Hartree Centre
Science & Technology Facilities Council

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THE HARTREE CENTRE'S INNOVATION RETURN ON RESEARCH (IROR) PROGRAMME:
MID TERM – PARTICIPANTS SURVEY REVIEW

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ACKNOWLEDGEMENTS

The Hartree Centre and Cambium would like to thank all those involved in the IROR programme, especially those that took part in the survey.

About the Hartree Centre:

The Hartree Centre is transforming UK industry through high performance computing, big data and cognitive technologies.

It is part of the Science and Technology Facilities Council (STFC), which is under UK Research and Innovation (UKRI).

About Cambium

Cambium specialise in accelerating adoption of data – enabled innovation that tackles high priority business-led challenges. For over a decade, they have enabled faster innovation by developing highly effective partnerships between public and private sector organisations using novel collaboration processes, such as InCEPT™.

GLOSSARY

AI	Artificial intelligence
CFD	Computational fluid dynamics
Digital asset	Software components that have been used and may be reused to address a business challenge / need.
HC	Hartree Centre
HPC	High Performance Computing meaning the practice of practice of aggregating computing power to deliver very high performance and solve large complex problems in science, engineering, or business
InCEPT™	Industrial Collaborative Engagement for Proof of Technology. A collaborative innovation process used by Hartree Centre to accelerate translation of research to satisfy real business challenges and create digital assets
IROR	Innovation Return on Research – a challenge-led industrial engagement programme that aims to translate research in data centric technologies into beneficial and measurable impact
JDA	Joint development agreement
ML	Machine learning
MNC	Multinational corporation
PaaS	Platform as a Service
Participants	Commercial organisations that have participated in the IROR programme
SCD	Scientific Computing Department at STFC
SME	Small or medium sized enterprises – The usual definition of small and medium sized enterprises is any business with fewer than 250 employees
SOW	Statements of Work-relating to each of the domains identified for the IROR programme. That is Chemistry & Materials, Science, Engineering & Manufacturing, Life Sciences and Enabling Technology
STEM	Science, technology, engineering and mathematics – usually referring to skills or expertise
STFC	Science and Technology Facilities Council, part of UK Research and Innovation (UKRI)
TRL	Technology Readiness Level – method of estimating technology maturity across different types of technology
UQ	Uncertainty Quantification, the science of quantitative characterisation and reduction of uncertainties

EXECUTIVE SUMMARY

Innovation Return on Research (IROR) is a challenge-led industrial engagement programme for the translation of research in next generation data-intensive technologies into digital assets and UK economic impact. The type of business challenges being addressed through IROR are complex and involve higher risks than any individual company would be able to undertake in isolation.

This review is based on a detailed survey of nine industrial organisations (Participants)[1], from a potential pool of 20. The Participants also represent a diverse range of business sectors, organisation size and business models. Close engagement with these Participants during the first six to 18 months of the programme has indicated that the research outcomes in their projects are closely aligned to their business challenges.

[1]Where the term 'Participants' is referenced in this report it refers to the nine organisations interviewed. For clarity, a further 11 organisations remain engaged in the programme but are at an earlier stage in terms of assessing potential benefits.

Survey scope

The report, produced by Cambium, covers the work carried out in three industry application domains (referred to internally and within this document as Statements of Work or SOWs):

- Science, Engineering & Manufacturing (SEM)
- Chemistry & Materials
- Life Sciences

The programme of work also includes development of enabling technology which underpins all three areas but is not included as part of this review.

This report forms part of a review by the Hartree Centre as part of the five-year IROR programme. Consequently, each project area is still in progress, therefore the analysis describes the benefits acquired from the Participants' involvement to date. For the most part, this analysis refers to the Participant's views of the expected future benefits of the research rather than to impacts experienced so far.

To date, IROR has enabled a clearer, better informed view of these potential benefits. In many cases the scope of individual research projects has introduced key milestones to assess and validate these outcomes.

However, this review should not be seen as an impact evaluation of the benefits delivered through IROR, rather it provides strong qualitative indicators of how valuable the programme will be to industry.

Findings

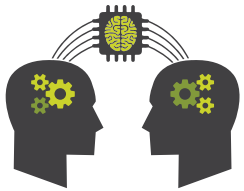
Feedback from the nine Participants on the anticipated business value of their individual projects indicates that there is a solid commitment and enthusiasm to continue with the programme. From the data gathering and analysis (See pages 11 - 17) the most important areas of anticipated impact identified by Participants were improved outcomes in:

- Time to market / implementation
- Skills dependency
- Knowledge capture and retention
- Reduced costs / improved resource efficiency

EXECUTIVE SUMMARY (CONTINUED)

Time to market / implementation was the highest rated likely future benefit. The individual drivers of this advantage varied across the IROR programme, but expectations included, greater productivity in research processes and improved predictability of research time to business value. Anecdotally, these gains are expected to be significant e.g. development time reduced from two years to two months in some cases. These benefits were cited by Participants of all sizes who form part of a number of supply chains for goods and services of organisation. Consequently, these expected impacts offer the potential for scale up of productivity and economic benefits.

Skills dependency was highlighted as an early positive impact due to the high-quality expertise provided as part of the IROR programme. This includes deep knowledge of artificial intelligence (AI) and machine learning (ML). The InCEPT™ process used for IROR industrial engagement, (see Appendix 2 – page 24), ensures these high-quality skills are applied more effectively to mutually-agreed, high priority, challenges with lower business risk than alternatives options for skills acquisition (e.g. PhD studentships). The effectiveness of this data-intensive digital skills enablement facilitated by the IROR projects underpins Participants' enthusiasm and commitment to the IROR programme.



Knowledge capture and retention was also highly rated as an important source of potential productivity gains by enabling more effective use of research and STEM talent to maintain and maximise competitive advantage. Participants believe this will be achieved through, firstly, enabling less skilled researchers to complete research tasks (now made more routine) and, secondly, by mitigating the risk of knowledge loss through improvements in the transfer of skills and knowledge to new STEM talent. It was also recognised that the introduction of the technologies developed in IROR will catalyse a more proactive approach to the management of data assets.

Reduced costs / improved resource efficiency here the benefits were projected to cover a wide range of areas from reduced testing costs (e.g. materials, staff and high cost computing time), improved use of resources in operations of the products and in manufacturing processes.

EXECUTIVE SUMMARY (CONTINUED)

Recommendations:
The following recommendations are based upon an analysis of the survey feedback and follow-up interviews with Participants. These are described in more detail within the main report (see page 21).

In summary, it is recommended that consideration is given to:

1. Instituting a mutually agreed monitoring and impact evaluation process as part of individual IROR projects and the IROR programme.

2. Ensuring all IROR projects have the regular involvement of an executive sponsor from each Participant so that there is high level business visibility and support for the full adoption of the technology.

3. Establishing a more detailed and transparent understanding of the value of the digital assets being developed by the Hartree Centre as part of IROR projects.

4. Identifying best practices that maximise the Participant identified gains / benefits in:

    - Time to market / time to implementation
    - Reduced costs / improved resource efficiency
    - Skills dependency
    - Knowledge capture and retention

Leveraging the lessons learned from IROR to establish a scalable enablement facilitated by the IROR projects to the practical application of AI and ML.

INTRODUCTION

This report, produced by Cambium, summarises the findings of a qualitative survey of IROR Participants' progress and emerging benefits of the IROR programme. It examined the following areas:

- The level of support and commitment offered by industrial collaborators to the IROR programme.
- The anticipated business value of IROR from the Participant's perspective to derive an early indication of the potential benefits of the project in the context of their business, sector or the wider economy.
- The status of the IROR programme to support the development of ideas to create more value for all stakeholders as the programme evolves.

The Hartree Centre and the IROR Programme

The Hartree Centre's mission is to "transform the competitiveness of UK industry by facilitating and accelerating the adoption of high performance computing, big data analytics and cognitive technologies". In 2015, the Hartree Centre began a programme of collaborative work with IBM Research called Innovation Return on Research (IROR) to deliver on this mission. The technologies deployed as part of this transformational programme comprise state of the art techniques in artificial intelligence, big data analytics, computer modelling and simulation, machine learning and visualisation. These technologies are collectively referred to as 'data-intensive' technologies within this report.

The role of the programme is to provide 'proof of technology' applied to business challenges as part of the process of translating research ideas from early Technology Readiness Levels (TRL) e.g. 1-3 to later stages of the innovation process e.g. 4–7. As a challenge-led initiative, the programme looks to address areas where the complexity and level of risk of developing a successful technology solution is too high for any single business or organisation to undertake alone.

Key to this programme is the engagement of industry partners to select business relevant challenges, where the data-intensive technologies can be applied.

These are then validated through proof of concept" projects. This industry engagement process was enabled and accelerated by a research translation process – called InCEPT™ (See Appendix 2, page 24 for a process overview). This was applied to three challenge-led domains:

- Science, Engineering & Manufacturing (SEM)
- Chemistry & Materials
- Life Sciences

Most projects are still at an early stage of implementation, so this report primarily refers to the expected business benefits of the research rather than to specific outcomes and impacts achieved so far. However, the programme has already enabled a clearer view of these potential benefits and in many cases the scope of individual research projects has begun to set up key milestones to assess these anticipated outcomes. These projects follow a common three stage pattern of:

1. Testing the technology on a problem closely aligned to a Participant's business challenge, but where the test is conducted using open or anonymised data.

2. Completion of a custom test of the technology using the Participant's private data

3. Assuming progress is maintained, the technology is then validated by a real-world application or a pilot within the IROR Participant's operations.

SURVEY APPROACH

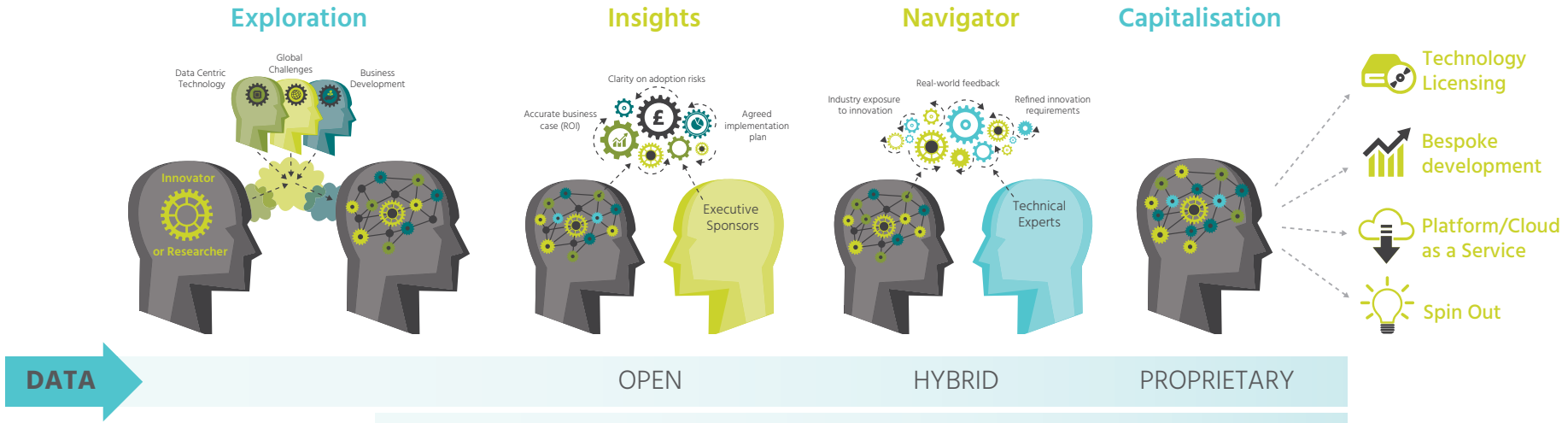
From the work completed on the IROR programme to date, nine organisations across the three domain areas (SOWs) and representing both SMEs and large-scale enterprises were interviewed using a semi-structured interview process based on a pre-set questionnaire template covering a broad range of business benefits.

The template was based on information gathered from previous work within the InCEPT™ engagement process and used as an initial guide to identify the areas of greatest value for the participating organisations. These areas were:

1. Time to market
2. Time to implementation / deployment
3. Reduced costs
4. Reduced waste / improved resource efficiency
5. Reduced carbon footprint
6. Improved product / service features
7. Skills dependency
8. Talent attraction and retention
9. Knowledge capture and retention
10. Regulation – license to operate

Any areas identified as high value were discussed with the Participant in more detail.

The scores were compared by overall areas of greatest/most important impacts to the business, by SOW domain and by individual Participant. For commercial confidentiality reasons, only the anticipated business value aggregated across all Participants and by SOW are included in this report.

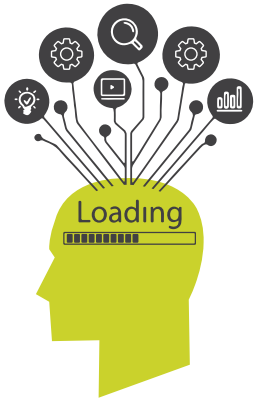


SUMMARY OF SURVEY FINDINGS

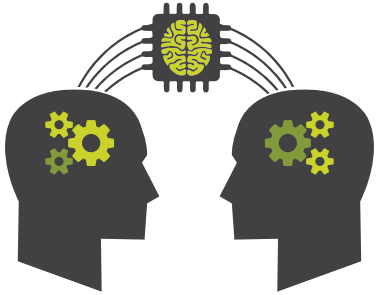
The survey results identified four significant areas of important early business value:

- **Time to market**
  Defined as the time taken from the product/service being conceived, to it being available to be promoted in a market or implemented and placed into production.

- **Skills dependency**
  Participants are benefitting from access to new high-level skills relating to the technologies being used in the IROR programme. Participants are accessing skills and knowledge that are not available internally and reducing costs through not recruiting new skills (e.g. PhD studentships).



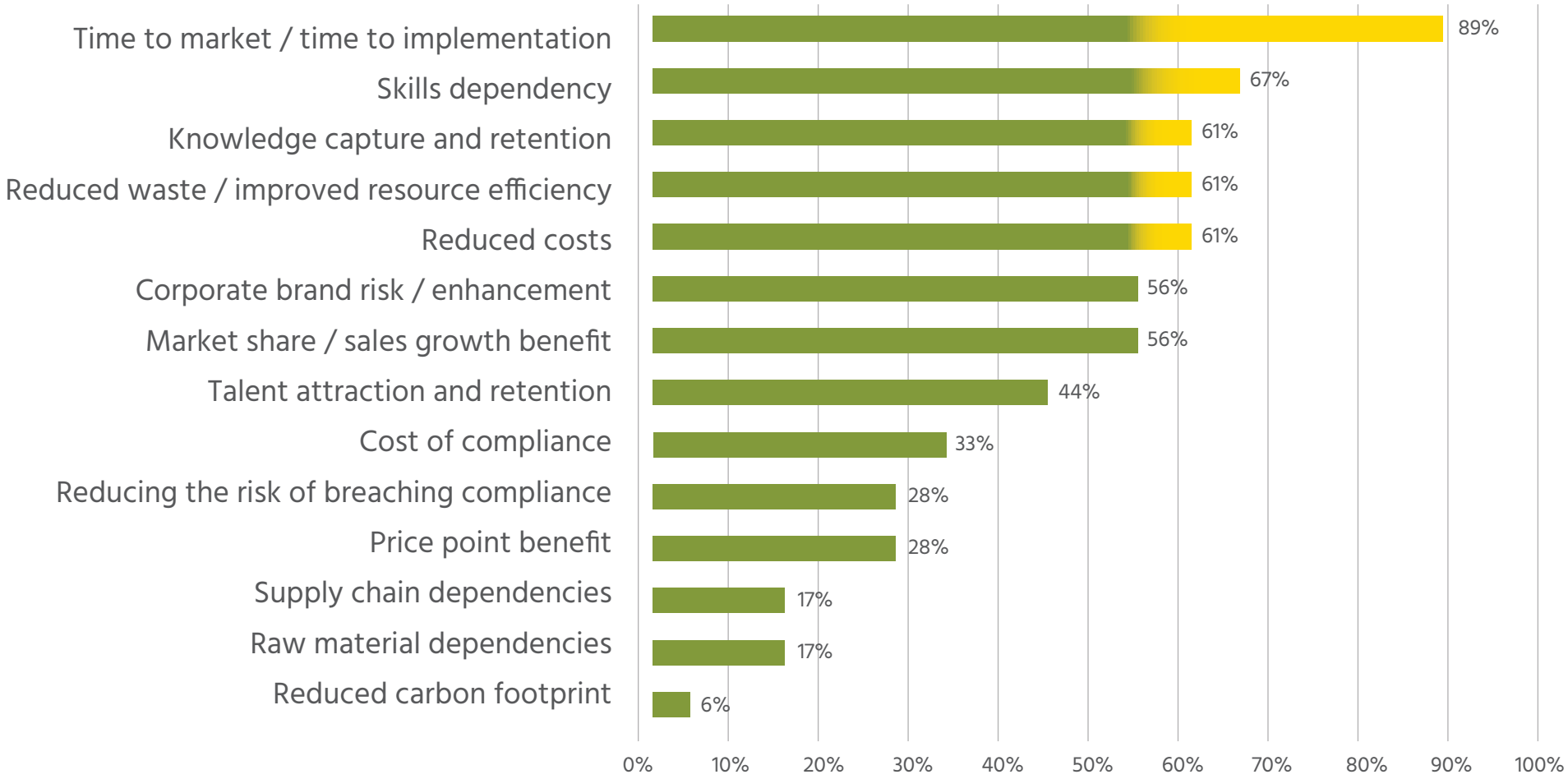
- **Knowledge management & retention**
  Knowledge capture and retention practices vary between Participants. Nevertheless, this expertise is seen as being important to the business competitiveness. Using knowledge effectively is recognised as a potentially fertile, untapped source of new products or services.



- **Reduced costs**
  The technologies used within IROR are enabling higher accuracy simulations and more 'intelligent' screening of research options. Both project outcomes are in turn offering new opportunities for optimising use of resources and reductions in costs.

SUMMARY OF SURVEY FINDINGS (CONTINUED)

The bar chart below shows the ranked scores aggregated across all three SOW areas. The highest scores are highlighted in yellow:



SUMMARY OF SURVEY FINDINGS (CONTINUED)

The scores provided by each Participant were aggregated by each domain area (SOW). The table below shows the comparison of likely / perceived benefits across all three domains:

	Science, Engineering & Manufacturing	Chemistry & Materials	Life Sciences
Time to market / time to implementation	100%	75%	75%
Skills dependency	60%	75%	75%
Reduced costs	60%	75%	50%
Reduced waste / improved resource efficiency	70%	25%	75%
Knowledge capture and retention	60%	75%	50%
Market share / sales growth benefit	40%	75%	75%
Corporate brand risk / enhancement	30%	75%	100%
Talent attraction and retention	30%	25%	100%
Cost of compliance	30%	50%	0%
Price point benefit	40%	0%	50%
Risk of breach	30%	50%	0%
Raw material dependencies	30%	0%	0%
Supply chain dependencies	30%	0%	0%
Reduced carbon footprint	10%	0%	0%

ANALYSIS OF SURVEY RESPONSES

This section analyses the overall level of engagement of the Participants in the IROR programme and the highest-ranking anticipated business benefits. This section also highlights the implications for how these anticipated sources of value may be developed in the remainder of the IROR programme.

1. Engagement of IROR Participants

Overall IROR Participants, particularly at a technical level, remain enthusiastic towards both the programme and the potential benefits that may result. However, broader commitment involving more commercially focused colleagues and business decision makers is currently limited, particularly in larger Participant organisations.

Implications

- More involvement of commercial colleagues and business decision makers would further strengthen the validation of IROR benefits for each Participant. This increased sponsorship also improves the likelihood of successful projects that apply IROR technologies being commercially implemented within a Participant business.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)

2. Time to market / time to implementation

This relates to reducing the time it takes to get new products to market or, reducing the time to implement upgraded versions of products in active use. Time to market and implementation is the most important potential benefit from the IROR programme according to the research. Eight of the nine of Participants in the survey cited this as being likely to have a high impact on their business, with all interviewees confirming its importance. Participant feedback also reflected differences in market sectors and competition dynamics in the way the data intensive technology was being applied.

Some IROR Participants are improving the delivery of their products for a single public-sector client within a long-term capital-intensive programme. Here innovation advantage is anticipated from improved operational performance or through extending the lifespan of in-service components. This was particularly important for Participants operating in heavily regulated sectors, where any new or upgraded components must meet stringent standards before they can be adopted for operational use.

For other Participants, better screening of research candidates and more accurate simulations offer the real potential to improve researcher productivity. This uplift in researcher productivity is expected from improved predictability in the lead time for the development of new IP. For example, in Life Sciences, the Participants anticipate a reduction in the list of 'promising' candidate antimicrobial agents to be put forward for further development. Similarly, some Chemistry & Materials Participants anticipate benefit from better candidate materials identification. In this case the benefits would come from a reduction in mandatory regulatory testing.

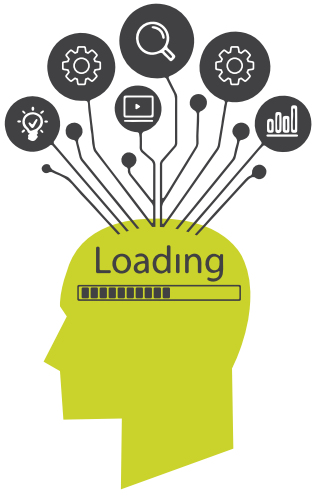
Implications:

- Time to market / time to implementation has potential to be a universally applicable evidence point of impact for IROR. It points to potential gains in both productivity and market advantage.

- The technologies have the potential to provide benefits across a range of sectors. In particular those where development costs are significant and where customers value faster or more predictable development times for new products. This potential value is already visible for Participants operating in markets where new innovations are subject to strong regulation.

- This business value therefore merits close attention so that the benefits of the programme can be monitored for progress. Markers such as the status of internal implementation or product launch project plans could be used as a proxy to monitor the level of progress and effectiveness.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)



3. Reduced skills dependency

This was seen as a strong benefit area across all three SOWs with five of the nine Participants scoring it as high impact and a further three as medium. All Participants cited the benefits of their organisation gaining early access to new skills relating to the technologies offered by the IROR programme.

The Participants noted the high quality of staff with relevant experience in advanced technologies, (e.g. Uncertainty Quantification or UQ), that was not available within their own organisation without further investment (for example, by funding a PhD).

The skills accessed via IROR were recognised as being of superior quality to those typically provided by a PhD student and equivalent to those in specialist contractors. These skills are rare and not readily available through the contractor market, as yet. Provision of these high-quality skills within IROR was seen as reducing the time for Participants to evaluate how these new, emerging techniques could be applied to their business challenges.

Participants indicated that the combination of high quality skills and experience in data-intensive techniques being applied to their recognised business challenges was enhancing the likelihood of wider adoption of these innovative technologies into their business.

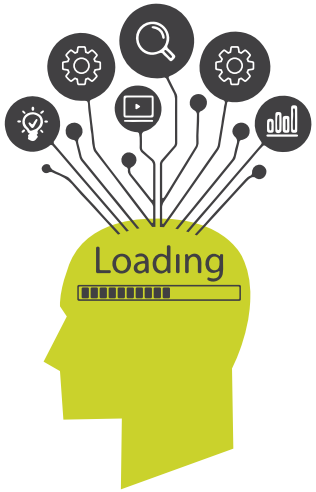
Several Participants quantified the costs and identified the risks of alternative modes of acquiring the skills and knowledge provided within IROR. For most Participants, the primary alternative is funding a PhD student – over 4 years this is estimated to be cost circa £100k. This does not include any:

- Quantification of the benefits of a research project focused on their challenges, where business benefit can commence immediately
- Estimate of the search costs for finding a university supervisor and student capable of completing a similar project
- Consideration of the risks and time delay to value delivered that were experienced through academic deviation from agreed industrial priorities

Overall, the deployment of specialist skills within the IROR programme is providing early value to the Participants by enabling earlier and more effective adoption of innovative data-centric technology. It represents a tangible cost saving over alternatives, such as providing the equivalent of a PhD level one-person allocation per participating organisation.

In terms of overall value, the IROR Programme is helping to accelerate strategically important projects which may not have otherwise progressed in the near term. The programme is helping Participants commit earlier to building their artificial intelligence skills, which also contributes to the building of skills capacity in this emerging technology within the UK economy. This case for skills development though IROR is likely to become stronger as Participants further realise the anticipated business value from their projects.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)



3. Reduced skills dependency

Implications:

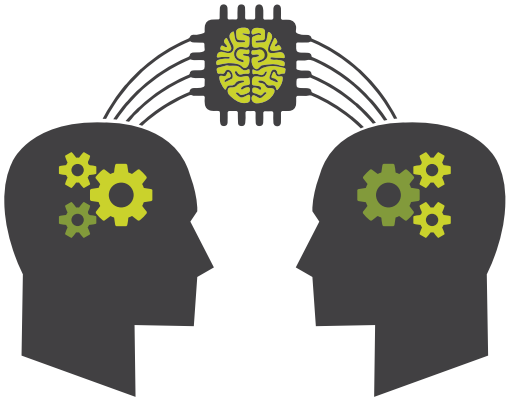
- IROR is already delivering effective skills development via the introduction and early adoption of data-intensive technologies.

- IROR provides Participants with a more effective, lower-risk alternative to university PhD studentships, at a significantly lower cost.

- The collaborative innovation process delivered through IROR has the potential to be used to augment the artificial intelligence and machine learning knowledge of existing PhD students.

- The IROR programme has the potential to play a bigger role in the faster scale-up of scarce AI/ML skills in the UK economy. This could be enabled by further collaboration with other academic institutions and PhD programmes by enabling recent post-doctoral personnel to acquire experience in the application of data-intensive technologies to real world business challenges.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)



4. Knowledge capture and retention

Knowledge capture and retention is expected to have a high level of business benefit by five of the Participants and medium impact by a further two. Knowledge capture and retention practices vary between companies, but it is generally seen as being important to the maintenance of business competitiveness and a potential source of high productivity gains.

Projected benefits for SEM Participants included:

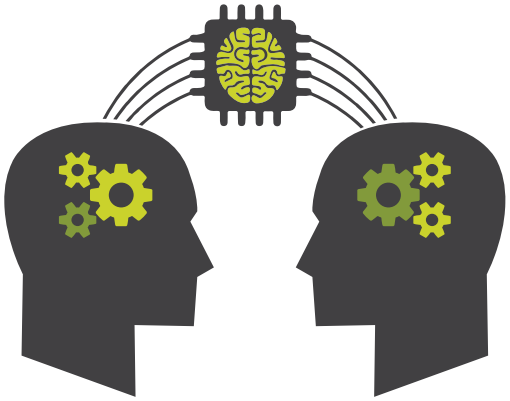
- Using the specialist expertise available within IROR, Participants can tap into and get evidence of the value of UQ techniques earlier and with lower risk. The ability to accelerate the value derived from UQ techniques without diverting their own valuable resources from existing priority projects is seen as a significant source of early value.

- For capital-intensive businesses, where the operational lifespan of custom-built plant and equipment is measured in decades, the capture and retention of knowledge is vital. Even more so when there is a shortage of skills and experience in data-intensive technologies within the business and wider economy. Many Participants face a knowledge retention challenge caused by the retirement of many of experienced engineers. These individuals often have detailed and unique knowledge of older plant infrastructures. In response, many organisations are implementing programmes of internal knowledge transfer, augmented by an aggressive programme of PhD recruitment. IROR projects offer the opportunity to use artificial intelligence and other data-intensive technologies as a vehicle to transfer skills from the more experienced staff. Successful results produced in the IROR projects are expected to contribute to this retention of key organisational knowledge by incorporating outcomes into these training programmes.

- The use of machine learning within IROR is also helping the capture and retention of key knowledge within the organisation. This technology offers the potential to enable less experienced engineers to make more progress with less supervision using new design tools that can access retained knowledge acquired in previous projects. This approach also frees-up more experienced engineers to tackle unsolved problems that are more challenging and of potentially higher value.

- For SME Participants, recruiting good people and getting them 'up to speed' and working productively quickly is vital to sustain growth. Some of the tools being developed by the programme offer the potential for smaller organisations to reduce their reliance on smaller numbers of key in-house personnel for knowledge transfer. The use of this technology offers the potential to improve the overall value such organisations can produce by making more of their existing knowledge and expertise.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)



4. Knowledge capture and retention

For the Participants in the Chemistry and Materials SOW, the impact of knowledge capture and retention was rated low – medium although, it was acknowledged that the programme creates a positive pressure to develop better methods of internal data management.

Knowledge capture and retention was seen as a high impact area for Life Sciences businesses with Participants seeing this as a major area of expected business value through the generation of more new products and licensing opportunities.

Implications:

- Better ways to manage and retain key knowledge is recognised by all Participants across all SOWs as an important potential enabler of business sustainability and competitive advantage. This value is important to businesses irrespective of their scale or size. Productivity benefits are projected from better knowledge management through:
    - Enabling the more effective use of researchers by empowering less skilled researchers to complete more research tasks aided by machine learning tools.
    - Evolving better ways to mitigate the risk of knowledge loss from ageing workforces by finding better ways to transfer skills and knowledge via learning and potentially to act as an attraction to new STEM talent.
    - 'Freeing up' more experienced staff to address higher value / more complex challenges.
    - Providing an increased focus on the management of each organisation's data assets.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)

5. Reduced costs

Reduced costs were anticipated as being a high or medium impact by seven out of nine of the Participants. The technologies used within IROR are enabling better starting points for research through more 'intelligent' identification and screening of candidate options. This has the potential to significantly reduce associated costs by enabling:

- More accurate proofs of the operational performance of existing components - reducing the need for real-world testing and extending the time between scheduled maintenance or replacement.
- Improved screening of alternative candidate solutions to reduce testing volumes.
- Improved use of resources in manufacturing processes.
- More efficient use of the high-performance computing infrastructure through reduced or optimised cycle times.

As an example, projected benefits for SEM included improved virtual testing of components through high accuracy simulations using techniques such as uncertainty quantification (UQ). The resulting improved accuracy of computational fluid dynamics (CFD) simulations contributes to lower costs by optimising designs earlier in the development process. This in turn results in improved plant performance and extension of the time periods between scheduled maintenance. IROR is also expected to improve understanding of the operational performance dynamics of existing components enabling an overall system to use available resources more efficiently.

The high accuracy simulation projects with an UQ component offer the potential to secure significant savings in testing costs, particularly in heavily regulated environments where the standards of proof required to extend the working life of components is high. In this context asset lifecycle extensions testing can cost in the region of £0.5m. The impact of reduced costs also extends to the design and construction of new facilities. The costs savings involved here, particularly for large capital-intensive projects are likely to be of the order of several millions or tens of millions of pounds.

The IROR programme is also expected to result in benefits through the optimisation of the computing resources needed to complete a simulation and the number of simulations required to get valuable outputs. These benefits can be taken as reduced costs and/or allowing more computing time for other important projects. Improved UQ techniques in simulations is also providing a better understanding of production tolerances, reducing waste and reprocessing costs.

ANALYSIS OF SURVEY RESPONSES (CONTINUED)

5. Reduced costs

In Chemistry and Materials projects benefits included improved screening of candidate product materials to reduce the need for testing. For instance, toxicity and biodegradation testing for a new chemical formulation typically costs £10k-20k.
For Life Sciences, the benefits are similar to the Chemistry and Materials companies. Candidate materials in this sector can be expensive to synthesize costing several thousands of pounds for a few grams. Generating candidate materials is a vital and expensive step in the research and development process. IROR Participants expect a significant cost reduction through the better screening of candidate materials. This will lower the cost barriers in generating new products and licensing opportunities.

Implications:

- A cost-benefit analysis generated from IROR projects can help Participant organisations better understand the returns on investment in these new technologies and allow their value to be assessed against alternative investment opportunities for the business.

- The programme could provide useful insight regarding the improved efficiency of IT facilities. Specifically, in the use of HPC and the deployment of data-intensive technologies.

RECOMMENDATIONS

This survey confirms that IROR Participants expect the programme to deliver positive benefits for their businesses with the most important areas being:

- Time to market / time to implementation
- Reduced costs / improved resource efficiency
- Knowledge capture and retention
- Skills dependency

Participants and stakeholders can increase the value that they derive from the IROR programme, by improving the overall governance of the IROR programme as follows:

1. Business value monitoring:

Institute a mutually agreed monitoring process, as part of both individual IROR projects and the wider IROR programme.

The early positive indicators of likely impact can provide an important source of learning and understanding of the potential value of the IROR technologies across a range of domains. A greater understanding of the mechanisms by which these technologies can catalyse new sources of business and economic value will benefit Participants, the Hartree Centre and the UK economy.

Acquisition of these insights will require a consistent mechanism to monitor benefits and value within the IROR programme. This monitoring will foster a deeper understanding of the high-level business benefits and can provide information to assist with estimating the economic value that may be accrued from the use of these technologies.

2. Increase executive sponsorship within IROR projects

Ensure all IROR projects have the regular involvement of an Executive Sponsor from each IROR Participant to provide feedback and mentorship relating to programme implementation. Given the potential positive benefits resulting from participation in the IROR Programme, it is recommended that an Executive Sponsor for IROR is appointed by each Participant organisation. The precise details of this role need discussion with IROR Participants, but typically may include:

- Review and feedback on bi-annual reports on progress within their IROR projects
- Receiving updates on the general insights captured and shared amongst all Participants resulting from the metrics monitoring process.
- Identification of business risk(s) from the deployment of IROR projects and to ensure that mitigation plans could be created at a Participant and IROR programme level.
- Validation of business benefits identified within each project and to determine which of these benefits that could be shared more widely.

This high-level business visibility also provides the opportunity to raise awareness and understanding of the potential sector impact and therefore the risks of the 'do-nothing' option. That is, what are the implications if other businesses develop and apply this type of technology.

3. Assessing the value of IROR digital assets

Establish a deeper understanding of the value of the digital assets being developed as part of the IROR projects.

IROR Participants may improve the value they derive from the IROR programme via a greater understanding of how the digital assets developed by the Hartree Centre are enabling business value within their projects. This deeper understanding will enable the Participants to provide feedback that can help focus Hartree Centre resources onto digital assets that are adding most business value within the projects.

RECOMMENDATIONS (CONTINUED)

A better appreciation of the impact of digital assets can also enable Participants to identify opportunities where the faster or additional development of digital assets could deliver even greater positive impact, business value and increased productivity across the overall IROR programme.

4. Best practices in the use of data-intensive technologies

By identifying best practices that maximise productivity, it is expected that Participants, the Hartree Centre and wider stakeholders can obtain a better appreciation of the common patterns and trends relating to how the IROR technologies impact business value and potential productivity improvements. The effect of improved governance and monitoring can deepen their understanding of how the technologies are creating these impacts and inform the strategic direction of digital asset development.

In relation to each of the most important benefit areas, this knowledge will help to improve the overall understanding of:

- Time to market / time to implementation

Identifying high potential areas where further competitive and comparative advantage may be captured through use of the technologies.

- Knowledge capture and retention

Capturing and disseminating lessons learned by Participants to develop knowledge capture best practices.

- Reduced costs / improved resource efficiency

Identifying new areas of cost savings enabled by the programme, e.g. best practice in the optimisation of expensive HPC infrastructure usage.

- Skills dependency

Capture and disseminate lessons learned by Participants during the IROR programme, that accelerate skills acquisition and development, e.g. through case studies describing the skills acquisition benefits relating to the adoption of data-centric technologies.

Next steps:

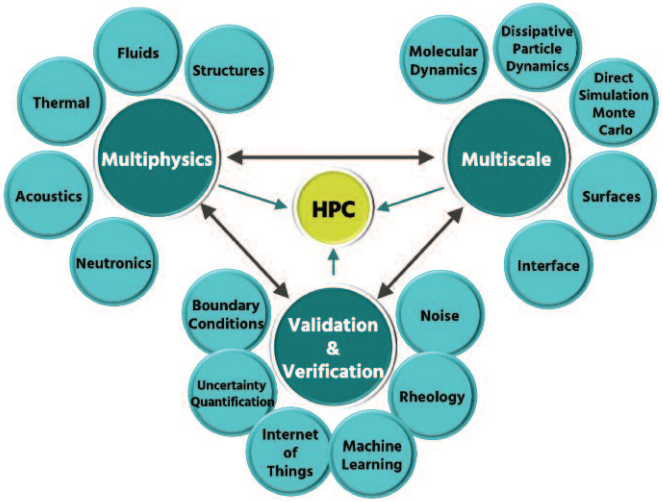
In support of the recommendations above, the Hartree Centre should build upon the early anticipated benefits of the IROR programme by securing the input and buy-in of IROR Participants to an ongoing IROR governance programme. This will ensure that progress is maintained during the remainder of the programme so that the early business value documented in this report is converted into tangible outcomes and impact that will benefit all programme stakeholders.

APPENDICES

APPENDIX 1 – Statement of Work (SOW) Models

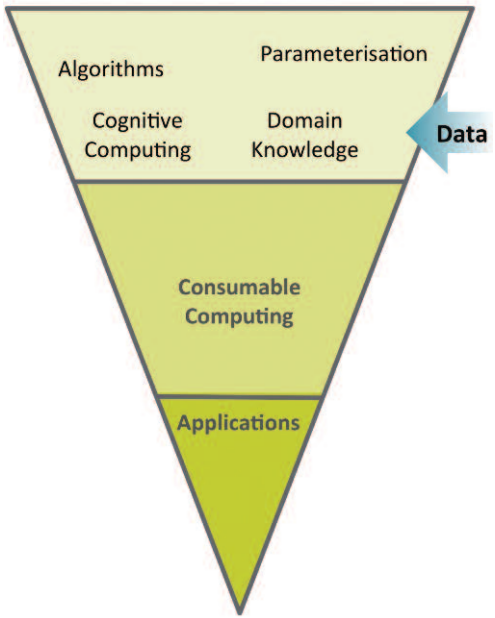
SCIENCE, ENGINEERING & MANUFACTURING (SEM)

The overarching vision for this programme is the creation of a 'digital' or virtual twin for physical components or systems. This requires the ability to extend the existing digital modelling capabilities to accommodate different length and time scales (multi-scale) and combine different engineering scales (multiphysics), e.g. deal with systems involving solid, liquid and gas interactions at the atomistic level through to the metre length scale. To be meaningful, all this needs to be achieved with a degree of accuracy to match the 'real world' twin and therefore would require on- going validation and verification).



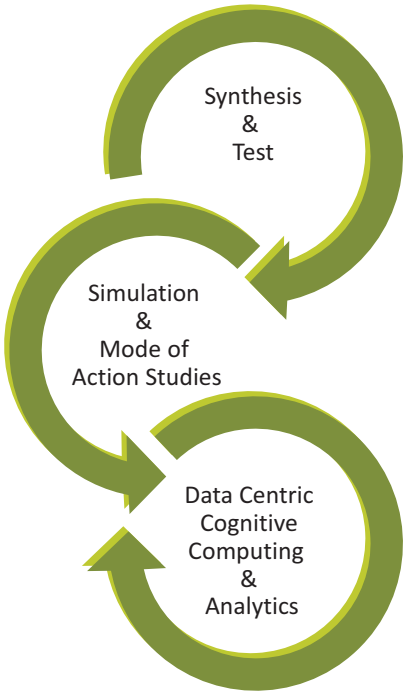
CHEMISTRY & MATERIALS

Development of an integrated data analytics, modelling, and simulation capability able to address a broad variety of chemical and materials problems with world-class scale and accuracy.



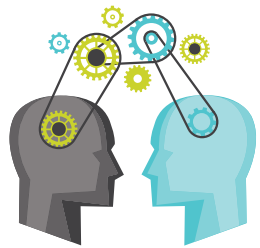
LIFE SCIENCES

Anti-Microbial Discovery (AMD) work consists of three integrated workstreams which combined create a 'learning loop' for accelerating anti-microbial discovery by better targeting of the most promising candidates through simulation and cognitive techniques.



APPENDICES

APPENDIX 2 – The IROR Industrial Engagement Process – InCEPT™



DISCOVERY	**TECHNICAL VERIFICATION**	**BUSINESS VALUE VALIDATION**	**BUSINESS VALUE REALISATION**
Matching Research Capabilities to Business Challenges	Validating Scope to Business Specific Needs	Assessing progress against Business Benefits	Range of exploitation options
Exploration	**Insights**	**Navigator**	**Commercialisation**

TYPES OF DATA	OPEN	HYBRID	PROPRIETARY
BUSINESS VALUE / IMPACT VISIBILITY	Testing technical /science know-how using public / anonymised data	Capture learning and validate business impact targets deliverable	Deploy technology on real-world project with real world data
	Mapping of Research capability to identify potential business value	Jointly agreed metrics to measure progress aligned to business value	Collect, analyse and share benefit areas and drivers of impact

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