such as Jaguar Land Rover and BAC Mono) and providing access to digital engineering and HPC through common platforms. The combined expertise and facilities of the VEC and the Hartree Centre provides a unique strategic asset to the UK.
- The Hartree Centre is one of the partners delivering technical support within the **Liverpool City Region LCR4.0** project. This is a part-ERDF funded initiative that connects SMEs to expertise and support from key knowledge assets – seeking to transform businesses in the manufacturing space through digital innovation. It plans to deliver fully-subsidised support to 300 SMEs in the LCR, enable collaborations between 200 businesses and partners, support 70 new product development cases across a number of firms and create 60 new jobs in supported businesses.

The SQW findings were echoed by some of our interviewees who believed that "organisations moved to the campus because the Hartree Centre was there", and who pointed to examples of companies (Atos Bull, Mellanox, OCF plc, OPTIS, etc.) that have chosen to locate at the Sci-Tech Daresbury site in order to be part of "something bigger." "They pay more for their rent than elsewhere in the region (a premium of perhaps 20%), because of the tech address and the people and facilities that are around the campus; but the Hartree Centre is arguably the 'cherry on top'." While the feedback we received was heartfelt and resonates with the SQW findings, we did not feel confident enough in the links between the centre and the growth of the campus to claim any part of the economic output or employment of tenant firms.

[24] Sci-Tech Daresbury Campus Impact Study (SQW, 2017)

Other users (not on site) have also highlighted the draw of the campus. WaveReach reported that one of the main attractions of working with Hartree is its location on the Daresbury Campus. The campus has been successful in encouraging innovative firms to locate there and collaborate, and the opportunity to be part of this ecosystem was a significant selling point for the firm. Similarly, Embecosm reported that there were reputational benefits associated with working on cutting-edge government research with a centre located on the very well-regarded Sci-Tech Daresbury campus.

The importance of the centre to the wider **Liverpool City Region** (LCR) has also been recognised as part of the recent Science and Innovation Audit (SIA) process. The 2017 LCR SIA summary report[25] highlights the significant role of the Hartree Centre in enhancing the region's world-leading HPC and cognitive computing capabilities, as well as the opportunities for the further development of the sector in its own right and as an enabling service for other industries and the wider regional economy.

7.2 Social benefits

While the centre has focused on industrial engagement, some of the products and services being developed with industry are likely to have wider social benefits. The centre has also done important work with public agencies and institutions that will impact on UK society. For example:

- **HR Wallingford** was commissioned to clarify the environmental impact of a proposed development in the Middle East, the modelling of which was at the margins of Wallingford's in-house computing resources. In view of the commercial pressures involved, the client needed to resolve this issue quickly, so HR Wallingford turned to the Hartree Centre to enable it to parallelise aspects of its modelling capabilities to carry out large numbers of modelling runs concurrently. This greatly reduced the amount of time needed to run 20 years' worth of wave and wind data using TOMAWAC, a 3rd generation wave transformation solver.[26] The outcome was a better understanding of local wave behaviour in terms of key physical phenomena such as wave propagation and their implications for coastline erosion. The required data was also produced significantly faster than would have been possible using conventional computing resources
- The **Met Office** is working with the centre (through the LFRic project, a follow-on to GungHo) on a new software code for numerical weather forecasting using algorithms that will scale to millions of cores. The software is being written so it can be configured to run efficiently on different next-generation computers. The new code is intended to replace the dynamical core of the Met Office's Unified Model (UM) from 2025. The UM is the principal UK tool for both weather and climate prediction (hence "unified") and is also used by other weather services around the globe (e.g. Australia, New Zealand, South Korea, India and the U.S. Air Force). The new code is necessary to harness the power of next-generation computers for weather and climate prediction and will mean more accurate forecasts to better cope with severe weather and adapt to climate change, maintaining UK leadership in environmental prediction. The rapidly developing climate services agenda involves major economic opportunities, and this action is essential to ensure the UK can play a leading role[27]

In addition, while it is part of phase 3 activities, it is worth also highlighting recent work with **Alder Hey Children's Hospital**. Here, a collaboration with IBM Watson and the Hartree Centre has led to a new software app that is able to anticipate and answer questions from patients and their families before they come to hospital. This should reduce patient anxiety levels, as well as the amount of time clinical staff need to devote to answering questions about non-clinical issues. The business case for the Alder Hey project covers benefits such as reducing missed appointments, increased referrals, happiness and best use of 'golden time' with clinicians. The cost of the development of the app was supported by the Hartree Centre and NHS England (NHS Digital) and has the potential to be rolled out to other hospitals across the NHS (and possibly internationally in time).

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[25] https://www.liverpoollep.org/wp-content/uploads/2017/09/LCR-SIA-Summary-FINAL-September-2017.pdf

[26] TOMAWAC is a component of the TELEMAC system, an open source suite of scientific codes, developed by an international consortium including energy company EDF SA (France), government agency BAW (Germany) and HR Wallingford (UK, sole distributor of the TELEMAC system), together with the Hartree Centre (UK).

[27] http://www.stfc.ac.uk/files/developing-next-generation-climate-and-weather-forecasting-models/

8 Economic impact

8.1 Introduction

This chapter presents a discussion of the economic impacts being realised as a result of the Hartree Centre's creation and early operation, drawing on findings presented in previous chapters.

We first discuss economic impact in terms of **commercial benefits among industry users** and then go on to assess the additional economic impact relating to the **Hartree Centre's operational expenditure**. We have sought to be comprehensive as regards to the types of economic impacts included (within the limits of the data available) and to be clear about the basis for our estimates (the source of monetary estimates, the related assumptions and likely sensitivity of the estimates).

We have focused only on the impacts of past work (investments made and work undertaken during phase 1 and 2). However, the centre continues to expand and is beginning to see some outcomes from its phase 3 cognitive computing work. As such, we would expect future economic impact to be greater.

It is worth highlighting again that the £19M investment in phase 2 – energy efficiency / data exploitation – was focused mainly on novel R&D (e.g. through the Energy Efficient Computing programme), rather than on short-term industrial engagement and support. As such, significant economic benefits were not expected to emerge from this phase of investment within the timeframe of the study. There are already a number of phase 2 research projects completed, with various outputs that provide good learning and useful showcases for a wider client base, but this is a long-term area of work and more time will be needed for the wider (economic) impacts to be realised.

8.2 Economic impact on industry users

We estimate that **the Hartree Centre will generate a net economic impact of between £7.4M (lower) and £27.5M (upper bound) in commercial benefits among its phase 1 and 2 users**. These estimates are based on the following formula, which is detailed more fully below.

Total Net Impact (£27.5M) Upper Bound	=	Direct impacts (£46.6M) + Induced impacts (£6.1M) + Indirect impacts (£30.8M)	x	100% - Attribution (0%) x 100%-Deadweight (40%) x 100% - Displacement (55%) x 100%-Leakage (0%)
Total Net Impact (£7.4M) Lower Bound	=	Direct impacts (£12.6M) + Induced impacts (£1.6M) + Indirect impacts (£8.3M)	x	

8.2.1 Gross direct impact on industry users

Our industry survey and interviews found that the majority of clients believe their work with the Hartree Centre during phase 1 and 2 has had (or will have) a positive impact on their commercial performance. While there is likely to be a response bias, our additional client interviews and desk research (e.g. enCORE testimonials) encompass more than 30 of the 43 clients in the overall population; these two additional sources suggest that around half of clients can expect to see an increase in income attributable to their collaboration with the centre.

Overall, most client companies found it difficult to attach an economic value to the developments that had been made possible through their use of the centre; our surveys, interviews and case studies produced largely qualitative feedback describing the benefits. There were, however, a minority of clients that could estimate the scale of commercial benefits deriving from their use of the centre:

- **Unilever** prepared two case studies specifically for this impact assessment, which are summarised below (the company also provided estimates on the impact to their turnover, which have been included in the overall impact assessment, but these are highly confidential and not included in this report):
  - The virtual pouring test has the potential to benefit a significant proportion of Unilever's global laundry liquids portfolio. To date it has been applied to three laundry pack designs and the huge benefits are already apparent. In one project alone, optimising packaging through five design iterations took just two weeks compared to 20 weeks for a traditional prototype-based process and hence generating considerable extra sales revenues.
  - Together with STFC Unilever has been developing a computer aided formulation tool to help bench scientists to pre-screen a number of options to focus on fewer better actual experiments. The tool, implemented as a computer application, allows the company's chemists to test various scenarios without the need to purchase or synthetically make a new molecule for inclusion in a novel formulated product. The in-silico formulation approach leads to economic gains via two routes: incremental sales and in market innovations directly via in-market performance (including, for example, delivering consumer benefits not previously possible); and direct savings and benefits from the development phase (due to speed to market and more rapid development of formulation designs).
- **OCF Plc** (an SME in Sheffield that offers high performance computing, storage and data analytics services) estimates that their work with the Hartree Centre has resulted in £150,000 of additional turnover (attributable to the centre)[28]. This equates to ~1% of the company's turnover in 2017

We have used this case-based evidence to inform our assumptions about likely effects across the wider client portfolio. We have set two main dimensions for our scenario building:

- Turnover growth attributable to the centre: We have assumed an average increase in attributable annual turnover of between 0.01% and 0.05% (large companies) or between 1% and 5% (SMEs)
- Sustainability of growth: We have assumed that the additional income would be sustained for a three-year period on average, before the additional benefit is competed away by the market

Based on these dimensions and UK sales figures for 33 of 43 client companies[29], we estimate attributable turnover of between £36.9M (lower) and £137.1M (upper scenario) for these users.

The HM Treasury Green Book recommends the use of gross value added (GVA) (instead of turnover) as a measure of gross impact on sales. GVA is a better measure because it discounts the added value generated along the supply chain and avoids double counting. We have used standard GVA:turnover ratios published by ONS for the UK economy (1:0.34) to estimate that the gross direct impact of the Hartree Centre on phase 1 and 2 industry users is between £12.6M (lower) and £46.6M (upper bound).

8.2.2 Gross indirect and induced impact on industry users

The direct impact generated through industry users has a knock-on effect on the wider economy, via:

- Indirect impact – the employment and activity supported across the client's supply chains, which is generated by their additional attributable sales. Using national statistics (on the ratio between turnover and the purchase of goods and services), we estimate that the indirect impact of £12.6M in additional sales will be £8.3M (GVA), while the indirect impact of £46.6M will be £30.8M.
- Induced impact – the additional economic activity supported by people directly employed by the Hartree Centre's clients (and the suppliers to these clients), who spend their wages on goods and services in the wider economy (and help support other jobs). This final induced effect can be

[28] Information was obtained via our industry user survey

[29] There are 10 client organisations that are not captured in FAME business register (e.g. a sole trader; the Met Office) and their trading figures have therefore not been included in the analysis.

calculated using an income multiplier[30] applied to the additional direct (£12.6M) economic activity among clients, which will induce a further £1.6M of consumption in the wider economy. For the upper bound (£36.9M) direct benefit, the induced impact is £6.1M.

The three linked estimates (direct, indirect, induced) amount to an estimated total gross impact on the UK economy (through phase 1 and 2 users) of between £22.5M (lower) and £83.5M (upper bound).

8.2.3 Total net impact on industry users

The Green Book recommends that gross effects be adjusted (discounted) for several other factors to arrive at an estimate of *net* impact, including[31]:

- Attribution (the extent to which measured change among beneficiaries can be attributed to the intervention). This is already embedded into our calculations, as our assumptions on growth only take into account the potential additional income generated thanks to the use of the Hartree Centre facilities. We have therefore zero-rated attribution in our adjustment of gross impact.
- Deadweight/counterfactual effects (firms may have realised some of the benefits anyway as a result of their own investments, which may have been crowded out by public support). From study consultations, 66% of users said that the work would not have happened and the benefits would not have occurred without the Hartree Centre. Consequently, we have applied a conservative deadweight factor of 40% (i.e. 60% of the benefit would *not* have materialised otherwise).
- Displacement (increased sales among assisted firms are largely accounted for by losses among their competitors elsewhere in the economy). Many of the Hartree Centre's clients operate in highly competitive global markets, with strong UK-based competitors too, while other (often smaller) clients provide rather niche products in markets with relatively few direct competitors. A detailed analysis of displacement is beyond the scope of this study. We have instead assigned a value of 30% to well-established companies (i.e. a displacement factor of 70% of existing economic activity) and 100% to smaller, innovative start-ups and tech companies (i.e. no displacement). The overall displacement rate for the whole portfolio of large and small users is 55%.
- Leakage (where benefits to UK-resident businesses flow out of the region or country where the taxes were collected that paid for the support). Already embedded in our calculations since we focus exclusively on improvements to client companies' turnover in the UK. Given the number of multinationals, benefits emerging will almost certainly flow to operations abroad – but these would be additional and would not exclude or dilute benefits in the UK. We therefore apply a leakage factor of 0% (100% of estimated benefits relate to the UK economy). Similarly, we apply 0% leakage to indirect and induced effects, as these are based on UK structural economic data.

After accounting for these factors, we estimate that the total *net* impact of the Hartree Centre through the positive commercial benefits generated to its phase 1 and 2 industry users is between **£7.4M (lower) and £27.5 (upper bound).** These benefits are expected to be realised over the course of three years (from the point in time at which they concluded their project with the Hartree Centre).

These are already strong results for a young and relatively small centre. The upper estimate of £27.5M in commercial benefits is already approaching the £37.5M initial capital investment to establish the centre[32], and this is before we include the economic impact generated by the centre's operational expenditure (estimated in the next section to be an additional £7.1M).

[30] Based on an income multiplier of 0.13, as used in the "Sci-tech Daresbury Campus Impact Study" (SWQ, 2017).

[31] A full discussion on these parameters is presented in Appendix C

[32] The additional £19M investment for phase 2 was focused mainly on novel research and development, rather than on short-term industrial engagement and support. Significant commercial benefits were not anticipated within the short term.

8.3 Economic impact from centre operations

We estimate that **the Hartree Centre generated £7.1M in net economic impact because of its operational expenditure during the first two phases**. These estimates are based on the following formula, which is detailed more fully below.

Total Net Impact (£7.1M)	=	Direct impacts (£10.2M) + Indirect impacts (£63.1M) + Induced impacts (£1.3M)	x	100%-Deadweight (90%) x 100%-Leakage (5%) x 100% - Displacement (0%)

8.3.1 Gross impact of Hartree Centre operations

We start our analysis by looking at the gross economic impact. We follow a similar methodology to that used in the ISIS Lifetime Impact Report (Technopolis, 2017) and the Sci-tech Daresbury Campus Impact Study (SWQ, 2017). Based on this, the **total gross impact** of the Hartree Centre's operations over 4 years is estimated to have been £74.6M. This includes:

- Direct impacts of £10.2M, arising from the payment of salaries to Hartree Centre employees;
- Induced impacts of £1.3M, resulting from employees spending their incomes in the economy, thereby helping to create further economic activity (based on a standard income multiplier)
- Indirect impacts of £63.1M, triggered by the centre's operations, which generate additional economic value in the supply chain through the purchase of goods and services. This includes: *revenue expenditure* over four years (on utilities, licences, professional services, etc.) and *capital expenditure* during phase 1 and 2 (e.g. on scientific equipment and buildings);

8.3.2 *Total net impact of Hartree Centre operations*

We then take account of a series of parameters[33] to arrive to an estimate of **net impact**:

- Deadweight/counterfactual – accounting for benefits that would have been realised anyway. One could argue that a substantial share of centre's capital expenditure would have happened anyway, as the government would have allocated the resources elsewhere. By comparison, operational expenditure (salaries and revenue expenditure) is funded by other sources (e.g. client contract income; R&D grants), most of which would not have materialised in the absence of the centre. Consequently, we apply a deadweight factor of 90% (i.e. we assume that only 10% of the total gross impact generated by the centre's operations would not have happened in its absence.
- Displacement – accounting for any reduction in activities and benefits elsewhere in the economy. One could argue that some services provided by the centre (e.g. Platform as a Service) displace the activity of some other cloud-based HPC providers. However, those displacement effects (where they exist at all) are likely to be realised outside the UK because the only alternative providers of similar quality and capacity (Amazon, Google, Microsoft, etc.) are based abroad. This may change in the future as new players enter the HPC on-demand market, however, for now we assume there is no displacement of economic activity in the UK. Other services, such as code optimisation and cognitive consulting are quite niche, with few other UK-based organisations, private or public, providing similar services. Consequently, we have used a displacement factor of 0% (i.e. we assume that benefits emerging from centre operations do not displace other UK economic activity).
- Leakage – accounting for the economic benefits that are accrued outside the UK. Based on supplier data, we estimate that only 0.5% of the centre's total capital and operational expenditure was spent with firms outside the UK. Consequently, we apply a leakage factor of 5% (i.e. we assume that 95% of the direct benefits will take place within the UK).

Applying these parameters to total gross impact, we estimate that the Hartree Centre has generated a **total *net* impact of £7.1M from its operational expenditure in Phase 1 and 2.**

[33] A full discussion on these parameters is presented in Appendix C

9 Relative effectiveness of Hartree Centre services

As part of the evaluation, we were additionally asked to compare and contrast the relative effectiveness of the Hartree Centre's main client-facing functions, and Table 7 presents our light-touch comparison of each. It is a largely qualitative assessment, as the evaluation has found many promising developments, but it is still rather early days as regards widespread measurable economic impact.

We have not included the substantial programme of internal research and development that is designed to develop the Hartree Centre's capabilities and international networks, rather than deliver client benefits directly. Indeed, one could argue that the centre's decision to pursue external collaborative research funding has even diverted staff attention away from the more pressing needs of business development and project execution. Although we appreciate that there are longer term benefits, as well as examples of projects (e.g. the DNV GL Innovate UK project on modelling wind farm layouts) where third-party grant funding has underwritten the cost of the Hartree Centre's involvement.[34]

We have outlined the particular strengths from the perspective of UK plc and indeed the likelihood that the centre can scale up sufficiently in each area. This last point is perhaps the single most challenging issue, with some of the most promising contributions tending to get caught up in issues of ownership and rights to reuse more widely.

The strategic relevance of the Hartree Centre's offer to UK business reflects a wider reality, and is a challenge because the centre is in direct competition for people and skills with the strongest and most dynamic sectors of the economy. Whether it is tech companies in Shoreditch, financial services titans in Edinburgh or biomedical superstars in Cambridge, the Hartree Centre has to compete with salaries and conditions that are above the level allowable within STFC. There are locational factors too; Northern Powerhouse notwithstanding, it is tough for Halton to compete with London or Edinburgh. This labour-market disadvantage is compounded by the government's tendency to invest more narrowly in science capital, assuming the operating costs can be covered from other sources or even through commercial income. This is deeply challenging and the Hartree Centre's strategic partnerships with the likes of IBM Research and its links with others private services companies, like OCF and Virtalis are a creditable response to the internal financing issues; there is however the need to achieve a minimum level of capacity to ensure the whole system can function and evolve. The agreement to use SCD staff flexibly has helped, immeasurably in several cases, but it is still a source of uncertainty and risk.

Unsurprisingly, there is no one set of activities that stand out as the single best way forward for the Hartree Centre. As with most knowledge-intensive business service operations, clients appreciate a full-service offering. The spread means that the centre is able to satisfy the needs of a cross-section of users, whether that is individuals looking to improve their technical knowledge and career prospects through a summer school or a multinational technology business looking to steal a march on its global competitors through the transformation of one or other of its key business processes. Our surveys and interviews also make clear that the broad service offering provides an opportunity for a client business to progress from the least demanding activities, like a training course, (lower costs, lower commitment of senior people) through to the more involved consultancy projects and all the way through to quite fundamental, collaborative research programmes, or indeed vice versa.

- **Platform-as-a-service** is delivering notable benefits to the greatest number of client businesses, and in particular to smaller technology companies allowing them to compete on an equal footing with larger firms. It is also helping recruit clients for other Hartree Centre services. The partnership with OCF has helped to overcome internal capacity constraints. This has also been a route by which to reach a very much larger number of UK-resident businesses. The challenge will be to keep abreast of service level and infrastructural developments, in what is a crowded marketplace, without further major capital investment

[34] By contrast, there are other externally-funded collaborative research projects where the Hartree Centre's involvement has been provided on a largely pro bono basis, such as the Met Office GungHo project.

- The **software development and optimisation work** is also delivering strong benefits, however, this is heavily staff-intensive work and not easily scaleable. The optimisation of existing software codes is clearly hugely beneficial for individual clients, however, work on new / open source software may deliver more value and could link more strongly to the PaaS
- The **externally-funded collaborative R&D** is delivering new opportunities and new capabilities, however, it is also creating additional pressures on the Hartree Centre team to satisfy requirements defined by other public bodies (e.g. Horizon 2020)
- The **education and training activities** could usefully focus more heavily on business, however, STFC headcount constraints, will mean that the Hartree Centre has to be even more creative with its partnerships with major industry players like Atos, Intel® and IBM. At the time of writing, the Hartree Centre does not have an explicit education and training strategy, however we understand that this will be developed in 2018. This is an increasingly important component of the centre's activities, with more and more courses being offered, while the level of demand is growing all the time. This additional outreach work could be delivered at relatively low cost, albeit the Hartree Centre is cash constrained, however, such an expansion would directly address its core mission to increase awareness and use of HPC across the UK.

In phase 3, the **IROR** work looks hugely promising, but it is clearly resource intensive and long-term. It is arguably the single most important function and the one channel where the Hartree Centre could find a way to bring key players together – pre-competitive – to help UK businesses seize the **benefits of AI, machine learning and big data several years before they are likely to do so left unsupported**. Digitisation of R&D is clearly important, but there are also important opportunities in other areas (e.g. advanced process modelling techniques are helping organisations to identify tens or even hundreds of millions of sterling in additional value through rigorous optimisation of process design and operation. They are also helping to significantly accelerate innovation). The challenge here is twofold, around scaleability (and cost) and the sensitivities with regard to the further use / diffusion of the resulting IP.

It is not the remit of this study to offer advice on where the Hartree Centre should go next. However, it does feel that while the Hartree Centre has the potential to make a real difference in the region and nationally, it will need to overcome its **resourcing issues** and **achieve a sufficient scale of activity** if it is to exploit this opportunity. The Hartree Centre is the only supercomputing centre in the UK with industrial engagement as its primary role, and its combination of cutting-edge machines and world-class computer scientists mean it is able to provide businesses with access to hardware and technical support services that mainstream commercial providers cannot match.

However, while this may be true now, it may not be in five years. There are a growing number of cloud-based HPC providers offering on-demand services to businesses around the world, and increasing competition is driving down prices. Private providers tend to focus on the hardware, exploiting their existing HPC capacity to improve utilisation rates and expand their client base; there are no major cloud-based providers offering the kind of technical support and development work undertaken by the Hartree Centre. There are a growing number of IT consultancies providing HPC-related technical support, however, these businesses tend to work with larger organisations that have their own clusters and a high-degree of internal competence.

Table 7 Relative effectiveness of Hartree Centre services (mid-2017)

	Platform as a Service	Software optimisation	Consultancy	Education and training	Cognitive problem solving
Current expenditure	15%	50%	30%	<5%	<5%
Demand	Strong	Strong	Medium	Strong	Promising pipeline
Scale of impact	Low to medium	Medium-to-high for immediate clients	Low to medium for direct clients	Medium for delegates Potentially high for employers	Potentially transformative for direct clients. Pre-competitive research may have more widespread impact
Added value	Medium-level over commercial HPC-on-demand providers (bigger facilities, dedicated user support and expertise). Possible displacement issues, with private providers	High-level over commercial software consultancies	Medium-level over private data analytics businesses	High level, with substantial synergies available through cooperation with SCD and strategic business partners	High, with unique offer (deep specialists, facilities, analytical software) not replicated in private sector (possibly in Digital Catapult)
Relevance	Widely relevant to all sectors of UK plc	Widely relevant to technology businesses in many sectors	Widely relevant to large and small firms across all sectors of UK plc	Widely relevant to all sectors	Potentially relevant to all sectors of UK plc, but larger / more sophisticated firms will likely lead in next few years
Scaleability	Highly scaleable, but high cost to maintain 'kit' as state-of-the-art. External providers allow the centre to greatly expand its industrial engagement activities	Low scaleability. Highly involved process requiring specialist skills (constrained by the Hartree headcount). IP rests with client; limits re-use of outputs	Medium scaleablity Highly involved process requiring specialist skills	Highly scaleable	Medium scaleablity, but quite involved process. Relevant skills in short supply globally and the Hartree Centre will be dependent upon IBM Research staff to deliver (in short-term)
Businesses reached	High tens of businesses, potentially many hundreds	Small number of individual businesses (<5) annually	Several tens of businesses annually	Tens of businesses annually, with the potential to address 100s	Small number of individual businesses (<5) annually (short term) Much larger possibilities with wider exploitation (long term)
Overall view of strengths and weaknesses	A good basis for promoting use of HPC, improves system utilisation rates and attracts clients to other functions. However, the centre may struggle to match the price (and growing service level) of cloud-based providers in the future.	This has been a core focus for the Hartree Centre in phase 1 and 2. The benefits to individual clients are impressive. Social benefits are less clear and are indirect. Could the Hartree Centre deliver more value to UK plc by focusing on open source software and tools? (though at the expense of income)	The centre has invested in specialist facilities and has also established partnerships with key data analytics and VR businesses. Could be expanded, to the benefit of very many younger tech SMEs. However, the Hartree Centre will need to fix its human resource issues or explore the creation of more strategic partnerships	Could be expanded, however, the Hartree Centre will need to lead any increase in engagement with industry. The Hartree Centre's industry partners may be prepared to do more, on a contribution-in-kind basis	Likely to deliver most profound impacts in the longer term. Strategic focus may allow novel (generic) solutions to be developed that can feed into the centre's other research and consultancy activities (i.e. tools that can be applied to other organisation's data or other sectors). However, cognitive clients will not allow the centre to automatically reuse tools and insights derived from work on proprietary data.

10 Future benefits realisation framework

10.1 Introduction

This chapter presents a recommended benefits realisation framework for the centre to use in future. It comprises:

- A restatement of the rationale and objectives for the Hartree Centre
- A more sharply resolved set of logic models, which track backwards from the Hartree Centre's mission and overarching objectives, to define a series of impacts, outcomes, outputs and inputs
- A set of suggested performance metrics, which derive from these logic models. These are designed to allow the centre to more clearly understand the extent to which it is making good progress against objectives
- A proposal for future data collection, based on the data requirements of the individual KPIs

10.2 Rationale and objectives of the Hartree Centre for phase 3 and beyond

We have assumed the **mission** will continue unaltered, and will focus on strengthening the global competitiveness of the UK by facilitating the adoption of high performance and cognitive computing by a larger number of businesses than would be possible otherwise. Indeed, with ongoing concern about the UK's productivity performance, it is likely that this will be even more central to the government's industrial strategy. We have also assumed the centre will make greater use of computing and cognitive technologies in the future, to complement its Platform as a Service / hardware oriented activities.

We understand the **rationale** for the future of the Hartree Centre to include:

- HPC-enabled applications having the ability to transform business performance, through digitisation of R&D on the one hand and reinventing business processes on the other
- Market provision of HPC-enabled services falling short of the service-levels required to deliver this kind of business transformation to the great majority of firms, which lack the internal skills and infrastructure to simply buy-in HPC computing resources
- A national HPC centre for business could support the development of 100s of UK businesses across multiple strategic sectors, which will in turn provide benefits to the wider economy
- A full-service facility being far beyond what the market will provide, as regards both its capital costs and specialist staff, and even though it has already been established and is generating industrial income, it is likely the centre will continue to need investment from government

We understand the **objectives** for the future of the Hartree Centre to include:

- Increasing the international competitiveness of UK-based business
- Contributing to the diffusion of HPC, big data and cognitive computing across UK business
- Contributing to the realisation of tens of new innovative products or services annually
- Contributing to the digitisation of clients' business processes, improving productivity
- Creating digital assets for re-use by the Hartree Centre

10.3 The Hartree Centre logic models

The following tables present the three Logic Models we have developed for the Hartree Centre. The first relates to phase 1 and 2, and has been used to guide our own impact assessment (a simplified version was presented earlier in the report, without the associated indicators and evidence sources). The second and third models relate specifically to the Cognitive Accelerator and IROR programme. All three are presented here as the basis for an improved monitoring and evaluation system in the future.

Figure 13 Logic model for phase 1 and 2 of the Hartree Centre

	Inputs →	Activities →	Outputs →	Short-term outcomes →	Long-term outcomes
Item	• Income / Expenditure • Resourcing (staff / suppliers) • Hardware / Software / Facilities	• Commercial – Software development / optimisation – Platform as a Service (HPC access) – Data analytics (simulation, visualisation) • Research – IoT demonstrator – Energy efficient computing – Next generation data analysis • Training and skills – Summer schools – HPC training – Workshops / events / talks – Masters / Apprenticeships – Engagement / support	• New or improved software • New or improved knowledge and skills • New or improved products, services and processes	• Improved competitiveness of Hartree Centre users / clients • Improved economic performance of Hartree Centre users / clients • Improved innovativeness of Hartree Centre users / clients	• Help keep UK at forefront of industrial innovation • Help UK industry fully embrace and accelerate application of HPC / big data / cognitive computing
Indicator	• Commercial revenue • Grant income • Government capital investment • Number of staff days used (Total / FTE) • Estimated value of client resource input (e.g. staff days)	• Number of projects, by type • Number of clients / partners • Number of training beneficiaries	• Number of published papers / articles • Number of IP-related outputs • Number (and potential value) of digital assets • Users reporting different types of direct benefits (faster R&D, reduced costs, improved knowledge and understanding, etc.)	• Users reporting (realised / anticipated) longer-term benefits / outcomes: – Cost savings (one-off, recurring) – Increased efficiency – New / improved products, services or processes – Increased competitiveness – Increased turnover / profits – Reduced time to market – Improved market position – New markets / market expansion	• Output / employment of UK digital tech industries • Digital employment within non-digital sectors • UK position in EU / global ranking for industrial innovation • Users reporting wider benefits / impacts – Consumer benefits – Societal benefits – Environmental benefits – Economic benefits (jobs, GDP)
Source	• Hartree Centre Finance Team • User survey	• Hartree Centre management information system (including project forms)	• Hartree Centre management information system (including project forms) • User survey / case studies	• User survey / case studies	• Innovation scoreboards • National statistics • User survey

Figure 14 Logic model for the Hartree Centre – Cognitive Accelerator

	Input indicators	Output indicators	Outcome Indicators	Impact indicators
Hartree Centre Cognitive Accelerator Three pillars: • Cognitive value enablement for industry – introducing cognitive technologies to UK industry (sales) • Cognitive centre for entrepreneurship and innovation – democratising cognitive technologies to start-ups and SMEs (ecosystem) • Cognitive grand challenges – developing innovative solutions for clients (research)	• Number of (Hartree Centre, IBM, STFC) staff days used on projects (FTEs) • Value of commercial income, related to activities • Value of grant income, related to activities • Estimated cost to provide the services, including any fractional value of the IBM IP used • Value of client resource input (e.g. staff days)	• Number (and details) of projects, completed and live • Total value of projects, completed and live • Number of clients, public and private sector • Number of clients, economic sector • Share of projects focused on commercial applications • Number of visitors to the cognitive demo centre	Number of clients reporting the following (realised / anticipated), as attributable to working with Cognitive Accelerator: • Financial savings • Additional sales • Additional employment • Productivity gains (output per capita) • Innovative new products and services brought to market • Innovative new tools or processes implemented Estimates for the following (realised / anticipated), attributable to working with Accelerator, for all completed projects in the portfolio: • Total net savings • Total additional sales income • Total additional employment • Total number of innovative products brought to market • Total number of innovative tools or processes implemented Number of clients reporting improved awareness, knowledge and understanding of HPC	<u>Competitiveness</u> Number and % of UK-based firms using cognitive computing routinely Number and % of UK-based firms that judge CA has enhanced their competitiveness <u>Economic output</u> The value of additional national income, linked with cognitive computing applied to big data <u>Job creation</u> Number of additional UK people employed as a result of product and process innovations based on CA technologies
Data sources	• Hartree Centre finance and HR • Project forms • Statements of Work • IBM finance and HR • Client surveys	• Hartree Centre management information system	• Hartree Centre management information system • Client surveys / case studies	• UK-wide landscape review (baseline, mid-term and ex post sample-based surveys)

Figure 15 Logic model for the IBM Research / Hartree Centre Research programme

	Input indicators	Output indicators	Outcome indicators	Impact indicators
IBM Research / Hartree Centre research programme • Chemistry • Engineering • Life sciences • Enabling tech	• Number of (Hartree Centre, STFC, IBM) staff days used on research projects • Value of UK government income (capex) • Value of grant income • Value of IBM contributions (software, hardware, people) • Value of IBM IP accessed	• Statements of work finalised • Number of events / attendees • JDAs signed • Number of research projects started / completed • Number of projects completed, from each SOW • Number of SOW projects completed on time • Digital assets created	• New research papers (and citations) • New reference data • New tools developed • Definition of industry target problems • Recruitment of new commercial partners to the research programme • Number and (potential) value of contracts signed • Income from digital assets (grants, projects, licences) • Paid consultancy engagements on a research basis	• Company case studies / statements as to benefits <u>Innovation</u> • Number of derived tools and reference data that progress to commercial application by the Hartree Centre cognitive computing team • Number of industry research partners that progress to become commercial clients of the Hartree Centre <u>Skills development</u> • Number of Hartree Centre staff trained in the use of Cognitive Computing • Number of UK data scientists familiar with cognitive computing techniques <u>HPC digital assets</u> • Number of new tools developed through the research programme, which materially advance the state of the art for cognitive computing • Number of strategic assets created at the Hartree Centre • Number of paid consultancy engagements, based on use of digital assets <u>International standing</u> • Hartree Centre expertise and computing facilities perceived as matching the best in the world
Data sources	• Hartree Centre finance and HR • IBM finance and HR	• Hartree Centre management information system	• Hartree Centre management information system and staff surveys	• Hartree Centre management information system • Staff and client surveys • International peer review

10.4 Inputs, activities and outputs

The following table teases out the main input and output data that we would recommend the Hartree Centre track as part of its management oversight. They build on the rationale and objectives for the Hartree Centre, and derive from our impact assessment work relating to phase 1 and 2. They are however intended to cover all aspects of the Hartree Centre's operations, including IROR.

We have given an indication of what we believe would be a reasonable target for individual measures, however, these are mainly based on our thinking rather than any explicit advice from the Hartree Centre senior management team or indeed other stakeholders. They are presented for discussion; however, we do recommend the Hartree Centre develop baselines and time-based targets for each of its final KPIs.

Table 8 Recommended input, activity and output data to be monitored

Inputs
Staff and facilities (increase in FTEs)
Funding (increase in income)
Strategic partnerships (IBM Research; Intel®; ARM; Unilever; etc.)
Activities
Provide an industry-oriented, fully-serviced HPC facility; it must remain at the cutting-edge in terms of technology, infrastructure and people
Provide HPC-related services and technical consultancy to 100s of UK-resident businesses, within the context of clearly defined business-development projects
Provide business clients with access to more experimental AI programmes, which focus on solving complex and potentially transformational business problems
Conduct HPC-related research, to ensure Hartree Centre staff remain involved with developments internationally and the team can replenish its own digital assets (in addition to those of its clients)
Provide right mix of HPC functions (Commercial services [70%], education and training [10%], HPC-applied research [20%])
Implement sustainable business model (Target: price realisation > 80% of market price for technical consultancy; price / core hour)
Maintain strategic focus (thematic, high-growth potential businesses)
Maintain pipeline of businesses and projects
Outputs
Proportion of clients that report an increase in income (Target 20% today; 50% by 2025)
Proportion of projects completed, judged to have had a strongly positive effect on a client's business processes or competitiveness (Target: 50%)
Proportion of highly satisfied industry clients (Target: 80%)
Number of digital assets added to the Hartree Centre catalogue in the previous year
Number and value of digital assets owned by the Hartree Centre
Number and value of digital assets exploited by the Hartree Centre

10.5 Outcomes and impacts

The following two tables present our current proposals for a series of key measures for the Hartree Centre's outcomes and impacts. The second column then indicates the main data source for each indicator. These additional data collection exercises are detailed further in the next section.

Figure 16 Outcome measures

KPI	Future Data Source
Total number and share of Hartree Centre client businesses that report a significant **business development outcome**, attributable to working with the Hartree Centre (Target: >10; 20%) – A productivity gain – An improvement in time-to-market – An improvement in competitiveness – Introduction of a new product, service or process	Hartree Centre **annual client survey** (run an online survey addressed to all clients, past and present; participation and ongoing support should be a condition of contract)
Combined **value of additional income** (and exports) realised by Hartree Centre clients in the UK in the previous year, attributable to working with the Hartree Centre (Target: >£2M)	Hartree Centre **annual client survey**
Combined **value of cost savings** among Hartree Centre clients, attributable to working with the Hartree Centre (Target: >£1M)	Hartree Centre **annual client survey**
Total number of **new or saved jobs** linked with Hartree Centre projects, attributable to working with the Hartree Centre, attributable to working with the Hartree Centre (Target: >50)	Hartree Centre **annual client survey**
Proportion of **businesses aware of the innovation potential** of HPC services; % using HPC services (Target: 10% baseline; 10% annual growth; growth in NW double that for the North of England overall)	Hartree Centre **annual business survey** (CATI survey; 1,000 businesses across North of England)
Number of new HPC-applications / tools added to the Hartree Centre portfolio of tools and services (**digital assets**)	Hartree Centre annual report, with a descriptive account of highlights / new additions in the year and an appendix showing an **inventory of all digital assets** possibly with a balance sheet value and explanation of the basis of value)

Figure 17 Impact measures

KPI	Future Data Source
Global competitiveness of UK in selected strategic sectors (e.g. aerospace, chemicals, digital)	Co-financing of **sector studies** by UK Sector Councils / growth partnerships
GVA of selected UK strategic sectors	Co-financing of **sector studies** by UK Sector Councils / growth partnerships
Digitisation of UK business operations in selected strategic sectors (e.g. aerospace, chemicals, digital, biotech, ...)	Ad hoc **case studies** of selected clients, revealing the nature and extent of transformation (attributable to the Hartree Centre)

10.6 Additional data collection to support future monitoring and evaluation

Table 9 summarises our recommendations for a series of **five additional data collection activities** that would help the Hartree Centre to monitor the changing HPC landscape in the UK and track and count its own contributions to HPC-related industry benefits (and thereby evidence the various KPIs set out above). The table briefly describes each additional data collection activity along with a suggestion as to the frequency, scope and cost of those activities.

Table 9 Recommended data collection activities, to support future monitoring and evaluation

Data collection activity	Description
An annual, online **client survey**. If this were commissioned externally, it might cost on the order of £25K each year	• An annual client survey would serve many purposes, providing both feedback on customer satisfaction with the Hartree Centre as well as being a source of semi-quantitative data about the benefits of working with the Hartree Centre (e.g. on competitiveness, income, employment, innovation, etc.) • The cheapest solution would be to run an online survey addressed to all clients, past and present; participation and ongoing support for such an annual survey should be a condition of contract. A CATI survey would give higher response rates and may help with gathering quantitative data, but it will also cost more
An annual **business survey** A CATI survey of 10 minutes per call and delivering feedback from 1,000 businesses might cost around £75K for the data and a brief analytical report	• An annual business inquiry would allow the Hartree Centre to track trends in business awareness and use of HPC-related services. • A CATI survey would be necessary to secure a sufficient number of responses from a statistically representative sample, as these are not client businesses • The structured questionnaire would need to be short, with perhaps no more than five questions, to support response rates and contain costs
A rolling programme of **sector studies** A £100K budget should allow the Hartree Centre to deliver at least two strategic sector studies (on a multi-client basis) each year and refresh or reframe those studies every three years (e.g. aerospace, chemicals, financial services, ICT)	• A typical sector study might encompass an economic analysis of the sector in question (current levels and trends in output and employment nationally; internationally; and an overview of leading companies, along with recent mergers and acquisitions); an innovation perspective (new business models, technological innovation, etc.); as well as an account of the role of digitisation in the sector (where and what is digitized; what are the key trends; what are the investment levels, etc.) • The studies might be carried out on a multi-client basis, in order to reduce the cost to individuals. The Hartree Centre is involved with several relevant sector councils, which could be a good platform; this does however mean the management team would need to fit their information and timetabling needs to the requirements of a wider group. However, a typical £100K sector study might cost £50K or less with two more partners
A rolling programme of Impact **Case Studies** 3 in-depth cases each year, procured locally and working directly for the Hartree Centre, might cost £50K a year	• The Hartree Centre should be able to produce a small number of in-depth case studies that reveal the nature and extent of the transformation of parts of a client business' operations, which are attributable in large part to their work with the Hartree Centre • The cases will need to be prepared with the support of client businesses, as the interesting effects are always going to occur outside the terms of any specific contract. Each case study might focus on a body of work that has been done with the Hartree Centre (rather than a single project), as the larger impacts seem to result from multiple interactions; and they will need to be carried out after a sufficient time has passed • As a price guide, the REF impact case studies consumed 10-20 staff days on average, albeit they rarely managed to quantify the specific commercial effects of the research • Such case studies would be a good platform for showcasing the Hartree Centre's contributions to the world and prospective clients in particular, with the full versions kept confidential and used by future evaluations to improve on the estimation of total economic impacts • These impact case studies are different in their analytical depth and quantification to the case studies that the Hartree Centre prepares routinely, albeit these lighter descriptions of projects are still very powerful communication tools (and would provide a platform for selecting the cross-section of the more substantive, post hoc impact case studies)
Digital asset register or catalogue and associated management reporting templates Cost is unclear, but largely internal staff time. It may take several tens of staff days to get to (and maintain) a fully functioning inventory and reporting system [this is work that is already in progress]	• The Hartree Centre has begun work on tracking the digital assets it is involved with producing, and so it should be possible for the management team to finalise the creation of a register or catalogue of all digital assets within the next 6 months. The register would allow the management team to present several different data sets / perspectives on its digital assets. • A complete inventory of all digital assets made, owned and co-owned by the Hartree Centre, by type. It would be helpful if the inventory included a range of meta data about the origins of the asset, its ownership and usage terms and any co owners. • An annual compilation of new digital assets, with mini vignettes that could be included in published corporate literature (e.g. annual report). Over two or three years, it should be possible to arrive at a normative view of the level of re-use and typical (economic) value for each digital asset type, which would allow the Hartree Centre to value its overall portfolio of assets

Picking up on the last row in the preceding table: we heard repeated references to **digital assets, particularly in relation to phase 3,** but were not provided with a count of new data sets or software

tools produced, or with information about the numbers being re-used under licence or the income produced (as they are not the focus of this study). Table 10 presents a view of the centre's initial efforts to track digital asset production, albeit the table presents workflows and activities and is not a catalogue of digital assets per se. We understand that further work has since been undertaken to create a much more detailed view of digital assets produced / under construction, with a valuation in each case.

This would be a useful development for future evaluations, and would mirror wider developments in monitoring, where public institutions are cataloguing project outputs (e.g. publications). Ideally, the centre should also develop a view as to the typical value of a class of digital asset, possibly based on licence income[35], otherwise future evaluators will still need to research these issues from first principles.

Table 10 Tracking of digital asset production

Chemistry	Task description	Life Sciences	Task Description
1	Parameterisation Engine	1	Membrane Binding and Permeation Assay
2	Chemistry Workflow	2	Electronically Coarse Grained Biomolecular Simulation Method
3	Cognitive Accelerator	3	Omics Analytics Catalogue
4	Consumable Computing	4	HPC omics workflows as a service
5	Particle Dynamics Modeller	5	Precision Agriculture
Eng + Mftng	**Task description**	**Enabling Tech**	**Task Description**
1	Multi-physics & Multiscale code coupler	1	Code analysis and generation for HPC
		2	Cognitive Technical Computing as a Service
2	Cognitive Uncertainty Quantification toolkit	3	Machine Learning at Scale
		4	Cognitive Transportation Technology
3	Simulation Methods for Engineering Applications	5	Cognitive Knowledge APIs
		6	Cybersecurity at Scale
4	Cognitive Process Simulation	7	Data technology platform

Source: Hartree Centre director's presentation to the November 2017 Hartree Centre Advisory Board

We have **costed these various measurement activities** on the assumption that most if not all of them would need to be outsourced, and arrived at a global estimate for a new Evidence Programme that might cost around £125K a year at the lower bound and £250K at the upper bound (still with a view to buying as economically as possible).

There are no definitive pricing references to allow the Hartree Centre to determine what would be appropriate, however, other government departments might use 3-5% as a guide for the overall evaluation costs of a smaller research and innovation programme (<£5M) and 1-2% for larger programmes (>£10M). The Hartree Centre's operating expenditure level would place it in the smaller programme range, which would suggest the £125K price point. However, if one were to factor in the contributions-in-kind of IBM Research, the upper bound starts to look more appropriate.

We appreciate there are affordability issues, and would fully expect the £125K to be as much as could be contemplated in the first instance; we have made suggestions for several co-financing options and could also imagine looking to the Local Enterprise Partnership (LEP) or even university partners to provide help – in cash or in kind – with several of the data collection activities (e.g. impact case studies).

[35] The precise definition of what constitutes a digital asset is still something the world is wrestling with, and in particular how to value the manifold and rapidly proliferating types of digital content and information. There are fewer reference points when it comes to valuing a particular database or an algorithm; the diversity of digital assets means there may be no established market through which to obtain pricing information in the way one would for the Hartree Centre's building at Daresbury.

10.7 Future impact assessments and lessons learned

This particular impact assessment was a mixed experience, with strong support from the Hartree Centre senior management team and selected clients and stakeholders, which allowed the study team to progress our work without difficulty, at least up until the point we launched our surveys. From here in there was a real challenge as regards our ability to capture sufficient numbers of quantitative estimates of benefits relating to the work of the centre. The support of the STFC's internal evaluation team was also greatly appreciated, in helping the external team to secure access to data and people, while also providing an additional source of advice on the highly-specialised nature of the work and flagging a number of key issues around data sources and confidentiality.

We took away several lessons from this ourselves. The first is probably too obvious to spend much time on, however, as it is relatively new, the Hartree Centre still has a **relatively small pool of industry clients**. Very few of those clients had worked closely enough or long enough with the centre to have yet realised the sorts of business-changing effects we believe ought to be possible. This is partly a question of timing – with the impact assessment being launched not much more than three years after the centre's inauguration – and partly about the scope of industrial engagement. This is a baseline evaluation, intended to provide an early view of benefits that the centre is delivering through an assessment of its first years of operations. It should form the start of a longer-term evaluation programme, with a more substantive socio-economic study in another three to five years' time.

The second lesson is perhaps equally obvious, and relates to the **quality of the administrative and other monitoring data**, which was not set up for an evaluation. There were similar issues around the standard terms and conditions of contracts, and expectations that clients would support evaluations. It would be helpful if a simple – but meaningful – evaluation framework could be developed as part of the business case for any future investments (indeed, this is now a BEIS requirement), which can then flow through to a monitoring and evaluation plan, for the senior management team to implement.

11 Conclusions and recommendations

This baseline study set out to provide an early view of the benefits that the Hartree Centre has delivered through its first years of operations (phase 1 and 2 investments) and to develop an updated performance evaluation framework that can support the future monitoring and assessment of impact.

The evaluation has found many promising developments, but it is still rather early days as regards widespread measurable economic impact. The centre has established itself as a national centre of excellence, with a spread of core services that can satisfy the needs of a cross-section of users. It completed over **100 collaborative projects** with a wide range of industrial partners in its first four years and users have confirmed the relevance of the centre's approach to working with industry.

The centre is clearly **helping firms to innovate** (and to do so more effectively and efficiently) and it has already made significant contributions to the design and development of new or improved products, services and processes. The centre has also delivered newly-optimised versions of various modelling and simulation codes that will continue to deliver analytical and productivity benefits to users. Already, half of industrial users have seen an increase in sales income, or expect to do so soon.

The centre has delivered **skills outcomes** through its training courses and skills-development activities, as well as by enhancing the knowledge and capabilities of its direct clients. It has also helped to raise awareness about the potential of HPC, **change views** as to the business-critical nature of HPC-related services and support businesses in seizing the opportunities that these offer.

The centre has also participated in a **wide range of research projects** as a means by which to develop its internal capabilities and tools, as well as its cutting-edge technical support to clients. Through its Energy Efficient Computing Programme, the centre has explored different aspects of power use in computing and ways to achieve step changes in efficiency, with various outputs that provide good learning and that can serve as useful showcases to a wider client base. The centre has also worked with several academic groups and played an important role in computer science studies.

We estimate that the Hartree Centre will generate a **net economic impact** of up to £27.5M in commercial benefits among its phase 1 and 2 users. This is in addition to £7.1M in net economic impact that the centre has generated as a result of its operational expenditure during these first two phases.

These are **already strong results** for a young and relatively small centre of excellence, with total economic impact already close to the £37.5M initial capital investment in the centre. Just four years after opening, the full economic benefits of early activities will still be working through the system, while in some areas (e.g. phase 2 EEC), impacts are only expected over a much longer timeframe.

It does feel that the Hartree Centre has the **potential** to make a real difference nationally. As the centre's interactions with client businesses develop – more joint projects, more time elapsed – we expect to see a greater number and proportion of clients reporting positive commercial results, and for the economic benefits to intensify. However, it will need to overcome its **resourcing issues** and achieve a sufficient scale of activity if it is to exploit this opportunity fully.

The costs of maintaining state-of–the-art HPC facilities are significant and if these were fully reflected in the fees charged to clients it would likely push prices above the level that many would tolerate. While the centre has been increasingly successful at generating industrial (and other) income, it is likely to continue to need government investment, with this ongoing public expenditure balanced against the wider social benefits of improved industrial productivity and competitiveness.

Evidence of the impact generated from past investment is essential for maintaining this support. The current baseline evaluation should therefore form the start of a **longer-term evaluation programme**, with ongoing monitoring and evaluation activities, as well as a more substantive socio-economic study in several years' time.

We have developed a **proposed benefits assessment framework** as part of the evaluation study, which we recommend that the senior management of the centre adopt as the basis for future performance assessment. This includes a series of **suggested metrics**, designed to allow the centre to more clearly understand (and demonstrate) the extent to which it is making good progress against objectives, as well as proposals for **additional data collection activities** that will help to provide the necessary evidence of achievements. This new Evidence Programme would include an annual client survey, an annual business survey, an inventory (and valuation) of digital assets, case studies of business transformation, and a rolling programme of sector studies. As part of this, we believe there is also a need to allocate greater resource to persuading industry clients to contribute to evaluation activities, to share information on business improvements and to quantify these where possible. We have costed the suggested new data collection activities at around £125K a year in total. We appreciate there may be affordability issues with this and have made suggestions for several co-financing options.

Appendix A Glossary

Term	Explanation
AI	Artificial intelligence
CAF	Computer-aided formulation
CFD	Computational fluid dynamics. A branch of fluid dynamics that uses numerical analysis and data structures to model, solve and assess problems associated with fluid flows.
Compiler	Computer program that translates source programming language into another performing language (the target language)
Compute node	An individual computer, part of an HPC cluster
Core	Part of the CPU (see below). A core is capable of running processes, and has its own processing logic
CPU	Central Processing Unit, the chip that performs the actual computation
EEC	Energy Efficient Computing
GPU	Graphics cards contain Graphics Processing Units (GPUs), for processing visual data. These processors have a different architecture from standard CPUs, and are able to run parallel processing
HPC	High performance computing is the term often used for large-scale computers and the simulations and models which run on them
Internet of Things (IoT)	Network of appliances and physical devices that are embedded with electronics, software, sensors and network connectivity which allows these objects to connect and exchange data.
IP	Intellectual Property
IROR	Innovation Return on Research
Memory requirement	The amount of RAM needed to successfully run an application. It can be specified per process for a distributed application
Molecular dynamics (MD)	A computer simulation method for studying the physical movements of atoms and molecules
Multicore application	A multi-core application uses more than one core during its execution by running multiple threads, also called a shared memory application.
Node	In traditional computing, a node is an object on a network. For example, on a home network, your computer and printer might be nodes. Supercomputers are essentially networks, with nodes that communicate with each other to solve a larger problem than any single computer could manage in a reasonable amount of time.
NPD	New Product Development
Process	An independent computation running on a computer. It may interact with other processes, and it may run multiple threads. A serial and shared memory application run as a single process, while a distributed application consists of multiple, coordinated processes.
RAM	Random Access Memory. Used as working memory for CPUs
SCD	Scientific Computing Department
Storage requirement	The amount of disk space needed to store the input and output of an application, expressed in GB or TB.
Thread	A process can perform multiple computations, i.e., program flows, concurrently. In scientific applications, threads typically process their own subset of data, or a subset of loop iterations.
TRL	Technology Readiness Level. A type of measurement system used to judge the maturity level of a particular technology

Appendix B List of user / supplier organisations consulted

Table 11 Overview of survey and interview responses

Group	Contacted	Respondents (where not confidential)				Response rate
Industry users	43 companies	3DSIM DNV GL Dstl / Marriott Embecosm Falcon Project	GSK KnowNow IBM Met Office Novidec	Optis Renuda Rolls-Royce Tracsis Trendalyze	Unilever Victrex Waters WaveReach	24 / 43 (56%)
Academic users	16 academics	Durham ErasmusMC		Liverpool (x3) Strathclyde		6/16 (38%)
Suppliers	102 companies	Applepark The Britpos Co. Cambium IBM		JPF IT No barriers OCF Limited		8/102 (8%)

Appendix C From gross to net economic impact

Net impact industry users

As mentioned in Section 8.2, our estimates of net impact to industry users account for attribution, deadweight, displacement and leakage. The paragraphs below explain in detail how we have arrived to estimates of each factor.

- **Attribution:** A key element when assessing the impact of a public investment is understanding the extent to which any (measured) change in economic activity among beneficiaries can be attributed to the intervention (in this case their use of the Hartree Centre), taking into account that there may be various contributing factors that help to achieve a final result.

  We already have the attribution factor embedded into our calculations, as our assumptions on growth only take into account the potential additional income generated thanks to the use of the Hartree Centre facilities. Additionally, we have used the most conservative scenario for attributable growth, to take into account the fact that other investments and resources (including the users' own) would have contributed to achieving the commercial benefits. We have zero-rated attribution in our adjustment of the estimate of gross impact

- **Deadweight / counterfactual:** Another key element when assessing the impact of a public investment is to understand what difference it made in supporting that specific activity. For instance, one needs to measure how different the final outcome (e.g. GVA) would have been without the public investment. This is the so-called *counterfactual scenario*. Put differently, we need to calculate what proportion of the outcomes would have happened anyway in the absence of the support provided by the public investment. That proportion is the deadweight factor.

  To analyse the extent to which the companies would have achieved the same results anyway (via other means), we turn to the evidence collected via our industry survey. Of the 15 survey respondents, three said that without the Hartree Centre the work would not have happened and the benefits would not have occurred. Another seven said they would have used other resources (e.g. university researchers and/or facilities). The feedback from our interviews and case studies was broadly similar, albeit there was an acknowledgement that this route would have probably been more time-consuming and expensive, and there is no certainty that the same results would have been achieved. This means that, overall, more than 66% (10 out of 15) of industry users declared that the same results would not have been achieved. Consequently, we have applied a conservative deadweight factor of 40%, i.e. we assume that 60% of the estimated gross benefit would *not* have materialised in the absence of the work with the Hartree Centre

- **Displacement:** Another key element is the extent to which a public investment has reduced other activities and benefits elsewhere in the economy. Displacement could happen when, for instance, public support benefits specific organisations at the expense of other players in the national market. The Hartree Centre's activities, while being positive for its clients, may be detrimental to their immediate competitors in the North West or elsewhere in the UK. In this case, the positive impact on sales could merely be a redistribution of sales income and market share within the economy, with no net additional benefit to the overall economy.

  Many of the Hartree Centre's clients operate in highly competitive global markets, with strong UK-based competitors too, while other often smaller clients provide rather niche software and electronics related goods and services, in markets with relatively few direct competitors (e.g. OCF). A detailed analysis of displacement is beyond the scope of this study. We have, instead, assigned a value of 30% to well-established companies (i.e. a displacement of 70% of existing economic activity) and 100% to smaller, innovative start-ups and tech companies (i.e. a displacement of 0% of existing economic activity). We have then applied those factors to our estimations of direct impact. This gives an implicit displacement factor of 45%, i.e. we assume that 55% of the economic benefits generated through the Hartree Centre has *not* displaced existing economic activity

- **Leakage:** Finally, economic estimates of impact should also take into consideration the extent to which the public investment benefits those outside the geographical area of the intervention, in this the case the UK economy.

  This parameter is also embedded in our calculations since we focus exclusively on improvements to client companies' turnover in the UK. Given the number of multinationals on the Hartree Centre's books, we believe the benefits emerging from the work at the Hartree Centre will almost certainly flow through (spillovers) to benefit the company's operations abroad. However, these benefits where they occur would be additional and would not exclude or dilute benefits here in the UK, and so we have not attempted to capture this global added value in our calculations. Consequently, we apply a leakage factor of 0%, assuming that 100% of our estimate of direct benefits relates to the UK economy only. The indirect and induced effects are also UK only, by virtue of the use of UK structural economic data

Net impact of Hartree operations

As mentioned in Section 8.3, our estimates of net impact of Hartree operations account for attribution, deadweight, displacement and leakage. The paragraphs below explain in detail how we have arrived to estimates of each factor.

- **Deadweight/counterfactual and attribution,** one could argue that a substantial share of the direct expenditure (salaries) would have happened anyway, as the government would have allocated the resources available to the Hartree Centre somewhere else in the economy. However, the Government investment relates mostly to the capital expenditure, and does not directly fund the operational expenditure of the centre. Operational expenditure (salaries and revenue expenditure) are funded by other national and international sources (e.g. client contract income; R&D grants), most of which would not have materialised in the absence of the centre. The operational expenditure represents 11% of the total gross impact.

  Consequently, we apply a conservative deadweight factor of 90%, which means we assume that only 10% of the total gross impact generated by Hartree Centre operations would not have happened in the absence of the centre. This is quite a high discount however there a so many potential investment routes for the government's science capital, that these seems appropriate

- **Displacement**. In terms of whether the Hartree Centre has reduced other activities and benefits elsewhere in the economy, one could argue that the services provided by the centre (e.g. "Platform as a Service") do displace the activity of some other cloud-based HPC providers such as Amazon, Google or Microsoft, however, those displacement effects where they exist at all are likely to be realised outside the UK. This may change in future as new players enter the HPC on-demand market, however, for now we assume there is no displacement of economic activity in the UK. Other services such as code optimisation and cognitive consulting are quite niche with few other UK-based organisations, private or public, providing similar services.

  Consequently, we have used a displacement factor of 0% i.e. we assume that benefits emerging from Hartree Centre operations do not displace other economic activity in the UK.

- **Leakage.** Again, this relates to the extent to which economic benefits accrue to those outside the UK rather than within the national economy. Based on the supplier data available to the study team, we estimate that only 0.5% of the Hartree Centre's total capital and operational expenditure was spent with firms outside the UK, for example, with companies located in Germany, Poland, Ireland and the US.

  Consequently, we apply a factor of 0.5% to account for leakage, i.e. we assume that 99.5% of the estimated direct benefits will take place within the UK economy.[36]

[36] A leakage factor of 0.5% is possibly too generous, as while the great majority of the Hartree Centre HPC cluster comprises equipment purchased from UK-based businesses, such as Atos Bull, Intel® and IBM, these are sales operations in the main, with their principal manufacturing operations located outside the UK. As such, there is likely to be a high import content associated with the computing and storage parts of the capital investment (not the buildings), and a substantial fraction of the wider economic benefit of these purchases is likely to have accrued to business operations elsewhere in the world

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