Complexity, Challenges and Opportunities for Carbon Neutral Digital Research

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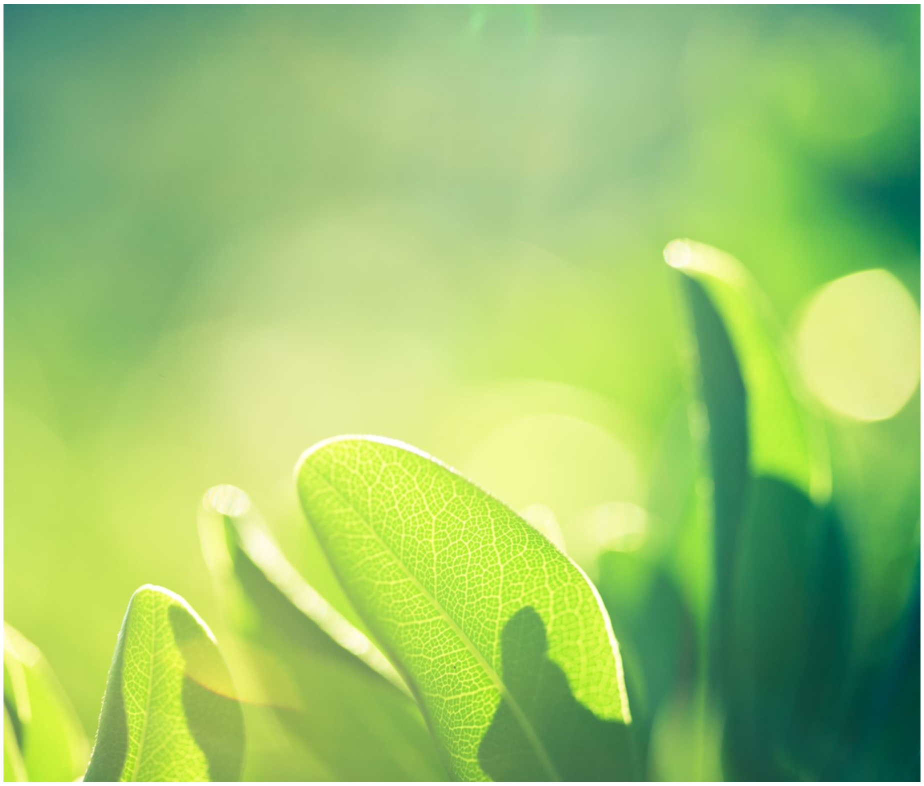

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Preface

Introductory words from Prof. Stephen Mobbs
Director of the National Centre for Atmospheric Science (NCAS)

Society is faced with an ever more urgent necessity to adapt to a new world where "Net Zero" is pervasive. This presents enormous socio-economic and technological challenges but the certainty of catastrophic climate change if nothing is done means that our response is imperative. Science and engineering has a huge part to play in making that response possible.

UK Research and Innovation has placed the net zero transition at the top of its priorities (UK Research & Innovation 2020). This has two implications. Firstly, UKRI supports research which develops and identifies solutions which create advances towards a new net zero world. At the same time, UKRI recognises that its activities and the research it supports have an adverse environmental impact.

As part of its strategy for creating world-class research and innovation infrastructure, UKRI supports a wide variety of digital research infrastructure (DRI). As UKRI notes, "Digital research infrastructure underpins the research and innovation ecosystem and is a critical system for researchers, policymakers and innovators." Digitally-enabled research and data science open up new avenues for scientific investigation, supported by rapidly expanding streams of sensor, measurement and observational data. This research has a large part to play in enabling the net zero transition.

However, at the same time, digital research infrastructure comes at a considerable cost to the environment. The availability of sufficient electrical power is now one of the principal factors limiting high performance computing. The pervasive use of computers of all types in research and innovation means that the very research itself can have a considerable environmental impact.

Recognising the critical roles of digital research infrastructure in its strategy, UKRI has determined that the infrastructure programmes should be fully a part of the UKRI net zero targets. An approach is now needed which both enables the provision of the infrastructure itself to be achieved sustainably and at the same time, policies need to be developed which avoid inadvertent and negative consequences of investment decisions which drive the use of digital research infrastructure.

In order to develop a comprehensive strategy for net zero digital research infrastructure, the Natural Environment Research Council (NERC), acting on behalf of UKRI, has commissioned a 19 month scoping project (CEDA 2021; UKRI 2022b) to identify all the principal factors which such a strategy should encompass and to advise on the most effective ways forward. This report describes progress made at the mid-point of this scoping study.

The report presents interim results from the Net Zero DRI scoping project based on a literature survey. Recommendations drawing on existing best practice in many areas already provide some guidance for UKRI funding decisions.

Within the scope of this study are actions fully under UKRI control and actions over which UKRI has no direct control. The report recognises that there are areas where UKRI can act unilaterally but also highlights the areas where UKRI can only work with others. However, these cooperative actions will be crucial in order to meet net zero targets.

The Net Zero DRI scoping project is also undertaking a wide range of technical studies in order to inform future recommendations. These are being undertaken with a wide range of partners and stakeholders, through workshops and small commissioned projects. Future reports will include outcomes from these studies.

Contents

The Executive Summary

E1 Introduction

This report is addressed to UKRI Digital Research Infrastructure (DRI) stakeholders in UK Research and Innovation (UKRI), its constituent Research Councils and in the Universities and other institutions which own and operate many digital research facilities which are majority funded by UKRI.

The aim of the UKRI Net Zero Digital Research Infrastructure Scoping Project (hereafter "the project") is to report on evidence and make recommendations for a roadmap to a Net Zero UKRI DRI by 2040 or sooner. The project, via this interim report and future reports, provides recommendations for reducing and avoiding carbon emissions. It also reviews options for dealing with unavoided emissions through carbon capture, biochar and offsetting.

The project considers the full range of carbon emissions associated with the computational facilities which are owned or majority funded by UKRI. These range from High Performance Computing (HPC) resources providing a national service to institutional machine rooms hosting a small number of server racks to support local research activities. The HPC centres have high footprints and visibility, and also have highly efficient systems following years of effort aimed at mitigating power costs and optimising utilisation of expensive resources. Estimates of the aggregate impact of institutional machine rooms will be gathered before the end of the project.

In terms of the scale, the carbon footprint of UKRI as a whole is broadly comparable with a large UK university, and the footprint of the UKRI DRI is broadly comparable to a large university department.

In many areas the UKRI DRI is at the leading edge of societal transformation, and now has to face transformation itself. The question of sustainability has suddenly gained prominence in a discipline which has long been driven by technical targets as the debate shifts from mitigation and adaptation to an emergency response. The environmental responsibility of the UKRI DRI often merges with the broader responsibilities of UKRI and the research sector.

This report looks at what needs to be done, both within the research sector and working collaboratively with others, in order to deliver the UKRI DRI net zero roadmap.

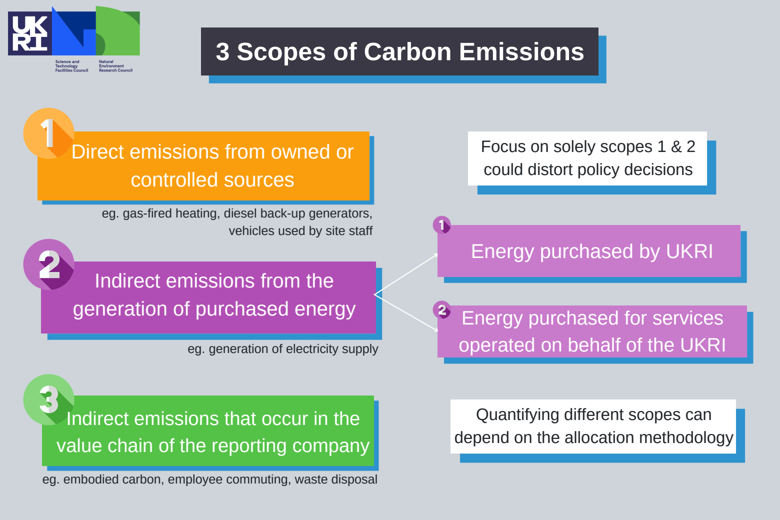
E2 Overview

The key areas of emissions are from the purchase of electricity, the manufacture of hardware and the mining of minerals going into the hardware, flights and other emissions associated with the operation and use of the UKRI DRI, and, last but not least, the impact of the UKRI DRI on societal emissions through research outcomes.

Responsibility for emissions is often shared, leading to considerable uncertainty in numerical allocation of emissions.

The largest footprint uncertainties are in the supply chain and in the impact of the UKRI DRI on society. Both of these are included within the Scope 3 emissions (see Figure E1) of the Greenhouse Gas Protocol. Treating local emissions as fully equivalent to emissions associated with mining activities at the other end of the supply chain creates many intractable problems, but ignoring those remote emissions is clearly incompatible with the high ambition of UKRI.

Figure E1: The three scopes of emissions defined by the Greenhouse Gas Protocol form the basis of national and international reporting requirements. When carbon emissions cannot be attributed uniquely to specific products of activities the allocation approach can be used, though results depend on methodological choices (e.g. Ernst and Young 2020).



The many complexities of the technology, supply chains, economic, political and social contexts should not divert us from simple truths:

- The climate extremes and the wave of extinction that are threatening to engulf us are now recognised as emergency and crisis situations demand an emergency response.

- UKRI has both an immense intellectual capacity and a mission to transform society.
- Society is going through a communication and information revolution powered by digital technology: UKRI can exploit its leading role in digitally enabled research to demonstrate how the information revolution can fit with net zero targets.

There is a growing recognition of the urgency of taking action, and a wide range of national and international activities are already making significant progress. The Science Based Targets Initiative (SBTi) is rapidly gaining recognition as a focus for setting consensus and has recently set the first globally recognised corporate net-zero standard and, with a UK focus, the Alliance for Sustainability Leadership in Education (EAUC) is bringing the SBTi principles into the university sector as part of its work to make sustainability 'just good business' in the post-16 education sector.

The SBTi standard recommends that organisations plan for 90% reduction in emissions relative to the start of their net zero journey, and commit to using carbon capture to compensate for remaining emissions. There is an immediate problem here as we start our journey with substantial uncertainty around our Scope 3 emissions, though there is little doubt that they are well above 10% and increasing. There are strong indications that focus on ad hoc metrics can be counterproductive and we should be keeping focus on the target of achieving net zero carbon balance and going beyond that to stabilise the climate.

E3 Key findings and initial recommendations

This section covers the various key themes of the report:

1. Building Consensus
2. Leading
3. Technology and Capability
4. User Efficiency and Market Rebound
5. Electricity Supply
6. Procurement of Equipment and Services
7. Estates and Travel
8. Offsetting, Sequestration and Biochar
9. Wielding Impact
10. Creating and Delivering the Roadmap

Initial recommendations are formatted in bold.

E3.1 Building Consensus

There is a firm consensus that something should be done, but behind the agreement on broad objectives there is considerable diversity of opinion about what should be done, and by whom. In the global context, every UKRI employee and every UKRI funded researcher is in a privileged and influential position: if we can start to focus that influence on the net zero challenge, we have the power to shift the transition into a positive phase. Care needs to be taken to ensure that potential negative consequences are not overlooked or underestimated and all views are taken into account. There needs to be an evidence-based discussion about the relative roles and footprints of physical experiment compared to digital research. The critics of a policy may provide the most valuable insights needed to establish resilience and eventual success. **The UKRI DRI needs to ensure that investment decisions are backed by a deep understanding of the views of the research community**.

Although SBTi recommendations rely heavily on a nominally precise quantification of emissions, there is a significant body of research suggesting that this approach is counterproductive. Many commentators are linking "net zero" to greenwashing because of the perception that organisations are using various forms of offsetting to delay or avoid making meaningful change. **UKRI DRI should exploit the UK research community capacity in social sciences, arts and humanities, and in economics, to understand the range of societal views, the avenues of consensus which open-up potential for accelerating transition and the emerging (or exploding) discords which can block or reverse change**.

Excellent organisations and networks are already emerging to support the transition to net-zero. The **UKRI DRI should work with emerging leaders, providing both intellectual input and operational experience at the same time as exploiting the standards and communication opportunities that emerge from these networks**.

E3.2 Leading

The creation of leaders is central to UKRI's existence and there are thousands of UKRI funded leaders making impacts across the spectrum of sustainability research, but the challenge of achieving net zero also needs a centre, a focus of activity with the capacity to engage at the national and international level. The UKRI DRI epitomises the need for activities to be joined up across the research sector, with much of the UKRI DRI activity hosted in universities and operating within their policies and governance. **A focal point which can bring together the strands of activities across the research sector is needed in order to enable a coherent approach on the Net Zero UKRI DRI roadmap**.

The UK research sector includes many leading climate scientists who have, for years, been warning of the seriousness of the climate crisis. There is a clear consensus that urgent action is needed. **The Net Zero target needs to be treated, like Health and Safety, as something that concerns everybody in the research sector. The response must reflect the recent recognition of a climate emergency**.

E3.3 Technology and Capability

The rapid development of ICT technology is bringing many opportunities. There is a rapid increase in the potential of the UKRI DRI to open up fantastic opportunities. There is also an increase in the diversity and complexity of our HPC resources. Efficient management of the resources on these complex systems require multiple layers of independently managed and operated software which is creating new scientific disciplines and new technical specialisations. **The UKRI DRI needs to invest in the development of capability to deliver effective scientific throughput in a rapidly evolving digital landscape**.

These new disciplines and specialisations need to find their space in the community and in the UK research funding envelope. The choice of placing new activities in either "infrastructure" or "research" will impact on the net-zero roadmap because it potentially limits or empowers the ability of grant holders to effectively exploit efficiency gains. **The UKRI DRI needs to take steps to minimise barriers to adoption of potential efficiencies arising from new technologies in hardware and software**.

E3.4 User Efficiency and Market Rebound

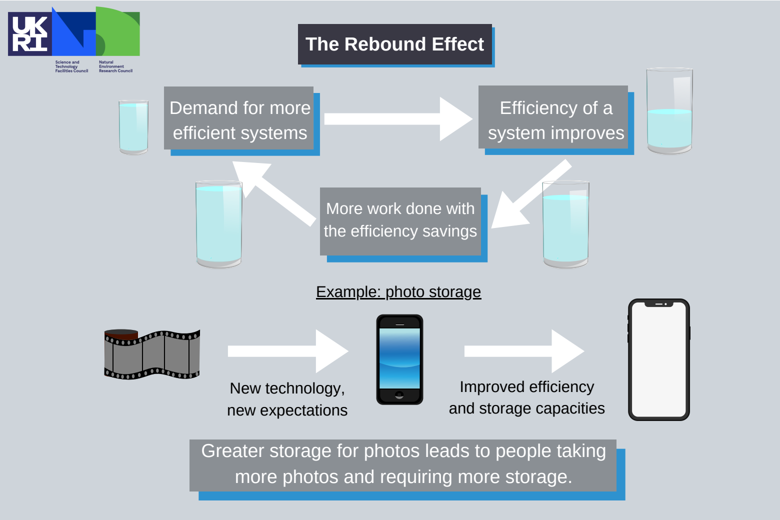
There is a broad consensus that users of digital services in general and the UKRI DRI in particular can improve their efficiency of resource usage if they are given both more reliable and relevant information and also appropriate training and tools. New hardware capabilities can present users with a bewildering array of opportunities and new challenges which will not have been covered in their previous experience. Inefficient use of facilities impacts negatively on both the carbon intensity of research outputs and the effective use of research staff time. **The UKRI DRI needs to ensure that the introduction of new technologies is matched by appropriate resources for training and expert user support**.

There is extensive literature discussing the potential for efficiency gains to lead to an expanding scope and hence greater resource usage, rather than the hoped for resource savings. This is known as the rebound effect which is illustrated in Figure E2. Within the research community, it is clear that HPC facilities are run at capacity with a power consumption that is, to a large extent, independent of the efficiency of user applications. Efficiency gains can only impact on UKRI DRI carbon footprint if they can be taken into account at the procurement stage. **The UKRI DRI needs to ensure that the procurement framework enables the conversion of efficiency gains into carbon savings**.

E3.5 Electricity Supply

Electricity is the largest single element of the carbon footprint for most UKRI DRI services and facilities. Green tariffs are often cited as being carbon-free but are also seen by many as falling short of a serious commitment to move towards sustainability: the green tariffs exist within and are an intrinsic part of a power distribution network with a massive carbon footprint. **Best practice for an individual institution is to**

Figure E2: The rebound effect reduces or eliminates the expected resource savings from new technologies or efficiency savings.



adopt 100% off-grid renewable electricity supply, but there are limitations of scale and location. More general solutions include:

- the **adoption of multi-year power purchase agreements with renewable investment clauses**,
- **construction of grid-scale battery storage** matched to the institutional power demands to eliminate use of diesel back-up generation and capable of reducing or eliminating power draw from the grid when demand is leading to high levels of gas usage,
- **building on-site renewable generation and grid-connected power storage** to mitigate load on the national grid.

E3.6 Procurement of Equipment and Services

UKRI must consider both what it procures and how it procures. The moment a large computer is procured, decisions about how to deliver and achieve a scientific throughput will be constrained within the tramlines of technical targets. UKRI procurement needs to include metrics that can be related to strategic objectives of societal benefit and the net-zero target (and, in many cases, still need to be invented) not technical targets. **Institutions making purchases on behalf of UKRI must be empowered to balance investments in efficiency against investments in energy intensive infrastructure**.

The carbon emissions associated with the manufacture of digital hardware are substantial and immediate measures need to be taken. Current best practices include:

- the inclusion of **sustainability clauses in procurement contracts** to ensure that suppliers are adopting and following a plan for emissions reductions,
- **building relationships along the supply line** to work on mutually beneficial solutions, and
- looking at the **whole life cycle of equipment and opportunities to extend the life and re-use potential of equipment**.

E3.7 Estates and Travel

The on-site use of fossil fuels, perhaps in the form of back-up power generation or heating offices, is a minor component of the overall UKRI DRI carbon footprint, but is also, from a technical perspective, the easiest to eliminate. Fossil-free on-site operations should be established in the near term. The **project** will evaluate the scale of the challenge in the context of the UKRI DRI, but specific options will vary from site to site. **Eliminating on-site use of fossil fuels will require a clear timeline. This should be developed by 2025**. This may include, for instance, the use of grid-scale batteries discussed above (§E3.5) or, for backup generators which are rarely used, biodiesel.

Travel, particularly by air, carries a significant carbon footprint. It is not a major component of the UKRI DRI footprint, but we know that the current pattern of flying is not compatible with any credible roadmap to net zero. The UKRI DRI community needs to explore avenues for maintaining the necessary level of international communication and collaboration with reduced dependency on air travel. Electric aviation is advancing rapidly, but unlikely to have a major impact on intercontinental travel by 2040. **The UKRI DRI should facilitate and promote digital collaboration tools and awareness to reduce carbon intensity and enhance access to the research programmes**.

E3.8 Offsetting, Sequestration and Biochar

When carbon emission cannot be avoided, a range of options are being discussed. It is important to remember that the phrase "cannot be avoided" is highly subjective. As leaders in knowledge and societal responsibility, **UKRI needs to be exhaustive in exploring what can be avoided before, during, and after taking steps to deal with unavoided emissions**.

Offsetting of emissions through, for example, tree-planting, restoring peatlands, and, more recently, managing the coastal shelves, can take carbon out of the atmosphere for a modest price of around £15 per tonne of carbon dioxide equivalent. It is seen by many as being inadequate because there is a near total lack of guarantees of long term stability, it cannot scale to the level of current emissions, and the price has been and currently remains too low to incentivise change.

Sequestration involves the storage of carbon dioxide extracted from the atmosphere in secure geological reservoirs. A commercial service is currently available at a price of £1000 per tonne, which can certainly incentivise change. It is, unfortunately, unclear whether the technology can scale from the limited capacity of a single small-scale provider who started operations in 2021 to a fully functioning global industry in 2022. Best practice is to **adopt carbon offsetting now and implement a plan to transition to sequestration before the net zero target date**.

Biochar is an emerging intermediate approach, with greater long-term stability than offsetting and lower costs and fewer technological barriers than sequestration. The process involves creating charcoal from wood or other plant material and then burying it in soil. Research is needed to ensure that secondary emissions do not overwhelm the benefits.

Given the uncertainty, particularly around scalability, of all these options, UKRI needs to pursue a broad strategy and **couple investments in carbon removal projects with research into their sustainability**.

The economic sustainability of the institutions taking responsibility for carbon removal also need to be considered. The offsetting industry is made up of many enthusiastic companies but none appear to have exploited legal governance mechanisms (such as trusts) that would ensure their viability in the long-term. **UKRI should ensure that any offsetting investments are linked to guarantees of institutional continuity, e.g. through a trust**.

E3.9 Wielding Impact

UKRI has a huge impact on society. Research impact is defined in terms of academic impact, of impact on the economy and society: there is currently no requirement for researchers to consider that their research could have a negative impact on sustainability. **The existential crises that face us in climate and biodiversity need to be reflected in every grant application as a key element of ethical and societal responsibility**.

E3.10 Creating and Delivering the Roadmap

The expertise and innovative capacity needed to convert scoping study recommendations into protocols, guidance documents and training materials for all stakeholders is spread across many research institutions. The distributed decision making which is inherent in the ethics of the research community, giving researchers a significant degree of autonomy in deciding the appropriate methodologies for their research, will mean that responsibility for delivering the net zero roadmap is spread across the entire research community. **The UKRI DRI must ensure continuity of activities which can assess best practice and deliver guidance to all those involved in funding, procuring, operating and using digital research infrastructure**.

E4 Summary of Recommendations

The list of recommendations in Table E1 was discussed at a stakeholder feedback meeting (Woodward, Townsend, and Juckes 2022).

Table E1: Interim Recommendations

Recommendations	
Building Consensus	
1	The UKRI DRI needs to ensure that investment decisions are backed by a deep understanding of the views of the research community.
2	UKRI should use its capacity in social sciences, arts and humanities, and in economics, to understand the range of societal views, the avenues of consensus which open-up potential for accelerating transition and the emerging (or exploding) discords which can block or reverse change.
Leading	
3	Create a focal point which can bring together the strands of activities across the research sector to enable a coherent approach to delivering the Net Zero UKRI DRI.
Technology and Capability	
4	The UKRI DRI needs to invest in the development of capability to deliver effective scientific throughput in a rapidly evolving digital landscape.
5	Steps must be taken to minimise barriers to the adoption of potential efficiencies arising from new technologies in hardware and software, e.g. ensuring adequate crossover between experts of science and experts of the technology.
User efficiency & Market Rebound	
6	Ensure the introduction of new technologies is matched by appropriate resources for training and expert user support, particularly training scientists in use of new technology.
7	Ensure the procurement framework enables the conversion of efficiency gains into carbon savings rather than simply resulting in higher usage.
Electricity Supply	
8	Best practice for an individual institution is to adopt 100% off-grid renewable electricity supply, but there are limitations of scale and location
9	Adoption of multi-year power purchase agreements with renewable investment clauses
10	Construction of grid-scale battery storage matched to the institutional power demands
11	Building on-site renewable generation and grid-connected power storage to mitigate load on the national

Procurement of equipment and Services	
12	Institutions making purchases on behalf of UKRI must be empowered to balance investments in efficiency against investments in energy intensive infrastructure.
13	Add sustainability clauses in procurement contracts
14	Build relationships along the supply line to work on mutually beneficial solutions
15	Look at the whole life cycle of equipment and opportunities to extend the life and re-use potential of equipment.
Estates and Travel	
16	Eliminating on-site use of fossil fuels will require a clear timeline. This should be developed by 2025.
17	The UKRI DRI should facilitate and promote digital collaboration tools and awareness to reduce carbon intensity and enhance access to the research programmes.
Offsetting, Sequestration and Biochar	
18	UKRI needs to be exhaustive in exploring what can be avoided before, during, and after taking steps to deal with unavoided emissions.
19	Given uncertainty in the scalability of biochar and other carbon removal innovations, the UKRI need to couple investments with research into their sustainability.
20	UKRI should ensure that any offsetting investments are linked to guarantees of institutional continuity, e.g. through a trust.
Wielding Impact	
21	There is currently no requirement for researchers to consider that their research could have a negative impact on sustainability. The existential crises that face us in climate and biodiversity need to be reflected in every grant application as a key element of ethical and societal responsibility.
Creating and Delivering the Roadmap	
22	The UKRI DRI must ensure continuity of activities which can assess best practice and deliver guidance to all those involved in funding, procuring, operating and using digital research infrastructure.

E5 Risk Assessment

Organisational transitions are complex projects and require a detailed risk assessment framework. Here, we highlight a few high level strategic risks. This will be expanded in the **project** final report.

	Strategic Roadmap Risk
1	The rapidly evolving landscape of climate drivers, technology and societal perceptions of appropriate responses could derail policy. It is important to base policy on firm foundations and not be tied to specific details of policies which may continue to evolve as the climate crisis and the public perception of urgency evolve.
2	Lack of consensus on appropriate measures may lead to poor implementation and adoption. Beneath the surface of shared concern on climate, there are many different views on what should be done.
3	Resource bottlenecks and transition costs can delay adoption of best practice. Investment decisions can commit organisations to patterns of usage and behaviour which are not optimal for a net zero perspective.

Table E2: Strategic risks which will need to be monitored and mitigated through the course of the roadmap.

Chapter 1

Synthesis

The following sections provide a synthesis of the key areas covered in the literature survey, with links to sections (indicated by "§") containing detailed discussion of individual papers in subsequent chapters.

1.1 Overview

The carbon emissions associated with the operation of Digital Infrastructure are significant and growing (Hopper et al. 2020; Royal Society 2022, §1.4), and the UKRI Digital Research Infrastructure is no exception. This report provides evidence and recommendations for a net-zero roadmap. The material presented here is largely derived from a literature survey. It will be updated in 2023 with material from proof-of-concept studies and workshops to be held later this year. Actions that will be tackled by the project in future reports are indicated with blue boxes throughout this section

This report is intended as advice to UKRI DRI stakeholders. Many of the actions needed to deliver real change in the carbon footprint are outside the direct control of UKRI, so dealing with the areas of indirect control will be vital. Broadly speaking, we can think of these in terms of team activities, in which UKRI needs to work with partners within the institutions that host the UKRI DRI, and crowd activities, in which the UKRI DRI needs to work with the commercial and public sector, nationally and globally. The fact the the UKRI DRI cannot directly control the crowd activities does not mean that there are no opportunities for leadership. If anything, the reverse is true: in confronting net zero it is leadership in the crowd that is particularly important. Providing leadership in the crowd is business-as-usual for UK scientists. It was, for instance, a British scientist, John Houghton, who led the first three IPCC reports which laid the foundations for the global adoption of a net zero target.

The 'net zero' objective is often treated as an objective and physically measurable target, but there is an increasing body of literature treating it as an emerging social norm (see discussion in §**??** below). This brings risks, challenges and opportunities. The central challenge can be posed in terms of the need to meet the expectations of a social norm that is evolving rapidly in response to the developing climate emergency.

There is a great opportunity for UKRI here to deploy the full range of knowledge across the research sector to understand.

> The science is unequivocal: a global increase of 1.5° C above the pre-industrial average and the continued loss of biodiversity risk catastrophic harm to health that will be impossible to reverse.
> …
> Targets are easy to set and hard to achieve. They are yet to be matched with credible short- and longer-term plans to accelerate cleaner technologies and transform societies. *Atwoli et al. (2021)*

Nevertheless, the total carbon footprint of the UKRI DRI is tiny in comparison with the IT sector as a whole, and the whole sector is a small component of the global emissions. The limited scale of potential emissions reductions does not create a significant platform for UKRI to demonstrate leadership, but there is potential in the breadth and excellence of the academic community in UKRI which can be brought to address the problem acting as an agent of change (cf. Radinger-Peer and Stoeglehner 2013).

The net zero target has a clear objective meaning when applied to global emissions, but precise interpretation becomes ambiguous and controversial when applied to organisations because of fundamental ambiguities about allocation (§2.6) and compensation measures through offsetting and capture (§3.9). On deeper analysis, it becomes clear that the objective of exerting leadership is a safer guiding principle than any specific quantitative metric.

The UKRI DRI, and UKRI generally, is already showing leadership in addressing the challenge of the climate emergency. However, it is clear that there is a growing urgency as the "change" in climate has moved from crisis to emergency and some start to talk about catastrophe. The UKRI DRI should take steps to provide leadership in the global transition using both quantitative and qualitative approaches, avoiding risks associated with a narrow focus on any single metric (§3.2).

The overwhelming majority of emissions associated with the UKRI DRI are outside the direct control of UKRI (§2.5, §1.5). The largest component comes from generation of electrical power, and the power is procured not by UKRI but by the hosting organisations. The next largest components are procurement of servers and data transfers outside the data centres, though both are hard to quantify precisely. Procurement rules are set by broader institutional policies and constrained by competitive forces from the commercial world. It is clear that better quantification of the carbon footprint is important, but also that effective measures to reduce the footprint can be taken on the information available now.

There are many areas where the UKRI DRI has opportunities to exert leadership. For example, as operators of machine rooms with a significant power footprint, they should work with other major power users in the UKRI owned and majority funded research infrastructure (e.g. the particle accelerators at the Rutherford Appleton Laboratory) to ensure that the policies around the purchasing of power and the offsetting of emissions associated with generation and delivery of power (§3.2.5) are dealt with in a way which demonstrates leadership.

The UKRI DRI is undoubtedly a strong and hugely influential agent of change in UKRI. When discussing the transitions that are needed to address the Net Zero Challenge we are not talking about a system which would otherwise be static.

The most cost-effective approaches to net zero typically involve greater degrees of cooperation and lower degrees of potential direct influence. For instance, it makes little physical sense to buy equipment manufactured in a factory driven by coal-power and then compensate for the emissions through expensive carbon sequestration technologies, but, in unfavourable scenarios, the UKRI DRI may not be able to source appropriate equipment from cleaner sources.

PROJECT ACTION 1: Scenarios

Need to set out an initial approach to scenarios here, including both those in which UKRI can play a leading role, with others, in establishing the level of global cooperation needed to implement the most cost effective solutions and those in which UKRI can take a lead and implement changes within their own area of direct influence.

It is now well established that the organisations buying material from factories in countries with potential weak regulations have responsibility for ensuring that certain minimum standards are maintained, especially with regard to child labour and modern slavery.

Many institutions are prey to the temptation to consider scope 3 emissions as being in some sense less pressing to deal with. They are outside the direct control of the institution, it might be reasoned, and so not their direct responsibility. In commercial activities, however, the institution footing the bill cannot escape responsibility. Failure to account for scope 3 may well result in actual emissions going up despite strenuous efforts to clean up activities which are on site.

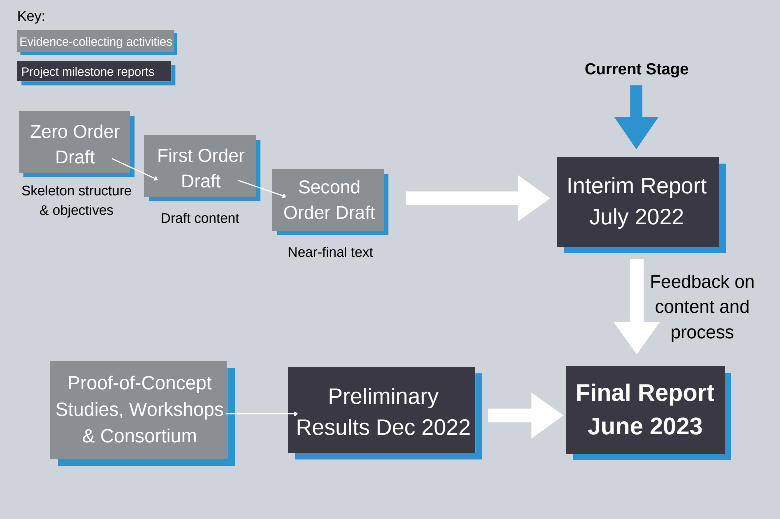
PROJECT ACTION 2: Clear statement of social responsibility

There is a need to formulate a statement on social responsibility. The UKRI DRI should recognise the social cost of carbon emissions. Estimates of the social cost of carbon, which reflects the projected cost to society of carbon emissions, are currently substantially higher than prices associated with offsetting or emissions trading schemes.

1.1.1 Report Development and Review

In order to achieve a good degree of community engagement, the development of the report includes multiple review stages shown in Figure 1.1. The review process for the interim report has a short time-line and, because of the challenging project schedule, limited time for review. The experience of generating this report will, however, feed into the design and implementation of a more extended review period for the final report.

Figure 1.1: Workflow for the preparation of the final project report. This document is the interim project report. The production of the interim report includes three review phases to allow plenty of opportunity for feedback on the structure and approach as well as review of the content. The production of the final report will take a similar approach, informed by feedback and taking advantage of an expanded time frame and additional input from other project activities.



PROJECT ACTION 3: Final review process

- Set a timetable for the final report review stages.
- Generate a lessons learned document for the interim report
- Create a timetable of critical meetings for input and decisions around the final report.

1.2 Leadership and Responsibility

> ❞ If we fail to identify and address greenwashing, we allow ourselves false confidence that we are already addressing the causes and treating the symptoms of the climate crisis *Howard Boyd (2022)*

The Net Zero UKRI DRI target cannot be achieved through technological

innovation alone, organisational change and transformation is also needed (§1.3). Our focus is on the footprint of the UKRI owned and majority funded digital research infrastructure, which does not fall under a single governance structure (§2.3). Instead, we have distributed responsibility spread between UKRI and the Universities, and there are important barriers in place to guarantee the independence of the Universities.

We start by setting out some assumptions about the nature and scope of the leadership challenge, then review a few potential role models.

The following elements will be important components of the leadership role:

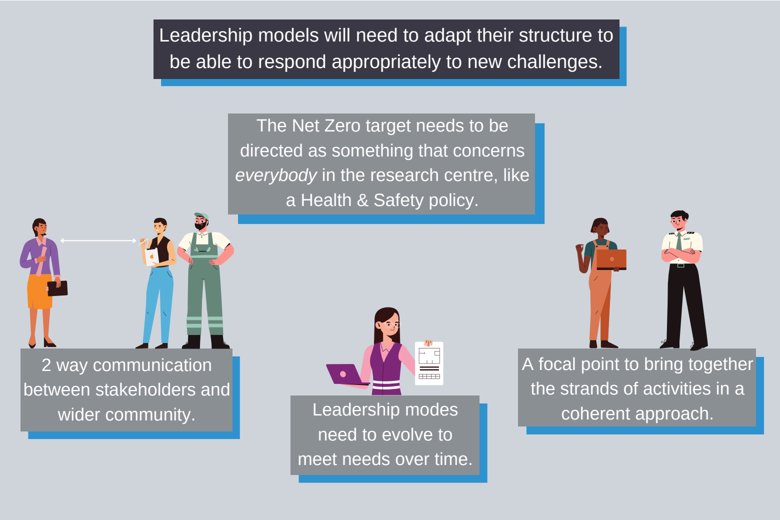
1. We will deliver on Net Zero, as we deliver on financial responsibilities, health and safety etc.
2. There are opportunities for leadership associated with ownership, with partnership and with being an active member of a community, and the UKRI DRI needs to exploit all three areas of leadership.
3. There is huge uncertainty in terms of the technology, the societal and the political context. The leadership model will need the capability to respond appropriately to new opportunities and challenges (§1.1).
4. Stakeholder interactions and community engagement are crucial because of the distributed decision making and societal responsibility.
5. The climate crisis is going to become more topical as climate change progresses (§2.3).
6. Adoption of best practise should take place in early stages of the roadmap (§1.7).
7. The roadmap needs to cover the whole chain, much of which is out of the direct control of the UKRI DRI, or even UKRI (e.g. being a responsible citizen, lobbying, etc.).
8. Multi-year planning will be essential (short, medium and long-term).
9. Establishing a leadership function will take years – need a learning and adaptable structure.
10. Change and transformation management will be needed (§1.3).

Different styles of leadership are possible, and will be relevant in different contexts (see Figure 1.2).

PROJECT ACTION 4: The project will convene a stakeholder meeting to review leadership options

Designing a leadership structure which can span Universities and Research Councils is clearly beyond the mandate of the project team, but we can convene a meeting to discuss options. Examples from among the role models reviewed here include, for example, the creation of an independent body through a Parliamentary Select Committee report or via a simple stakeholder decision.

Figure 1.2: Different leadership styles.



Leadership models will need to adapt their structure to be able to respond appropriately to new challenges.

The Net Zero target needs to be directed as something that concerns *everybody* in the research centre, like a Health & Safety policy.

2 way communication between stakeholders and wider community.

Leadership modes need to evolve to meet needs over time.

A focal point to bring together the strands of activities in a coherent approach.

1.3 Efficiency and Rebound

Efficient use of resources is clearly important when there are growing concerns about limitations on the supply of resources, but efficiency does not automatically lead to reductions in demand. Brockway et al. (2021) estimate that, across the economy, rebound effects which arise when greater efficiency boosts demand, will wipe out half of the expected gains from improved efficiency (see discussion of Jevons' Paradox in §2.12).

> It is wholly a confusion of ideas to suppose that the economical use of fuel is equivalent to a diminished consumption. The very contrary is the truth. As a rule, new modes of economy will lead to an increase of consumption according to a principle recognised in many parallel instances
>
> *Jevons (1871)*

.

In purely economic terms the rebound effect would be seen as positive, leading to an enhanced long-term return on investments in efficiency. In the context of sustainability, however, this effect can undermine attempts to preserve resources through efficiency gains.

The Jevons' Paradox is a consequence of the catena:

1. Cost of production determines supply;

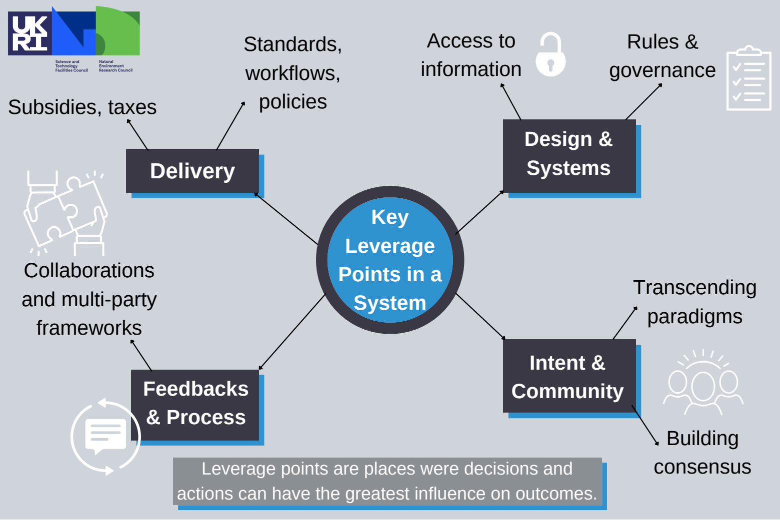
2. Supply determines final degree of utility:
3. Final degree of utility determines value.

In the Jevons analysis, the total demand will be determined by the balance between value and cost. Attempts to accurately identify the true cost of high energy use may be self-defeating, with many studies showing that adoption of a single metric can distort policies.

From the Jevons perspective, advances in energy efficiency lead to cost reductions which create more demand and can result in a net increase in energy use (also known as the rebound effect). In order to counter the feedbacks that can lead to such a rebound we need to look outside the machine room.

1.3.1 Protecting against Rebound

Figure 1.3: The four-realm concept of leverage points developed by Abson et al. (2017) formalises the stages between establishing goals and intentions and final implementation.



Recent reports from IPCC and IPBES (see §3.2.2) discuss the importance of considering multiple areas of action which can address the overriding objective of achieving net zero and then continuing to stabilise climate and the life-supporting biosphere. The areas of action have been analysed in terms of leverage points.

> Leverage points [are] places in complex systems where a small shift may lead to fundamental changes in the system as a whole
>
> *Abson et al. (2017)*

For complex multi-institution organisational structures with strong community engagement in decision processes, the journey from establishing a goal to achieving delivery is a complex one (Figure 1.3). Woiwode et al. (2021) argue that that Intent and Design are "deep" leverage points which must be used in order to achieve real transformation in an organisation and avoid the kind of policy failure predicted by the Jevons' paradox.

The Delivery realm includes the actions which can be taken by the UKRI DRI with a degree of independence, but these are also the actions which are considered by Woiwode et al. (2021) and others to have low leverage: that is, they will have low or moderate effect in the long term. The realms of Process, System, and Community require joint action with other UKRI and societal actors. The realm of Community includes actions which engage directly with the aspirations and concerns of individuals, independently of the organisational attachments. This is the realm in which organisations such as NC3Rs and Julie's Bicycle operate.

1.4 Arithmetic of Net Zero

The carbon footprint of the UKRI DRI is dominated by the emissions associated with the electricity supply. These can be characterised by an annual power consumption, for example JASMIN has an annual power consumption of about 1.5 GWh. This compares with a Typical Domestic Consumption Value (TDCV) OFGEM (2020) for a medium UK household in 2020 of 2.9 MWh.

The carbon footprint associated with loading a web page into a browser can be calculated using the Wholegrain Digital site. The CEDA home page, for instance, is mid-ranking with 1 g of CO_2 per page view. This would equate to around 1 tonne per year. Some savings are clearly possible (in an extreme case, the bare-bones approach of the Google search page yields a footprint of just 0.09 g CO_2), but these will be minor compared to the 400 tonne pa footprint of the JASMIN service. Greenwood (2019) gives some tips for improving website efficiency. CISCO (2019) estimate that 80% of global internet traffic by volume is due to video streaming in various forms.

The consumption is related to the carbon footprint through the carbon intensity. We consider three basic approaches to quantifying carbon intensity discussed in §2.6. Typical values are 213 g/kWh for the representative national average, 84 g/kWh for the location based carbon intensity in the North West on August 5^{th}, 2022, at 11:45 am (Carbon Intensity API), and down to zero for the contract based approach.

In 2020 the ARCHER supercomputer delivered peak performance of 2.5 PFlops with power consumption of 3.3 MW (Top 500 2022) (the average power draw in operation is significantly lower, close to 2MW, Alan Simpson, personal communication).

PROJECT ACTION 5: Authoritative information

UKRI DRI will need to ensure that stakeholders have access to authoritative information to back policy implementation. Many key parameters are continually evolving. Consistency in stakeholder decision making can only be achieved if there is a consolidated source of relevant information. The effort to achieve this may be modest, but it will be more efficient to have a single, authorised activity collecting and sharing information, rather than having multiple sources. The project will develop specific proposals through continued stakeholder engagement.

1.4.1 A standard for information exchange?

There are several possible approaches to defining the carbon footprint of the electricity which is at the core of the net zero data centre challenge (2.6). Each approach has some advantages. The fundamental problem, however, is not about deciding which is best for us, but the more intractable problem of arriving at global agreement so that everyone can reliably exchange information of carbon budgets, just as we all have a common understanding of money.

PROJECT ACTION 6: Information exchange

The project will discuss technical options for standardising information exchange.

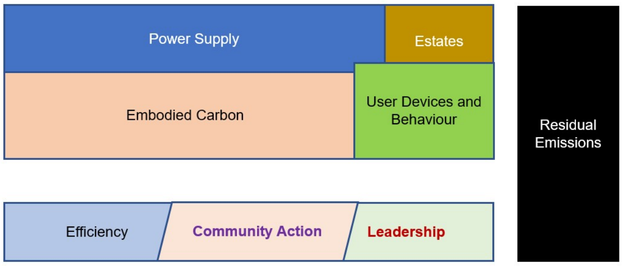
1.5 Challenges and Emission Scopes

The international reporting framework for carbon emissions is set in the context of three reporting scopes (§2.4). The first and second scope refer to the footprint associated with, respectively, emissions on site and emissions associated with the supply of electricity to the site. Scope 3 deals with a very broad range of additional emissions associated with both upstream activities such as procurement and downstream activities associated with service delivery. The scope 3 emissions associated with purchased goods are generally referred to as embodied carbon. The downstream emissions may be equally important (e.g., if a company is selling fossil fuel then the consequences of their customers burning that fuel are the downstream scope 3 emissions of the seller). The scope 3 emissions are defined in terms of the value chain of an organisation. See further discussion in §2.4 below.

PROJECT ACTION 7: Challenge areas

The project needs to clarify the nature of the four challenge areas. E.g. in dealing with embodied carbon, develop contractual arrangements which ensure clarity about the carbon footprint of purchased ICT equipment and work with suppliers to reduce the carbon footprint by 75% by 2030 (see Figure 1.4).

Figure 1.4: The net zero target can be split into four challenge areas.



1.6 Embodied Carbon and Scope 3 Emissions

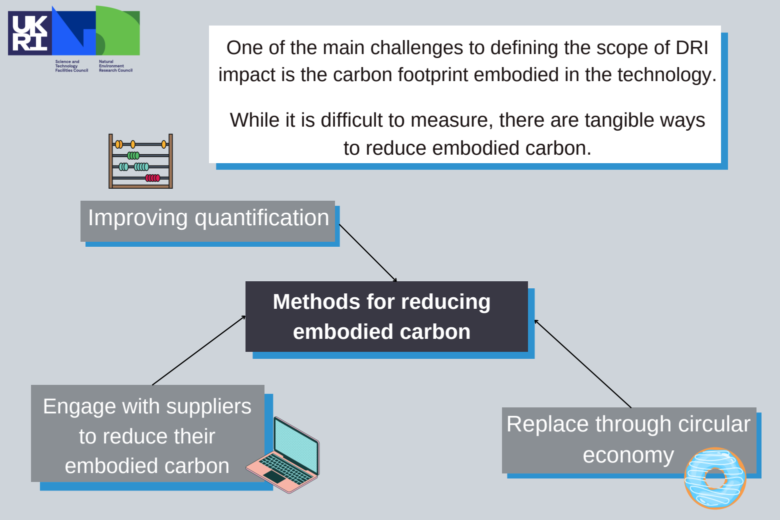
There are many difficulties in defining the scope of the impact of digital research infrastructure. Shehabi, S. Smith, et al. (2016) provide a useful taxonomy based on a range of sources. Potential impacts include increased energy consumption due to enhanced economic growth. Fortunately, there is now evidence that economic growth and energy consumption in the UK economy are now decoupling. Nevertheless, it is clear that work supported by the UKRI DRI should respect the ambition of the Net Zero commitment and should take steps to avoid promoting activities which lead to high carbon emissions. Approaches to addressing scope 3 are summarised in Figure 1.5.

1.7 Best Practice

Hale et al. (2022) review targets set by 203 countries, 806 states and regions, 1170 cities and 2000 companies. Among those entities that have net zero commitments, they find a wide range in robustness. Key frameworks are set by the UN Race to Zero (UNFCC) and Science Based Targets (SBTi 2020; SBTi). SBTi call for a 90% reduction in emissions, but it is not clear how this relates to ideas of equity. There are many calls for “real zero” rather than“net zero” (Stabinsky, Bhatnagar, and Shaw 2021; Thunberg 2020).

UK Government (2021) announces a new rule requiring companies bidding for major Government contracts to have a net zero target of 2050 or sooner. The 6th UK Carbon Budget suggests, in a balanced pathway, an approximately 4-fold reduction in carbon intensity over this time period.

Figure 1.5: The challenge of embodied carbon can be addressed by improving quantification of the embodied carbon, by working with suppliers to reduce known sources of embodied carbon and by working towards a circular economy (§2.8).



One of the main challenges to defining the scope of DRI impact is the carbon footprint embodied in the technology.

While it is difficult to measure, there are tangible ways to reduce embodied carbon.

Improving quantification

Methods for reducing embodied carbon

Engage with suppliers to reduce their embodied carbon

Replace through circular economy

PROJECT ACTION 8: Clarification of Best Practice

The project needs to do further work to clarify best practice or an approach to establishing best practice. The relevant expertise lies in the University sector, rather than within UKRI, so we envisage a consultation process. This should cover aspects of best practice illustrated in Figure 1.6.

1.8 Lessons from the Net Zero Scoping Project

The Net Zero UKRI DRI Scoping project is engaging with a broad range of stakeholders and bringing together new multidisciplinary teams to investigate the challenges at the confluence of two immense societal transformations: net zero and virtualisation. In addition to the technical outputs, there will be lessons learnt from the process and these will be reported on in full in a later report.

Figure 1.6: Best practice needs to be adopted in all areas of activity, not only in performance, but also in the development of technical capability and staff competence.

What does best practice look like?

Vision and potential

Sharing within the UKRI community

Staff competence

Experience

Development of technical capability

Ethics

Knowledge

Best practice needs to be adopted in all areas of activity.

1.9 UKRI and Net Zero

This report sets out recommendations and a pathway for the implementation of the UKRI Net Zero strategic ambitions within the Digital Research Infrastructure. The ambition is interpreted broadly: the overall aim is to eliminate carbon emissions from UKRI operations by 2040 not only as a necessary contribution to the national Net Zero target but also reflecting the role of UKRI in leading innovation and societal change.

The UKRI Sustainability Strategy (UK Research & Innovation 2020) sets out the target of net zero emissions by 2040, a decade in advance of the UK national target of net zero by 2050. The strategy includes the establishment of a carbon fund in 2021 to support emissions reductions in UKRI operated infrastructures.

A compelling science case for supercomputing in the UK is presented by Wilkinson et al. (2020a).

1.9.1 Scenarios

Scenarios for implementation of the national net zero ambition have been provided by Zero Carbon Britain (Allen and James 2019; CAT 2019; Climate Change Committee 2019). While there are differences, all see a major reduction in use of grassland for livestock as being a key element of the transition, enabling large areas of land to be used for carbon capture and biofuels. Poux and Aubert (2018), looking at a scenario for Europe, propose changing to less intensive agriculture rather than taking land out of use. CCC (2021) foresee an approximate doubling of UK national electricity supply between 2020 and 2050. The additional capacity in this scenario is needed to replace direct use of fossil fuels in transport and heating, so that the power supply available to existing electricity consumers is, in the national aggregate, expected to remain level. A similar pattern of change is seen in Allen and James (2019), though expressed in terms of energy use rather than generation.

The International Energy Agency (IEA) have published a global scenario for Net-Zero global electricity generation sector by Bouckaert et al. (2021). The UN (2022) define “net zero” as “cutting greenhouse gas emissions to as close to zero as possible” and taking steps to re-absorb the rest, but do not give precise information on what should be considered as possible. Some, particularly from communities with extremely low per capita footprints today and high expected impacts from climate change, see the logical interpretation as being “leave the oil in the soil, leave the coal in the hole” (Stabinsky, Bhatnagar, and Shaw 2021).

1.9.2 About the Net Zero DRI Scoping Project

The UKRI Net Zero Digital Research Infrastructure Scoping Project will:

- Collect evidence to inform UKRI Digital Research Infrastructure Investment decisions.
- Provide, as recommendations for UKRI and their community, an outline roadmap for achieving carbon neutrality in the UKRI DRI by 2040 or sooner.

- Enable UKRI to play a positive and leading role in the national and global transition to a sustainable economy.

The infrastructure elements in scope include all the UKRI owned and majority funded digital research infrastructure. The role of connected devices will also be considered, both in the context of the carbon footprint that users need to incur to connect to the infrastructure and as an indication of the direction and speed of technological change.

In addition to the roles of operator, procurer and service provider alluded to above, UKRI and their research community have a critical role as influencers and innovators. As a customer for computer hardware UKRI has a tiny leverage in the global market, but the influence of UKRI science on national and global attitudes to sustainability in general, and the net zero target in particular, is immense.

This project does not aim to place limits on researchers, but to develop a framework which can enhance the contribution that the community makes to a huge societal challenge. Just as national infrastructure investments are considered in the context of expected return on investment, we will consider the expected benefits of resources, including potentially limited power and offsetting capacity, allocated to digital research infrastructure.

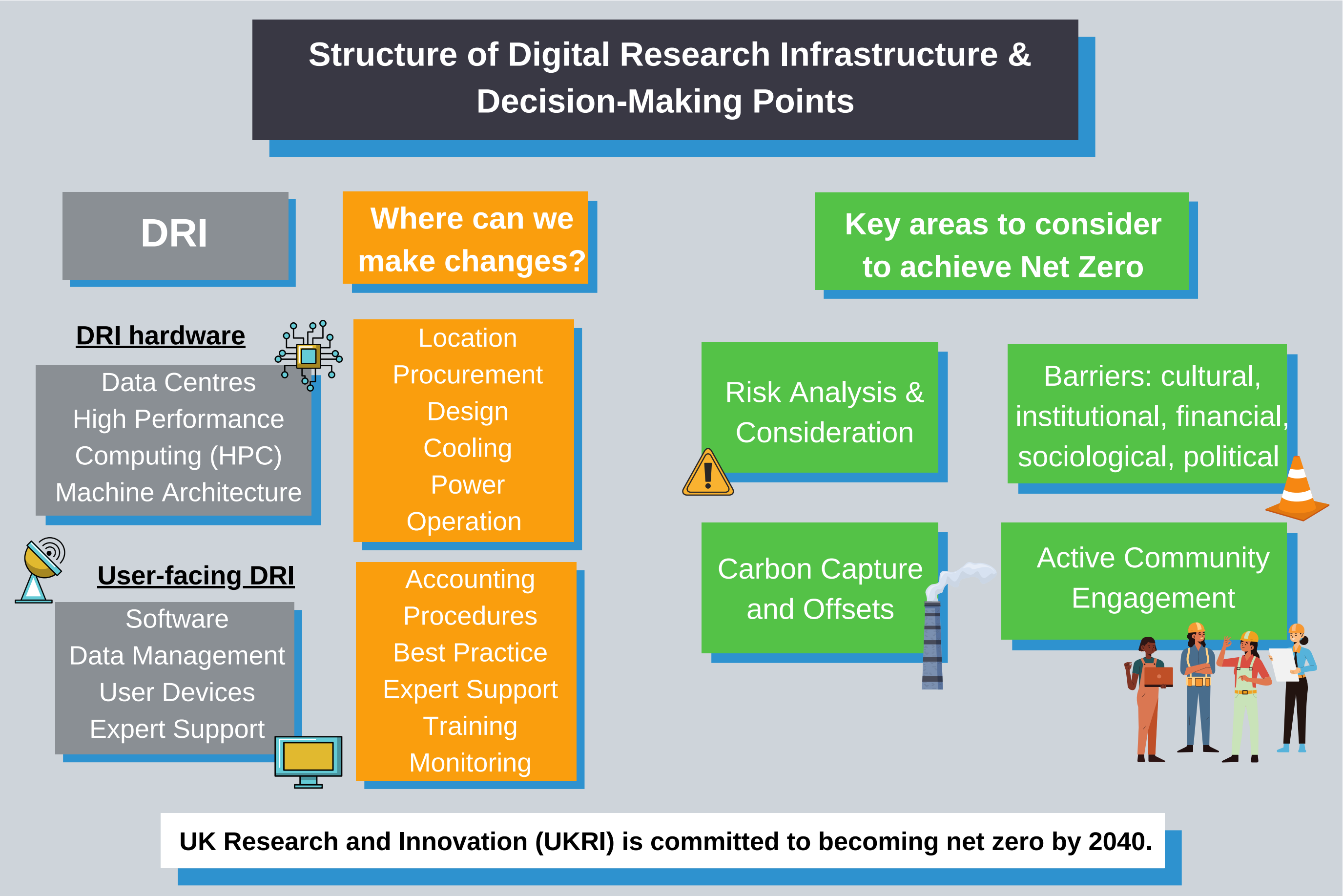
A substantial component of the current carbon footprint of the digital research infrastructure is electricity. We will explore measures to reduce electricity usage as well as measures aimed at procuring electricity with a low or zero carbon footprint. The manufacture of hardware also has a substantial footprint, and for laptops and phones this is the dominant component of the footprint. For well-run data centres, on the other hand, the electricity use tends to dominate, but the footprint of manufacturing, which includes both electricity to drive factories and emissions of volatiles released in integrated circuit manufacture remains to be addressed.

Measures to extract carbon dioxide from the atmosphere will also be considered, as a means to balancing any unavoided emissions.

With the role of UKRI as an agent of change (cf. Radinger-Peer and Stoeglehner 2013) in mind, all aspects of the project will be considered from a broad perspective, and will acknowledge the risk that policy intended to reduce emissions can often simply displace them.

We will look at the part that changes in behaviour can play in delivering net zero emissions (see Figure 2.1), and at the experience in other areas of delivering change in the research culture to adapt to societal objectives and expectations.

Figure 1.7: Overview of topic of interest.



Structure of Digital Research Infrastructure & Decision-Making Points

DRI

Where can we make changes?

Key areas to consider to achieve Net Zero

DRI hardware

- Data Centres
- High Performance Computing (HPC)
- Machine Architecture

- Location
- Procurement
- Design
- Cooling
- Power
- Operation

User-facing DRI

- Software
- Data Management
- User Devices
- Expert Support

- Accounting
- Procedures
- Best Practice
- Expert Support
- Training
- Monitoring

Risk Analysis & Consideration

Barriers: cultural, institutional, financial, sociological, political

Carbon Capture and Offsets

Active Community Engagement

UK Research and Innovation (UKRI) is committed to becoming net zero by 2040.

The evidence collected will take various forms, including direct quantitative evidence collected from current facilities, an extensive literature review, community workshops, proof-of-concept studies and other forms of expert consultation.

The UK is embarking on a transition to a sustainable economy with a target for net-zero carbon emissions. The evolving nature of the net-zero challenge for digital technology and lack of cohesion in the research and user community is limiting both research and innovation developments and policy benefits. The net zero target clearly raises transdisciplinary, transgenerational and transnational issues. Consequently, stakeholders are faced with multiple evidence streams leading to inconsistent analysis and inefficient application of new science to support policy and action. To address these challenges the programme will support a range of proof-of-concept studies and workshops.

1.10 Organisational Complexity

The UKRI Digital Research Infrastructure is a distributed organisation, majority funded by public funds. It is also a complex organisation in the sense that decision making is highly distributed with many independent but interrelated institutions and individuals taking part. For further discussion of the consequences of complexity, see §3.2.

1.10.1 Funding of the DRI

Public funding from the Treasury is delivered through BEIS, UKRI and UKRI's constituent Research Councils. The allocation of funds to operators is through science programs. The funds for capital investment and for operation of the services flow through different programmes within the Research Councils.

Funding decisions will depend on the ability of applicants to meet a range of criteria, including contributions to the broader UKRI objectives of delivering scientific excellence. Funding decisions for infrastructure investment are made through independent panels.

1.10.2 Operation of the DRI

The operation of the DRI is in the hands of numerous independent organisations. The facilities are located within Research Councils, Universities and in independent institutions such as EMBL-EBI. The flagship of the UKRI DRI is the ARCHER2 service operated by EPCC at the University of Edinburgh.

The UKRI DRI exists to support the UK scientific research community in their role of delivering research and innovation to advance knowledge and innovation to support the UK economy. Much of the work is funded through UKRI, but the decisions around funding allocations are distributed and operationally independent of decisions on investment in the DRI. There are also users in areas of policy guidance and implementation, e.g. from DEFRA and in connection with the COVID response.

Users of the DRI also have a complex interaction involving multiple independent decision centres. The process may start with a Principal Investigator (PI) creating a proposal for research work with an estimated allocation of resources needed from an HPC facility. The proposal will be evaluated by an independent review panel, judging both its scientific excellence and it's fit to aims set by the Research Council. The PI is unlikely to be a direct user of the DRI, that role usually being deferred to a post-doctoral research associate (PDRA) or Doctoral Student. The actual user may be involved in the proposal preparation or may become involved after approval of funding. The choice of algorithms and applications to be deployed in the project will be decided jointly between the project team, the review panel, any advisory bodies established in the project, and influenced by other actors in the research domain.

Chapter 2

Background

2.1 UKRI and Net Zero

This report sets out recommendations and a pathway for the implementation of the UKRI Net Zero strategic ambitions within the Digital Research Infrastructure. The ambition is interpreted broadly: the overall aim is to eliminate carbon emissions from UKRI operations by 2040 not only as a necessary contribution to the national Net Zero target but also reflecting the role of UKRI in leading innovation and societal change.

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2.1.1 Scenarios

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2.1.2 About the Net Zero DRI Scoping Project

The UKRI Net Zero Digital Research Infrastructure Scoping Project will:

- Collect evidence to inform UKRI Digital Research Infrastructure Investment decisions.
- Provide, as recommendations for UKRI and their community, an outline roadmap for achieving carbon neutrality in the UKRI DRI by 2040 or sooner.
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The infrastructure elements in scope include all the UKRI owned and majority funded digital research infrastructure. The role of connected devices will also be considered, both in the context of the carbon footprint that users need to incur to connect to the infrastructure and as an indication of the direction and speed of technological change.

In addition to the roles of operator, procurer and service provider alluded to above, UKRI and their research community have a critical role as influencers and innovators. As a customer for computer hardware UKRI has a tiny leverage in the global market, but the influence of UKRI science on national and global attitudes to sustainability in general, and the net zero target in particular, is immense.

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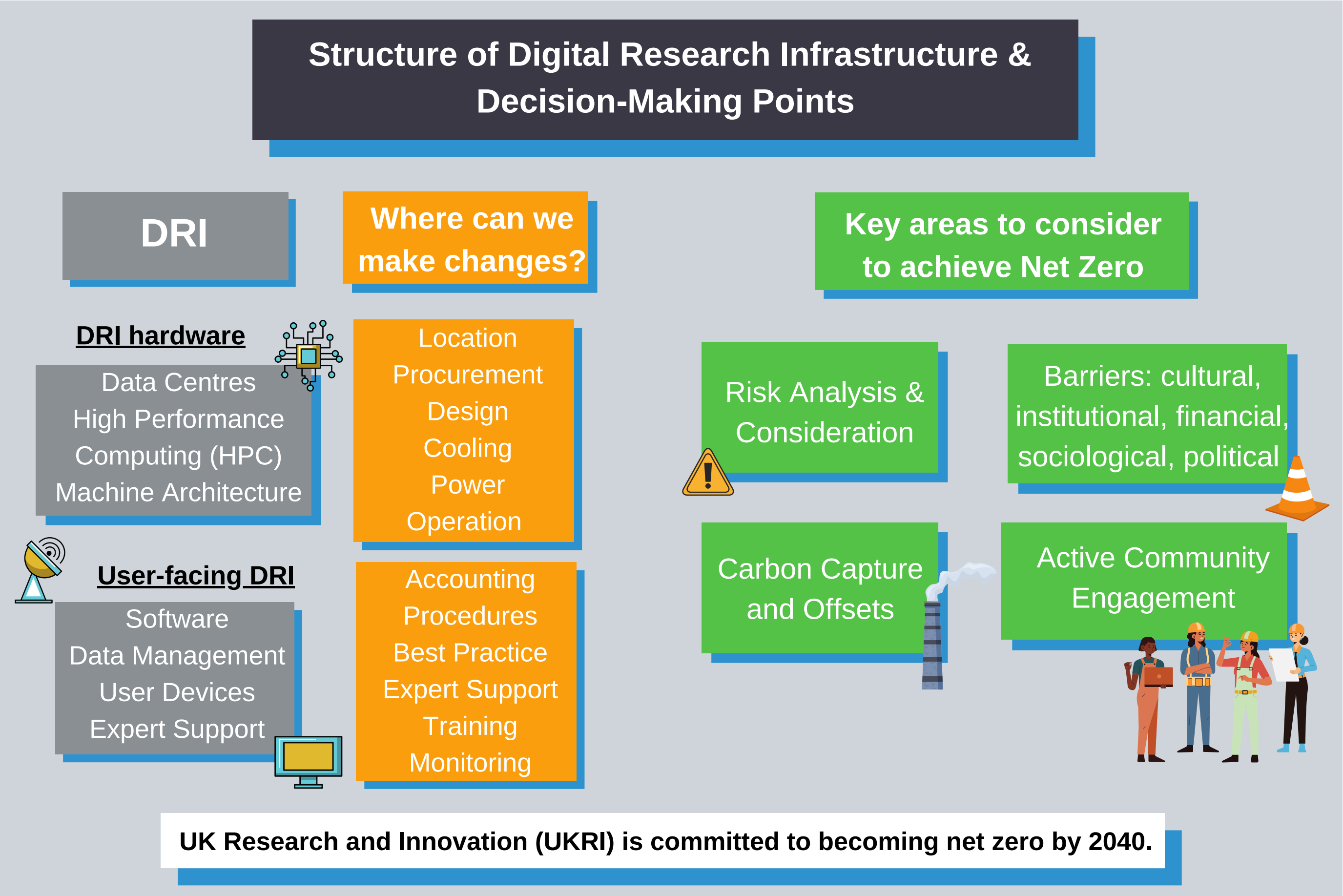

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High Performance Computing (HPC)
Machine Architecture

User-facing DRI

Software
Data Management
User Devices
Expert Support

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Location
Procurement
Design
Cooling
Power
Operation

Accounting
Procedures
Best Practice
Expert Support
Training
Monitoring

Key areas to consider to achieve Net Zero

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Users of the DRI also have a complex interaction involving multiple independent decision centres. The process may start with a Principal Investigator (PI) creating a proposal for research work with an estimated allocation of resources needed from an HPC facility. The proposal will be evaluated by an independent review panel, judging both its scientific excellence and it's fit to aims set by the Research Council. The PI is unlikely to be a direct user of the DRI, that role usually being deferred to a post-doctoral research associate (PDRA) or Doctoral Student. The actual user may be involved in the proposal preparation or may become involved after approval of funding. The choice of algorithms and applications to be deployed in the project will be decided jointly between the project team, the review panel, any advisory bodies established in the project, and influenced by other actors in the research domain.

2.3 The Digital Future in Research

The UKRI Digital Research Infrastructure (UKRI-DRI) supports a huge range of research. It includes high performance computing to support extreme simulations, multiple mid-range computing facilities supporting local or specialist communities, and institutional machine rooms supporting research departments and teams. Wilkinson et al. (2020a) set out a case for a capacity at the high performance end founded on research requirements, discussing key applications in the realms of astronomy, molecular physics, climate, extreme weather, the solid Earth, computational biology, medicine, digital humanities and mathematics.

A different perspective is given by Bichsel (2012), reporting results from an EDUCAUSE survey of US institutions showing that demand for digital research computing is driven in part by a competitive element: “having research computing resources makes an institution more competitive in recruiting and retaining faculty with research computing needs”.

BBSRC (2020) show that the proportion of ‘data-rich’ submissions to the BBSRC Responsive mode funding calls has risen from just over 20% in 2006 to over 50% in 2018. The NERC Digital Strategy (NERC 2022) announces an ambition to use “digital technologies to transform our understanding and management of the natural world”. Both BBSRC and NERC stress the importance of people and skills. The importance of people and skills is also highlighted by the ExCALIBUR programme (see also ExCALIBUR 2021).

There is a broader trend linking technological progress with economic growth, reductions in pollution and improvements in health outcomes, at least in OECD countries (Nghiem et al. 2021, – though these authors do not, unfortunately, include greenhouse gases in their analysis).

The DCMS digital strategy (DCMS 2022) sets out the national context for the digital sector, with a focus on the positive role that the digital sector can play in enabling the transition to net zero.

Stein (2008) discuss the role of cyberinfrastructure in genomics research, but two of their conclusions can apply equally across the whole academic endeavour:

> The most promising cyberinfrastructure systems combine a flexible, semantically driven framework for sharing information with a strong social and community-building component.
>
> The emerging biology cyberinfrastructure has the potential to be a great leveller, giving all researchers equal access to data and compute facilities regardless of their geographical location or data-handling abilities.

Hanson and Ludwig (2010) discuss the growing role of cyber infrastructure in the arts and humanities, reflecting a global movement of digital services from the fringes to the centre of society.

2.3.1 The Tiers of Digital Infrastructure

Digital research infrastructure can range from sophisticated systems with multiple levels of redundancy and load balancing to relatively simple stacks of servers. It is common practise to categorise the different systems in to different "tiers". In the context of European research infrastructure, a 4-tier system is used, ranging from "best across a continent" systems ranked as Tier 0 to institutional systems at Tier 4 (e.g. EPCC 2017; Wikipedia 2022b, : this is an emerging standard, there does not appear to be a formal definition). Ranking of commercial services, on the other hand, deals with the levels of service and ranges from, at the high-ambition end, Tier 4, with services supported at multiple sites allowing continuity of service when a whole machine room is taken out of action down to Tier 1 with basic uninterruptible power supply (UPS) and back-up generator to ensure reasonable continuity of service (UptimeInstitute 2022b).

2.4 The Greenhouse Gas Protocol and Emission Scopes

The Greenhouse Gas Protocol was jointly convened in 1998 by World Business Council for Sustainable Development (WBCSD) and World Resources Institute (WRI). They provide a range of tools to support businesses seeking to quantify and manage their carbon footprint. They provide a widely used definition of 3 "scopes" of carbon emissions (GHG Protocol 2004, 2011, 2013, 2019):

- Scope 1 emissions are direct emissions from owned or controlled sources.
- Scope 2 emissions are indirect emissions from the generation of purchased energy.
- Scope 3 emissions are all indirect emissions (not included in scope 2) that occur in the value chain of the reporting company, including both upstream and downstream emissions.

Within the GHG Protocol, the concept of the emissions consolidation approach gives an organisation a choice of 3 approaches to defining the boundaries of the emission scopes: based on 1. equity share, 2. financial control and 3. operational control.

There is some discussion of the ethical aspect of evaluating scope 3 emissions in a discussion of search engine choices by Reyes-Menendez et al. (2018). They note that the dominant element of the carbon footprint of a google search is the scope 3 element associated with the user laptop. Google (2021) exclude this from their figures, though the current GHG Protocol specification implies that it should be included. Google is, however, correct in stating that the data centre element of the footprint is small in this case, contrary to a huge number of online discussions attributing the footprint of the overall process to data centres. Figures for search footprint from online sources, such as Sterling (2009), appear to be based on power-hungry user devices from around 2000. Since then, most users devices have shifted to low-power technology and the primary footprint of the user activities is associated with the purchase of devices.

Cambridge University (2022b) and Google (2021) both distinguish between "Location-based" and "Market-based" scope 2 emissions in their annual reports. For Google, "location-based" scope 2 emissions which are more than 5 times higher than the "market-based" figure. Their market based emissions have declined steadily 2016 and 2020 while their location based emissions have almost doubled over that period. The "location-based" emissions are related to the physical power generation and delivery infrastructure which is delivering electricity to data centres. Cambridge University use a grid averaged factor for their "location-based" figure (Cambridge University 2022a), which may differ from a more local evaluation as discussed further in §2.14.4 below.

The GHG Protocol emission scopes form the basis of reporting requirements for UK companies and limited liability partnerships covered by the DEFRA (2019) guidelines. For Non-Departmental Public Bodies Greening Government Commitments (DEFRA 2021) are also relevant. The list of sub-categories of scope 3 defined in the GHG Protocol is listed in Table 2.1.

Table 2.1: Scope 3 emissions categories from the GHG Protocol

Stream	**Group**	**GHG Protocol Categories**
Upstream	Embodied	1. Purchased goods and services; 2. Capital goods; 3. Fuel- and energy-related activities (not included in scope 1 or scope 2); 4. Upstream transportation and distribution
	Waste	5. Waste generated in operations
	Staff travel	6. Business travel; 7. Employee commuting
	Leases	8. Upstream leased assets
Downstream	Products	9. Downstream transportation and distribution; 10. Processing of sold products; 11. Use of sold products; 12. End-of-life treatment of sold products
	Activities	13. Downstream leased assets 14. Franchises 15. Investments

Table 2.2: Illustration of partitioning between scopes along a value chain, taken from Oliver Wyman Forum (2022). In this idealised example the total footprint for each organisation is the same, but the partitioning between scopes changes.

	Coal extraction, processing and transportation company	Power generation company	Power transmission and distribution company	End consumer company
Scope 1	Emissions from the extraction, processing, and transportation of coal 5 t CO_2e	Emissions from the combustion of coal for power generation 100 t CO_2e	N/A (unless SF_6 is released from transmission and distribution)	N/A
Scope 2	N/A (unless electricity is used during coal mining and processing)	N/A	Emissions from electricity consumed during distribution and transmission to consumers 10 t CO_2e	Emissions from generation of electricity purchased and consumed by end consumer 90 t CO_2e
Scope 3	Downstream emissions from the combustion of coal sold to power generator 100 t CO_2e	Upstream emissions from extraction, processing, and transportation of coal 5 t CO_2e	Upstream emissions from the combustion of coal during power generation 95 t CO_2e	Upstream emissions from extraction, processing and transportation of coal and electricity consumed (i.e. lost) in transmission or distribution 15 t CO_2e

2.5 Key Elements of the Carbon Footprint

When dealing with regulatory and national reporting requirements, greenhouse gas emissions are categorised by scopes (§2.4) which reflect the positioning of the emitting activities relative to the governance and control structure of an organisation.

The link between reporting scopes and the organisational structure immediately confronts us with a problem in providing recommendations for a digital research infrastructure which is in the process of being established. From an administrative perspective it may be natural to consider the UKRI DRI emissions in terms of the reporting requirements of UKRI. This would immediately put the majority of emissions in scope 3.

Focus on scopes 1 & 2 could distort policy decisions, hence we adopt an activity based approach which looks at the operation of running a data centre and the steps needed to eliminate carbon emissions independently of issues about ownership. That is, we treat the UKRI DRI as a virtual organisation and, consequently, consider electricity usage in a UKRI-funded university facility to be equivalent to electricity usage in a UKRI facility.

Thus, we can look either at UKRI reporting scopes or aggregates of reporting scopes of the UKRI owned and majority funded services which comprise the UKRI DRI. The latter approach will aggregate, for instance, the power usage and the services delivered across all UKRI DRI services. This approach will provide an actionable view of the overall capacity and impact of the UKRI DRI.

Taking the facility-centred view, the dominant element of the carbon footprint will generally be the electricity supply (scope 2) with a significant additional element coming from embodied energy of computer hardware (scope 3). Scope 1 emissions (e.g. gas fired heating, diesel back-up generators, vehicles used by site staff) are generally small relative to the electricity supply and hardware footprints. When it comes to quantifying scope 2 and scope 3 emissions, specific values will depend on the allocation methodology adopted (§2.6).

When a reductive carbon budget approach is taken, reductions in the footprint associated with electricity consumption can be achieved either through reduction in electricity use or taking measures to reduce the Carbon intensity of electricity used. This approach suffers from the weakness of making policy options heavily dependent on arbitrary choices around the carbon intensity calculation methodology referred to above. Efficiency measures can be adopted to reduce the overall electricity use, but extreme care needs to be taken to avoid the rebound effect through which greater efficiency leads to demand growth which dominates over efficiency gains (§2.12).

Aujoux, Kotera, and Blanchard (2021) provide a detailed analysis of the carbon footprint of the Giant Array for Neutrino Detection (GRAND) project, and find the digital element dominates and is evenly split between data centres and user devices. Their projection for the future sees the hardware element becoming dominant in the future, albeit in a scenario which sees a 27-fold increase in carbon emissions of a time frame over which major funders are committed to a net decrease.

Some further examples are given in Tables 2.3 and 2.4.

Table 2.3: Some initial estimates on carbon footprints, covering some facilities and other items for comparison.

Item	Annual Power	Annual Scope 2 (kg)	Embodied (Scope 3) (kg)	Annualised Scope 3 (kg)	comment
JASMIN	1.5gWh	318,000	-	50,000	Based on grid-average carbon equivalent intensity of electricity generation (212g/kWh BEIS 2022) and sector-typical factor for scope 3 (16%)
Laptop	26kWh	8.3	321	80	Based on Dell Latitude E6530 DELL (2022), 4 year lifetime. Note, this is for the default system configuration.
Tree	-	-		-46	Based on 7.3 t ha^{-1} a^{-1} for poplars at 156 trees per hectare and a lifetime of 26 years (Cannell 1999).

Table 2.4: Some initial estimates on carbon footprints of a range of activities.

Item	Footprint	Comment
Search (service)	0.2g	Google search, ignoring user devices (Google 2021; Sterling 2009)
Search (activity)	7g	Google search using desktop
Simulating one year with a climate model (low resolution)	1 kg	Assuming around 10^6 mesh points (Balaji et al. 2017)
Simulating one year with a climate model (high resolution)	600 kg	Assuming around 10^8 mesh points (Balaji et al. 2017)
Scientific Publication	5.4kg	Case study at Dalian University of Technology (Song, Che, and Zhang 2016)
PhD	21 tonne	Achten, Almeida, and Muys (2013)
One hour of streamed video	16 g	Power use (0.077 kW) from Kamiya (2020) and 213 g kWh^{-1} from BEIS (2022). Kamiya also discusses much higher values which are widely cited and explains why they are unrealistic.
Regular Latte	400g	Maslin and Nab (2021) assuming dairy milk and air-freighted coffee

2.6 Allocation – or What is My Share?

When many users share products from one source, it can become unclear how much responsibility each of the users bears for the total environmental impact of the source. The concept of “allocation” is important in deciding how the footprint of a process, such as data centre operation or, more widely discussed, food production, should be distributed across many products. (e.g. see the report “Product Carbon Footprinting” Ernst and Young 2020). If a farm, for instance, is producing a combination of beef for human consumption, dairy products and meat for pet food, how do you decide how much of the carbon and methane emissions to allocate to each product?

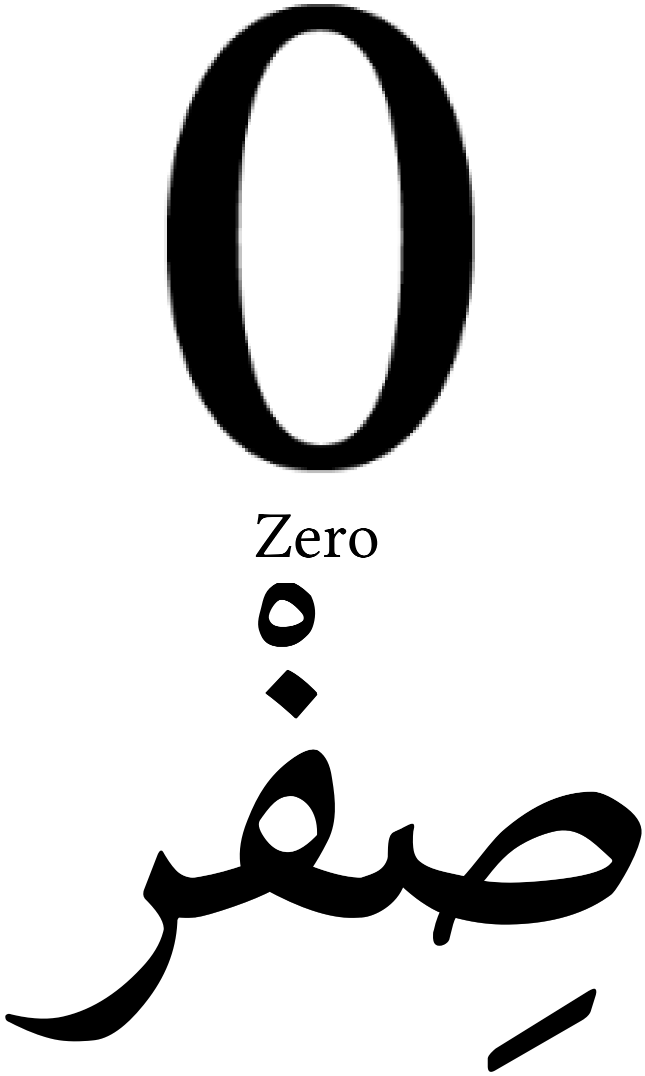
In particular, when it comes to drawing electricity from the UK National Grid we have a range of options for estimating our carbon footprint.

- BEIS (2021) suggest a blanket rate of 213g/kWh CO$_2$-eq[1]
- Carbon Intensity (Carbon Intensity API) (see 2.14.4) offer a service which allows users to track by the hour the carbon intensity of electricity in their region, calculated on the basis of data from plants delivering power into the grid at that time. At 9:17am on March 22nd, 2022, for instance, carbon intensity of power generation by region varies between 8 g kWh^{-}1 in the North East (dominated by nuclear power and imports from Norway) and 474 g kWh^{-}1 in the East Midlands (dominated by gas and coal). Note that Carbon Intensity use values of zero for carbon emissions from solar, wind, hydro and nuclear (Bruce et al. 2021). This neglects some emissions revealed in a full life cycle analysis (e.g. Pehl et al. 2017).
- Green Tariffs from UK electricity suppliers[2] offer customers promises of carbon neutrality on the basis of the contracts they have with generators.

PROJECT ACTION 9:

The UKRI DRI should exploit multiple metrics and use these to monitor responsibility for carbon emissions associated with a range of lines of influence. In particular, metrics based on location based, market based, and national average carbon intensity should be used to reflect the impact of the local demand on energy, the procurement of energy and the load placed on the national capacity. The Net Zero Roadmap should address all areas of influence.

Figure 2.2: The adoption of the concept of zero revolutionised scientific culture in Europe.



2.7 Net-zero and Actual-zero as Sustainability Targets

2.7.1 Zero as a Paradigm Shift

The introduction of zero (Figure 2.2) revolutionised scientific culture in Europe. The adoption of a net zero target heralds a similar deep change, marking a change from a gradualist approach attempting to address the climate crisis through incremental savings to a holistic approach targeting elimination of aggregate carbon emissions.

Zero as a mathematical concept started in the form as a placeholder in written representations of numbers, indicating an empty space. The first usage of zero as a number in its own right is attributed to the Indian mathematician Brahmagupta in the 7th century AD (Pogliani, Randic, and Trinajstić 1998). The use of zero was adopted by Persian and Arab mathematicians, and through their work arrived in Europe through their work.

Hogben (1989) remarks on the revolutionary impact of the humble zero (or "sunya" as it was first called in Hindi):

> The invention of sunya (zero) liberated the human intellect from the prison bars of the counting frame. Once there was a sign for the empty column, 'carrying over' on a slate or paper was just as easy as carrying over on the abacus…and it could stretch as far as necessary in either direction.

We are no longer evaluating carbon reduction measures against a range of potential alternative investment plans. Instead, we have the narrower, though still complex, question of balancing benefits of retaining residual emissions against the multiple costs of funding carbon extraction and storage to balance those residual emissions. This shift in perspective is a real revolution in the approach to climate impact mitigation.

The costs and implications of carbon extraction and storage in 2040 remain difficult to predict, but there are clearly defined physical constraints and opportunities which can be balanced against the physical constraints and opportunities for carbon emissions reductions.

2.7.2 Understanding the target

- Allen and James (2019), CAT (2019) - suggest 92% reduction in GHG emissions, similar to the 90% now recommended by SBTi, which might equate to 100% reduction in scope 2 (electricity) and 60% reduction in scope 3.

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[1] Often written as g CO_2-eq/kWh, but we keep to the SI interpretation of units and express the quantity separately from the units.

[2] In the UK the electricity suppliers are responsible for the contracts with the customers, but generally buy power from 3^{rd} parties and contract the National Grid to deliver the power

- Allwood et al. (2020) “We can’t wait for breakthrough technologies to deliver net-zero emissions by 2050. Instead, we can plan to respond to climate change using today’s technologies with incremental change. This will reveal many opportunities for growth but requires a public discussion about future lifestyles.” Allwood et al. also argue for “actual zero” emissions from electricity supply, but in their report this “actual zero” appears to neglect emissions associated with construction, maintenance and decommissioning of renewable power generation infrastructure. Eliminating direct emissions by combustion of fuel during power generation may eliminate 98% (e.g. see Harrison et al. 2010) but not 100%.

- Doyle and O’Mahony (2014) coin the phrase ”Nihil computing”, as opposed to ”net-zero” computing, for data centres which are run off entirely renewable resources separated from the grid. Their proposition is to combine renewable generation, batteries and demand management to fully avoid the need to draw power from the grid. Their approach shows considerable benefits from sharing work between geographically distributed data centres, taking into account latency constraints (e.g. not streaming videos from Ireland to California), but depends on an assumption that data centres can scale power consumption according to workload.

2.8 Circular Economy and Sustainability

The circular economy movement aims to drastically reduce embodied emissions and associated threats to sustainability by re-use of materials. The European Commission Circular Economy Action Plan provides some useful context (European Commission 2020). There are two companies trading IT equipment on circular economy principals in the UK: C2 IT; Circular Computing. Gåvertsson, Milios, and Dalhammar (2020) discuss the absence of any certification framework and its consequences. Schischke et al. (2020) discuss reuse of pre-consumer waste.

Although the specific challenges of net zero carbon need their own focus, there are linkages with other sustainability issues. If policy does not take this into account, carbon reduction targets may conflict with other objectives.

Bobba et al. (2020) and Ku (2018) provide a useful overview of the pathways through which a range of metals impact on ICT manufacture and on power supply.

2.9 Equivalent Carbon Dioxide

The “Net Zero” target refers not only to carbon dioxide, but all other anthropogenic greenhouse gas emissions associated with the manufacture, operation and decommissioning of digital research infrastructure. Of these, carbon dioxide is strongly dominant, but SF_6 (from power transmission) and PFC (per-flourinated compounds potentially released in integrated circuit manufacture, [§3.5]) are also of significance and will need to be addressed between now and 2040. These compounds have ex-

Table 2.5: Comparison of a range of different carbon prices

Item	Price (£ per tonne)	Price Date & Source	ΔPP
Ecosystem Storage	£5-25	Table 3.3	1-5p
Charcoal Storage in Soil	£300	§3.9	66 p
Deep Geological Storage	£900	See §3.9	£1.97
Market	£80	EMBER Viewer, 8th June 2022	17p
Social cost	£10000	Rogelj et al. (2018)	£21.93

tremely long atmospheric lifetimes, so that atmospheric levels will not re-equilibriate in this millenium, even if emissions are halted now.

The definition of equivalent carbon dioxide (CO_2e) depends on the specification of a timescale. Some gasses will persist in the atmosphere much longer than CO_2, others will be removed faster by natural processes.

The timescale of 100-years is often used. If we are aiming, at some point, to balance SF_6 and PFC emissions against CO_2 extraction from the atmosphere, we need to be clear about the timescale we use as a basis for our budgets.

For example, the Global Warming Potential (GWP) of SF_6, which is a ratio of the impact of a given mass of SF_6 to the same mass of CO_2, was estimated as $16,300$, $22,800$ and $32,600$ for timescale of 20, 100 and 500 years respectively (Forster et al. 2007). If we are interested in responsibility for the long-term impact, we should adopt the higher GWP associated with the longer timescale (implying that more CO_2 needs to be extracted to balance a given residual SF_6 emission).

This problem could perhaps be circumvented through adoption of SF_6 free substations (National Grid 2017).

2.10 Pricing Equivalent Carbon Dioxide

There are many approaches to attaching a price to carbon. The range of different prices reflects ongoing diversity in assumptions, processes and values that are applied to the sustainability challenge, with prices varying by close to a factor of 1000 between the highest and lowest.

In order to ease interpretation we also define and introduce here the quantity ΔPP which is the Change in the Price of a litre of Petrol resulting from adding the carbon cost. This is calculated assuming 2.19352 kg CO2 equivalent per litre, as cited for “Petrol (average biofuel blend)” by BEIS (2022).

Dietrich (2022) recommend avoiding reliance on carbon offsets because they are “problematic due to financial risks and quality and availability issues”.

The suggestion from Rogelj et al. (2018) that a social cost equivalent to almost

Table 2.6: Description of different approaches to costing carbon

Item	Description	Strength	Weaknesses
Ecosystem Storage	Removal of carbon from the atmosphere into biological storage through, e.g., planting trees.	There are many programs and projects using this approach, creating a well developed market.	It is difficult to quantify additionality and stability of carbon storage
Charcoal Storage in Soil	Conversion of carbon to charcoal (“biochar”) and burial in soil	Storing carbon as biochar gives better chance of long term storage. There are also marginal benefits associated with the way in which biochar stimulates biological activity.	Cost effective biochar production relies on availability of biological feedstock, and this is limited.
Deep Geological Storage		Relatively high level of long-term stability.	Limited capacity. Concerns that expanding volume might increase risk of accidental release. Low level of maturity relative to the scale of the challenge
Market	Systems such as the UK and EU Emissions Trading Schemes allow companies to trade allocations of carbon. The price is set by the market.	Allows companies to integrate carbon measures into existing financial planning.	Prices set by the market have been consistently very low relative to the levels needed to trigger change
Social cost	The projected cost to society of releasing additional greenhouse gasses		
Marginal Abatement Cost	The cost of taking measures to remove an additional unit of carbon dioxide	The marginal abatement cost is used in a wide range of contexts in which measures are taken to reduce environmental damage.	The different forms of abatement associated with different carbon reservoirs are not distinguished from each other in this quantity.

£22 on the price of a litre of petrol is needed to show the scale of the challenge. We do not, of course, need to take every number that occurs in the many thousands of pages of the IPCC reports as unquestionable facts. On the other hand, we certainly cannot ignore them. The question of changes in behaviour are important because it is clear that the capacity for actions to compensate carbon emissions is limited, and increasing demand for offsetting and sequestration could, in principle, lead to price increases which match these high social price estimates.

Table 2.5 shows some examples of carbon prices and Table 2.6 defines the categories.

2.11 The Kaya identity and related concepts

The Kaya identity (Kaya and Yokobori 1998) breaks down global greenhouse gas emissions into the product of four factors:

- F is global CO_2 emissions from human sources
- P is global population
- G is world GDP [per person]
- E is global energy consumption.

Variations on the theme can be applied to data centres. Bol, Pirson, and Dekimpe (2021) suggest a range of different Kaya-decompositions for different elements of the global ICT carbon footprint:

$$\text{CO}_2\text{ footprint} = \text{Population}\times\text{Technology Affluence}\times\text{Energy Intensity}\times\text{carbon intensity}$$

The concept of "Technology Affluence" here replaces the general measure of affluence represented by GDP.

2.12 Laws of Information Technology

Trends in information technology (IT) are often expressed in terms of empirical laws, some of which are listed here.

Moore's law is the observation that the number of transistors in a dense integrated circuit (IC) doubles about every two years (Moore 1998).

Koomey's law describes a trend in the history of computing hardware: for about a half-century, the number of computations per joule of energy dissipated doubled about every 1.57 years (Koomey, Berard, et al. 2010, 2011).

Jevons' paradox states that increasing efficiency will lead to increases in demand which result in a net increase in consumption (York 2006). Trincado, Sanchez-Bayon, and Maria Vindel (2021) review the Jevons' paradox (also know as Jevons' effect) in the context of European energy policy. A more recent analysis of the counter-intentional impact of efficiency gains, also known as the rebound effect, is given by Khazzoom (1980) and Saunders (1992).

2.12.1 Technology Readiness Levels

The concept of Technology Readiness Levels (TRL) will be key to tracking the progress of different technologies from invention to commercial exploitation. A reference table of levels is shown in Table 2.7.

Table 2.7: TRL Chart from the UK House of Commons, Technology and Innovation Centres, Science and Technology Committee (Science and Technology Committee 2011), taken from Ministry of Defence.

TRL 1	Basic principles observed and reported.
TRL 2	Technology concept and/or application formulated.
TRL 3	Analytical and experimental critical function and/or characteristic proof-of-concept.
TRL 4	Technology basic validation in a laboratory environment.
TRL 5	Technology basic validation in a relevant environment.
TRL 6	Technology model or prototype demonstration in a relevant environment.
TRL 7	Technology prototype demonstration in an operational environment.
TRL 8	Actual technology completed and qualified through test and demonstration.
TRL 9	Actual technology qualified through successful mission operations

These definitions will need some modification to fit the technical scope of the UKRI DRI, but the underlying concept of progression from outline design to robust operational service is sure to be useful. In planning for net-zero, we also need to consider issues beyond the TRL9 to look at scalability and sustainability.

S. Hallstedt and Pigosso (2017) discusses an approach which builds sustainability planning into the TRL approach, exploiting the Sustainability Compliance Index (SCI developed by S. I. Hallstedt (2017)) based on the Framework for Strategic Sustainable Development (FSSD):

> In the sustainable society, nature is not subject to systematically increasing
>
> I Concentrations of substances extracted from the Earth's crust
>
> II Concentrations of substances produced by society
>
> III Degradation by physical means and, in that society . . .
>
> IV People are not subject to conditions that systematically undermine their capacity to meet their needs.
>
> *Ny et al. (2006)*

A weakness of Hallstedt et al. is the lack of distinction between abundant metals and rare ones. The complex mix of elements in a typical server is not well characterised by the aggregate weight of metal.

2.13 Missions and Policy Options

Georghiou et al. (2018) set out the case for mission-orientated policy in which the identification of missions with verifiable objectives is used as a means of addressing societal challenges. The mission framework allows a range of activities and projects spread across multiple sectors of society to be coordinated and directed towards addressing a challenge.

Mazzucato (2018) makes recommendations for a mission-orientated approach for the European Framework Programme of research funding. The Net Zero target fits into this concept of mission well, addressing the challenge of sustainability.

It might be argued that, as a UK agency UKRI is obliged to adopt the BEIS reporting factor. There is some truth there, but stopping at that point would imply that UKRI had little or no agency to address the footprint of its electricity: a conclusion which is clearly not societally acceptable.

Equally, we could adopt the green tariff approach. However, because the green tariff is independent of facility location, this approach would hide the undoubted benefits of siting infrastructure in a region which has high availability of renewable power.

This conundrum may appear intractable, but we suggest that it only appears to be so if we choose to route our pathway through the policy territory mapped out by carbon audits. We need to ensure that early methodological choices do not create roadblocks for later progress.

Setting carbon audits and targets has been a mainstay of carbon mitigation policy for decades. Has it worked? Some recent literature casts doubts on these foundational assumptions (see §3.9.3). There are other possibilities, such as those adopted for health and safety, equality, diversity and inclusivity (EDI), or modern slavery, in which the priority is on eliminating a harm without setting a price on it.

2.14 Other Initiatives

2.14.1 Standards and Certification

CEEDA (CEEDA) provide certification to gold, silver and bronze standards, using a range of best practises, standards and metrics from Energy Star, EC Data Centres Code of Conduct (Acton, Bertoldi, and Booth 2022), The Green Grid, ETSI, ASHRAE. The governance process behind the CEEDA certification is not visible on their web pages.

ISO 13586:2006 comments that "no scientific basis for reducing Life Cycle Assessment (LCA) results to a single overall score or number". This and other remarks about the use of Life Cycle Assessment LCA) and Life Cycle Inventory Analysis (LCIA) reflect a concern about useful analytic tools being turned into misleading score tables.

The BREEAM (2016) report on construction identifies "building and building services which can play a significant role in facilitating IT equipment efficiency", but does not address the footprint of the IT equipment itself.

Saadi Ansari (personal communication, 2022): following a review of standards on behalf of NERC, concluded that CEEDA and BREEAM were the most relevant to data centres.

GRI provide a broad range of reporting standards, including GRI (2018) for energy. This is a framework standard designed to ensure basic consistency of terminology in reporting. For energy, there is a requirement to report energy intensity which is the energy used normalised by the units of production. This raises an interesting question about the units of production of data centres. For HPC, this could be Petaflop-hours (an execution rate of 1 petaflop for 1 hour), and for storage systems data holding and data movement units of production could be defined.

2.14.2 In UKRI

2.14.3 On-site Power Generation

STFC ran a 45kW wind turbine from 1990 to 2015 (ERU 2022a) and is currently running a 12kW turbine (ERU 2022b). The turbine feeds energy into the Rutherford Appleton Laboratory grid, but is primarily operated to support research.

The STFC Estates Strategy (STFC 2021, 🔒) sets out an "Environmental Plan" which includes objectives to set standards, deliver onsite renewable generation and publish utility usage for each building. STFC is now installing 9000 solar photovoltaic panels at the Rutherford Appleton Laboratory, forecast to produce produce 1900MWh per year (Munro 2022, 🔒). Comparable to annual footprint of JASMIN... but a small fraction of Rutherford Appleton Laboratory's entire site footprint.

Additional on-site power could be generated by a new generation of low visual-impact wind turbines. The mechanical efficiency of these small capacity generation plants does not match that achieved by the high towers of the large off-shore installations, but local capacity brings significant advantages, not least in terms of transparency around other impacts such as land-use.

2.14.4 UK Activities

Carbon Literacy provide training in carbon literacy, covering the whole range of basic information about climate science and sources of carbon emissions, for both individuals and organisations.

NBIP provides digital research services for four bioscience institutes (the John Innes Centre, The Earlham Institute, The Sainsbury Laboratory and Quadram Institute Bioscience).

The Green Algorithm project (Lannelongue, Grealey, and Inouye 2021; The Green Algorithms project 2022) is raising awareness about the carbon footprint of computational research and provides an online tool to aid estimation of emissions.

C. Woods (C. Woods) provides a tutorial in accelerating python.

Julie's Bicycle (Julie's Bicycle) has, since 2007, been mobilising the arts and culture, working with over 2000 organisations, to take on the climate and ecological crisis.

NC3Rs was set up in 2004, following the recommendations of Animals in Scientific Procedures (2019). NC3Rs is dedicated to helping the research community worldwide to identify, develop and use technologies and approaches for replacement, reduction and refinement of the use of animals in research. While the use of animals in research is a very different topic, NC3Rs is cited here because of their experience in facilitating an ethically driven change in research practise.

The Laboratory Efficiency Assessment Framework (Leaf) helps research laboratory staff to assess performance and follow good practice to reduce both cost and environmental impact (Krause et al. 2020) and has already been adopted by MRC (2021).

Carbon Intensity API monitor and forecast carbon intensity of power generation in the UK, and provide an API through which users can interrogate the data in order to integrate the information into to power consumption planning. Carbon Intensity is a service developed jointly by National Grid (National Grid), the Environmental Defense Fund Europe, Oxford Department of Computer Science and the "World Wildlife Fund". See also Section 2.6.

SIR is an innovative hub of expertise connecting companies with academia to find sustainable and effective solutions to manufacturing problems.

ICT Footprint is a service created by a Horizon 2020 project providing a range of resources which help organisations to deal with their ICT carbon footprint.

Other radical solutions include placing data centres off-grid in wind turbines (a process which is available commercially in Germany via windCores, though unlikely to fit requirements of research data centres with novel architectures and frequent access requirements) and in a tidal lagoon (Blue Eden project, under development, construction hoped to start in 2023: BBC 2022; Ingram 2021).

2.14.4.1 The EPCC path to Net Zero

EPCC, the supercomputing centre at the University of Edinburgh, has been a hosting site for the UK's national HPC services since 1994. EPCC currently house IT equipment worth £125 million, including ARCHER2, the DiRAC system Tesseract, the EPSRC-funded Tier-2 system CIRRUS, the Edinburgh International Data Facility (EIDF), as well as a number of smaller research systems and University equipment.

All the systems are hosted at the Advanced Computing Facility (ACF), a state-of-the-art data centre located 10 miles south of Edinburgh in Midlothian. The ACF has 4 compute rooms, each with its own plant room providing power and cooling. EPCC and the University of Edinburgh have invested heavily in the efficiency of the ACF, including infrastructure for direct liquid, adiabatic and "free" cooling, providing the capability to host many different types of hardware efficiently.

Power: The University procures its electricity through the Scottish public procurement electricity contract, which includes the power for the ACF. The University chooses the renewable energy option which is provided through certified renewable sources (Edinburgh 2022).

Cooling: Cooling HPC systems uses a non-negligible amount of energy and optimising the cooling infrastructure is key in making a data centre efficient. The Scottish climate (with its relatively low average temperatures in the summer and moderate winters) is ideal for data centres: it means that the ACF can utilise free cooling (the cooling of systems solely using outside air to cool via water pumped to fans on the roof) throughout the year. The infrastructure is set up in such a way that systems will automatically use this whenever outside air temperatures are sufficiently low. For significant amounts of the year the ACF uses free cooling solely. A mixture of chilled cooling, adiabatic cooling and free cooling is used during the warmer months. Wherever possible, the aim is to use direct water cooling to systems, which is the default for modern high-end system designs (such as ARCHER2). Where this is not possible, for example for much of the EIDF equipment, the systems are housed in climate-controlled racks, avoiding the need to keep the air in the machine room at a low temperature and maximising efficiency.

Geothermal heat battery: The by-product of liquid cooling is hot water. The location of the ACF in relative isolation means that using this heat directly is not viable (see Figure 2.3). However, the data centre is in an area of disused (and now flooded) mine workings, which stretch all the way to the southern edges of Edinburgh, an area of dense housing and commercial infrastructure.

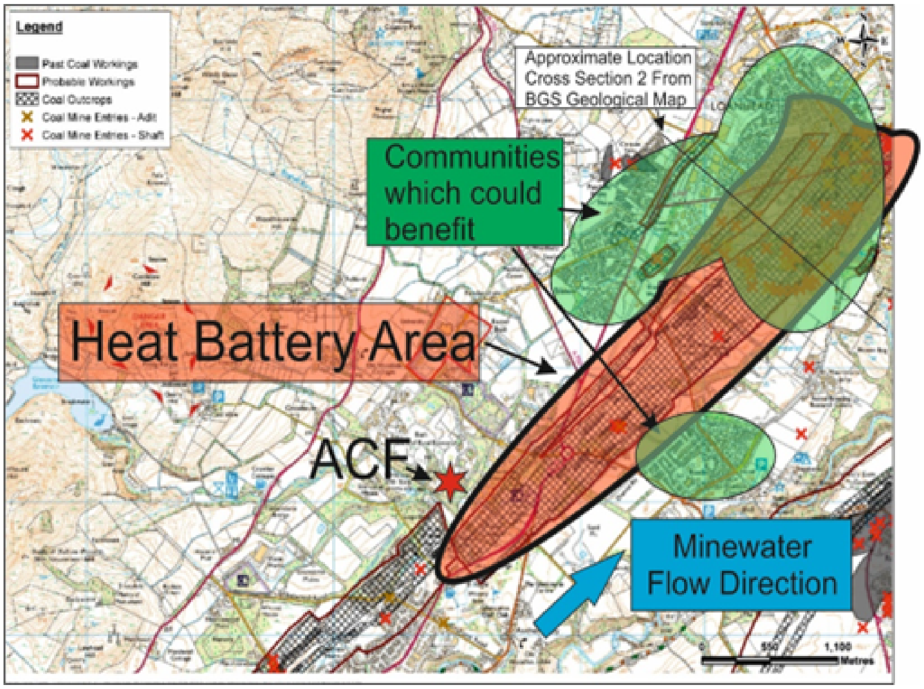
A detailed feasibility study was completed (Fraser-Harris et al. 2022) to assess whether it is possible to use the hot water to heat up the water in the mines (which is at 14°C) in order to create a geothermal battery (illustrated in Figure 2.4), with the aim to extract the heat (via ground-source heat pumps) to use in homes, public and commercial buildings. Funding has now been secured to drill 3 test wells (injection, extraction and test points) to explore the feasibility of this approach prior to a full development project being established.

2.14.5 The global context

The EMBER Energy Think Tank (EMBER; EMBER Viewer) is a UK Community Interest Company, founded in 2020. They provide information on current carbon prices in the UK and EU Emissions Trading Schemes.

"Climate Neutral Data Centre Pact" (CNDC) is a self-regulatory European initiative set up to ensure that data centres are an integral part of the sustainable future of Europe. Participating data centre operators and trade associations have agreed to a broad range of actions to make data centres climate neutral by 2030, including:

Figure 2.3: Geographical location of the EPCC heat battery



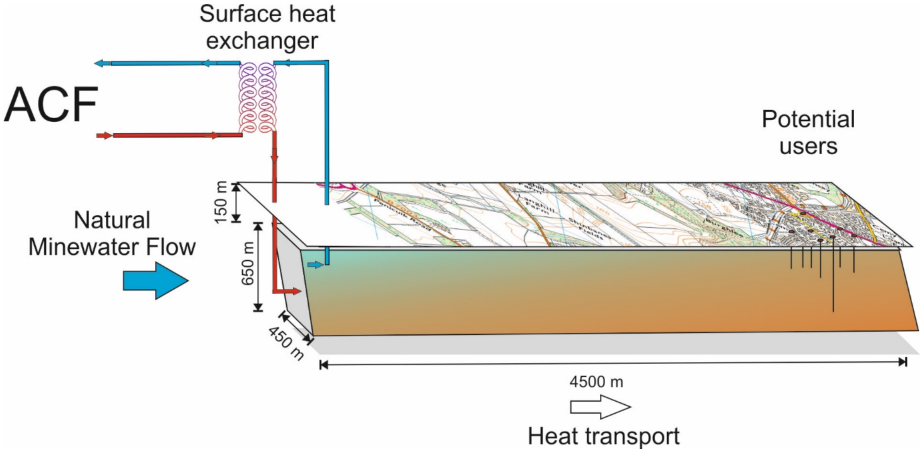
- PUE below 1.4 in warm climates, below 1.3 in cool climates.
- 100% renewable energy by purchase by 2030.
- “High bar” for engagement with circular economy.
- Proactively seeking opportunities for exploiting community heating.

While CNDC is clearly raising standards in carbon efficiency, we can see some ambiguities in these targets. The concern about the high carbon footprint of equipment manufacture is being addressed through the commitment on the circular economy, but this does not carry specific targets at this stage. The commitment to 100% renewables is excellent, but leaves open questions about the approach to allocation (2.6) and the embodied energy of renewable generation infrastructure (1.6,3.5).

“Cloud Infrastructure Services Providers in Europe” (CISPE) is a non-profit association with a goal of developing greater understanding and promoting the use of cloud infrastructure services in Europe. They promote use and uptake of cloud services and also support CNDC.

The *International Renewable Energy Agency* is, in their words, “is an intergovernmental organisation that supports countries in their transition to a sustainable energy future, and serves as the principal platform for international cooperation, a centre of

Figure 2.4: Schematic overview of heat flows in the EPCC heat battery concept



excellence, and a repository of policy, technology, resource and financial knowledge on renewable energy."

The *International Institute for Sustainable Development* is a think-tank "working to create a world where people and the planet thrive". Among many projects, they have been running the *Earth Negotiations Bulletin*, reporting on intergovernmental negotiating processes, since March 1992.

The Uptime Institute is an "advisory organization focused on improving the performance, efficiency, and reliability of business critical infrastructure through innovation, collaboration, and independent performance certifications". Their technical reports include guidance on reducing the carbon footprint (Dietrich 2022).

PACE catalyze global leadership from business, government and civil society to accelerate the transition to a circular economy.

Tseng et al. (2018) discuss the role of the Brigham and Women's Hospital's Digital Health Innovation Group (DHIG) in driving forward transformation in a multi-institutional environment through targeted support for innovators, though their focus is on exploiting digital innovation to enhance services and does not extend to explicit activities associated with environmental sustainability. The relevance here is as a model for driving organisational change across multiple linked organisations.

The Extreme Science and Engineering Discovery Environment (XCEDE) is a collaborative partnership of 17 institutions set up to promote inclusion and diversity in digital research (Akli 2018).

EDUCAUSE "is a nonprofit association whose mission is to advance higher education through the use of information technology."

Chapter 3

Key Findings

3.1 General

This section deals with system-wide aspects of the net zero challenge.

3.1.1 Evolving technical, societal and environmental context

The 20-year time span of the transition to net-zero will see many changes. The net zero ambition is driven by the climate crisis which will bring many changes in addition to the rapid pace of technological change in the information technology sector. The Strohmaier et al. 1993 site records a peak performance of 2.4 Exaflops for 2020, compared with 64TFlops in 2000. The historical rate of increase to the peak performance is a factor 200/decade, though this appears to have slowed to significantly to a factor 60 in the most recent decade. Looking forward we may expect our computational resource for HPC to increase by anything between a factor 4×10^4 and 2500 over the next 20 years[1].

See also Bol, Pirson, and Dekimpe (2021).

The environmental changes are equally unpredictable. The global scale changes in surface temperature can be foreseen with reasonable accuracy, but the consequences of those changes become increasingly uncertain when weather events and their consequences are considered.

> We have a choice. Collective action or collective suicide
>
> *UN Secretary-General, Guterres (2022)*

The large degree of uncertainty around these external factors make it inevitable that there will be a need for adjustments and continued evaluation during the transitions.

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[1] From the performance page, `https://www.top500.org/statistics/perfdevel/`, of the TOP500 project (Strohmaier et al. 1993)

Knowles et al. (2022) discuss the importance of placing constraints on resource use and the potential benefits and call for the “End of Digital Exceptionalism”.

Koomey and Masanet (2021) discuss the pitfalls of dealing with a rapidly changing system. Information may be accurate when published but can easily be misinterpreted if context and time of validity are not accurately stated. Fryer and Banach (2021) discuss the tendency for “inaccurate and sensationalist” claims to persist in public discussion. The importance of understanding the scope of reported carbon footprints is neatly illustrated by the range of figures reported for the footprint of a single google search, from 0.2 to 15g (Sterling 2009) (Sterling and many others attribute a 7g-per-search figure to Wissner-Gross based on a Times article (Leake and R. Woods 2009), despite the fact that Wissner-Gross published an explicit and robust denial of any responsibility for the claim within 24 hours (San Miguel 2009) and the Times added a clarification a few days later. Both are correct in their own perspective. The low figure (which is valid for 2009), from Google (Google 2009), represents emissions in scopes 1 and 2 and may include the upstream elements of scope 3 emissions, but explicitly excludes the user device. Google also note that user device footprints exceed the data centre emissions included in their estimate. They do not explicitly justify the decision to exclude user device emissions.

Koomey at el. make four recommendations which can be applied to the UKRI DRI:

1. Improve sharing of data about energy use.
2. Encourage accurate and precise reporting to avoid confusion about scope, location and time of validity.
3. Exercise restraint and be clear about assumptions.
4. Peer review processes need to be improved to reduce persistent reference to refuted results.

There are also pitfalls in the broader context of public attitudes. On the one hand, expert groups such as Atwoli et al. (2021) are talking of “risk catastrophic harm to health” and UN Secretary General, Antonio Guterres is talking of a choice between “collective action or collective suicide” (Guterres 2022), on the other hand, surveys of public attitudes in Europe suggest that, in 2017/18, the median level of concern was “somewhat worried” (Poortinga et al. 2019). Even when individuals are concerned and aware of the high impact of their choices, as, for instance, in the case of scientists flying for work, there are many reasons why the combination of awareness and concern does not translate into action (Whitmarsh et al. 2020, 2021).

3.1.2 Metrics and Evaluation will play a central Role

There is an extensive literature on metrics. A sample is listed here:

- J. Dongarra, Heroux, and Luszczek (2016) introduce the High-performance conjugate-gradient benchmark (HPCG 2022) to provide a more realistic guide to machine performance solving scientific codes. This complements the pre-existing and widely used High Performance LINPACK (HPL) benchmark (J. J. Dongarra, Luszczek, and Petitet 2003). Both the HPL and the HPCG metrics are used by the widely cited Strohmaier et al. 1993 project.

- Strohmaier et al. 1993 also provide a Strohmaier et al. 2013 list using energy efficiency measured as the Maximal LINPACK performance FLOPS(Rmax) per Watt of power.
- Balaji et al. (2017) provide a comparative assessment of performance of climate models run by many institutions on multiple platforms. Balaji et al. record HadGEM3-GC2T achieving 0.57 ASYPD (Actual Simulated Years per Day) with 180 million grid points, complexity of 66 and CHSY (core hours per simulated day) of 6504 running in ARCHER, a machine with 118,080 cores and LINPACK benchmark (Rmax) of 1.6 PFLOPS. That is 13.5TFLOPS per core. Timestep 15 minutes.
- Browne et al. (2000) describe the "Performance Application Programming Interface" (PAPI), which is a widely used tool for measuring the floating point count of an algorithm. A single processor operation may deal with multiple arithmetic operations, and PAPI provides a range of metrics to cover different applications (PAPI 2020, : the influence of Speculative Execution is also discussed here). Morris (2007) gave an analysis of two simple matrix operations and show how the compiler optimisation on the IBM BlueGene can fuse two multiplication operations into a single complex multiplication which is counted as a single operation by PAPI. See also Ahn (2008).
- BenchCouncil provide a range of metrics for HPC. Their big data suite has two metrics related to scientific computation: for FFT and matrix multiply. In general, their focus is on the type of workloads run in commercial data centres supporting commercial and public services.
- Peña-Monferrer, Manson-Sawko, and Elisseev (2021) discuss concurrent use of HPC and cloud, with the implementation of a workflow which executes a CF simulation on an HPC platform and runs concurrent visualisation on a cloud service connected over the WAN (both in the UK, within 200km of each other).
- MTBF : Mean Time Between Failure is an important metric of HPC performance. In HPC usage, the class of failure referred to here is a hardware fault which leads to a user application crash. e.g. Cappello and Bosilca (2019) "For example, GPU bus errors (disconnection of the GPU), voltage fault, kernel panic, PCI width degrade, machine check exception, and SXM (PCI) power off observed in Titan lead to process crashes" (see also Cappello 2009).
- The surface area of annual silicon chip production has been estimated at 3 km^2 in 2008 (Boyd 2012) and projected to rise to 10 km^2 in 2025 (University Wafer 2022).

Reddy et al. (2017) provide a comprehensive review of metrics which can be used to monitor energy efficiency in data centres and categorise them according their relevance to the concepts "Reduce (reducing resources), Reuse (reusing resources), Recycle (recycling resources) and Renewable (use of renewable resources)" and whether they target IT equipment or the facility as a whole.

Stanley, Brill, and Koomey (2007) advertise four metrics in their title, but actually provide four functions each of which can be tracked by multiple metrics. The four functions nevertheless provide a good basis for structuring discussion of machine room efficiency:

1. Strategy : business requirements, systems architecture and platform selection, data topology, and network.
2. Hardware asset utilization : e.g. retiring underused servers, enabling power saving features.
3. Energy and power efficient hardware deployment: purchasing equipment which will be efficient to run.
4. Site physical infrastructure overhead.

Shao et al. (2022) also review energy efficiency metrics for data centres and present a Kaya-like energy chain which in a typical data center means that 1 Watt of compute power translates into 27 Watts of data center power consumption. This results from multiplicative factors 5 (server utilization factor), 3.33 (processor power fraction) and 1.66 (PUE). With best practice they suggest that these can be reduced to 1.2, 2.33 and 1.33, which would reduce the total power requirement to 3.7 Watts of data center power to 1 Watt of compute power.

Some additional key concepts are listed in Table 3.1.

3.1.2.1 Metrics and Kaya Decomposition

The Kaya (§2.11) decomposition approach can be adapted to decompose the net zero challenge into a product of distinct efficiency factors. This approach makes it possible to analyse a broad range of activities in a consistent framework.

Kaya's identity can be used to analyse the different factors which can lead to overall increasing or falling overall carbon footprint. E is impacted by changes in the power supply to exploit more renewables and is on a downwards trajectory. PUE is influenced by machine room design and best practice is approaching an optimal value of near unity. U can be improved by consolidation of services. K is falling through technology innovation due to a range of factors. C and I are poorly defined, but there is a trend towards needing more computations to make a meaningful addition to scientific knowledge.

The ambition, A, is a critical factor: digital services are playing an increasing role. Table 3.2 lists a potential seven-fold Kaya decomposition of the carbon footprint of digital research.

3.1.3 Global Information and Communication Technology and Data Centre Trends

A substantial increase in emissions from the Information and Communication Technology (ICT) sector between 2000 and 2010 prompted a lot of interest in future trends.

Table 3.1: Some key concepts in the quantification of the net zero challenge.

Symbol	Title	Description	Units
$C_{E\|p}$	Operational carbon intensity of power generation allocated by purchasing contract	Measured in terms of the equivalent (based on 100-year timescale unless specified otherwise) mass of carbon dioxide emitted during operation. Neglecting embodied energy, maintenance and end-of-life.	g / kWh
$C_{E\|r}$	Operational carbon intensity of power generation allocated by regional usage	Measured in terms of the equivalent (based on 100-year timescale unless specified otherwise) mass of carbon dioxide emitted during operation. Neglecting embodied energy, maintenance and end-of-life.	g / kWh
	Floating Point Operation Count according to PAPI	Operation count as recorded by the PAPI suite. Requires specification of precision	1
	Tensor FLOP	Mixed-precision FP16/FP32 multiply-accumulate calculation commonly used in machine learning applications and specifically supported by some accelerators	1

Recent literature contains a broad range of results. Andrae and Edler (2015), Belkhir and Elmeligi (2018), and SRC (2021) give high estimates of 2020 global energy consumption ICT equipment at between 2,000 and 3,000 TWh , about 7%-11% of the world's total electricity consumption. Andrae and Edler (2015) include a worst-case projection for 2030 of a rise to 30,000 TWh, exceeding the current world electricity consumption. However, these studies appear to rely on out-dated projections. Belkhir and Elmeligi (2018) refers to a conference paper (Pickavet et al. 2009) which itself refers to projections from an earlier data and Andrae et al. use exponential extrapolation from 2010 figures.

Analysis based on more recent data such as Malmodin and Lundén (2018) for global ICT and Kamiya (2020), Malmodin (2020), Masanet et al. (2020), Shehabi, S. Smith, et al. (2016), and Shehabi, S. J. Smith, et al. (2018) for data centres identifies a flatting in the power use growth since 2010, with annual energy use stabilising at around 200 TWh for data centres (including network traffic) and 800 TWh for ICT excluding entertainment and media. Shehabi, S. Smith, et al. (2016) have estimated a growth rate of ICT energy use of around 4% over 6 years for the US market. This latter figure reflects a levelling off in the growth in the number of servers as capacity becomes increasingly focused in the hyperscale data centres of the major cloud service providers. Freitag et al. (2021) question, however, whether the evidence for a plateau

Table 3.2: A seven-factor decomposition of the carbon intensity of scientific work supported by the UKRI DRI.

Symbol	Title	Description
$\mathcal{E}$	Power Carbon intensity	The carbon intensity of power supply can be quantified in a number of ways. The power for most, if not all, data centres will come from a national grid providing power from a range of sources through complex physical, administrative and financial workflows. See §2.6 above.
PUE	Power Usage Efficiency	Data Centre energy use per computational energy use. Current values may be in the range 1-2, with best practice tending to 1.2 (Uptime Institute 2020)
$\mathcal{U}$	Machine utilisation	The amount of time that a machine is running scientific software
$\mathcal{K}$	Operational Joules per Computation	According to Koomey's law, the energy intensity of computation is falling by a factor 2 every 1.6 years. There is a wide spread of values depending on how the computation is defined.
$\mathcal{C}$	Computation per Information generated	Not all scientific computations are equal (e.g. see quantum computing in section 3.4.1.3 below). Measuring information outputs is likely to be subjective. We do not have a recommendation at this stage.
$\mathcal{I}$	Impact rate per information	The impact of research projects is routinely monitored by Research Councils, but these impact measures are not linked to resource usage. Consequently, we do not have direct information about the role of energy-intensity in contributing to the impact of the UKRI DRI
$\mathcal{A}$	Ambition	The targeted impact. There are good reasons to believe that digitally enabled research will have an increasingly central role in science as the power and versatility of computational services increase (see 3.10)

in data centre energy use is robust.

Significant improvements in the efficiency of ICT equipment usage are shifting the balance of the carbon footprint towards the embodied carbon associated with the manufacture of equipment and extraction of raw materials. There is considerable uncertainty around estimates of embodied energy (Freitag et al. 2021).

Global network traffic is dominated by videos, which account to around 80% by volume (CISCO 2019).

3.1.4 Short-term actions are needed if we are to meet the long term goals

The New Climate Economy report of 2015 (Jacobs et al. 2015) concluded that “The next 15 years of investment will also determine the future of the world’s climate system”.

Increases in computational efficiency have been offset by increases in affluence (Bol, Pirson, and Dekimpe 2021), resulting in a net increase in carbon footprint.

3.2 Dynamic Efficiency, False Equivalences, and Complexity Economics

Kattel et al. (2018) discuss the role of dynamic, rather than static or allocative, efficiency in tackling challenges over an extended period of time. They propose ‘Decarbonisation at least cost’, or ‘at most gain’, as a dynamic efficiency metric. The dynamic efficiency framework reveals real benefits which are obscured by the static approach, such as the potential to enhance innovation through constraints (e.g. review by Acar, Tarakci, and Knippenberg 2019). Kattel et al. (see Box 3 of their paper) identify three areas where a dynamic efficiency approach to decarbonisation can bring benefits:

1. Targeted taxation because the level of carbon levy needed to make an impact on use of fossil fuels in transport is much greater than that needed to impact on power generation.
2. Subsidies which drive long term growth.
3. Regulation which can create a framework for innovation.

> [Complexity economics sees] decision makers (or agents) as not super-rational, the problems they face as not necessarily well-defined and the economy not as a perfectly humming machine but as an ever-changing ecology of beliefs, organizing principles and behaviours
>
> *Arthur (2021)*

Carton, Lund, and Dooley (2021) argue that adopting institutional carbon neutrality as the primary target of an institutions carbon policy can lead to outcomes which are out of line with the national journey to net zero. Barron et al. (2021) suggest that widespread carbon accounting methodologies lead to false equivalences between different actions which can distort decision making.

Mercure et al. (2021) conclude that cost-benefit analysis is inadequate for dealing with the complexities of responding to the climate crisis and propose a risk-opportunity analysis as a better option. See also §E5 and §1.3.

Arthur (2014) discusses complexity economics which deals with non-equilibrium economics which is of particular relevance to a time when major elements of the economy are in transition. Arthur draws an analogy between the spontaneous appearance of traffic jams on busy roads and the potential for self-induced volatility in complex economic systems. His conclusion is that we should look for patterns of behaviour in the system rather than seeking a comprehensive deterministic solution.

Different metrics of carbon footprint, such as those based on different approaches to determining carbon-intensity of electricity supply, can be related to different pathways of influence.

Meyer and Lord (2021) discuss the need for individual and societal change to complement technological advances. From an ethical perspective, responsibility can be linked to the ability to influence outcomes (Page Center 2022):

> To be more specific, responsibility refers to more than just the primary function of a role; it refers to the multiple facets of that function, which includes both processes and outcomes, and the consequences of the acts performed as part of that set of obligations.

3.2.1 Risks of Involuntary Greenwash

There has been considerable discussion in both public media and the academic literature about "greenwash": the phenomenon of organisations which are perceived to fall far short of their public claims (e.g. Lyon and Montgomery 2015). Some suggest that greenwashing is often unintentional (Worldfavor blog) as a consequence of failure of a well-intentioned policy. The Triple Bottom Line (TBL) which expands business success metrics to include social well-being, the environment, and a just economy (the so-called three Ps of people, planet, and prosperity) has been proposed as a means of avoiding these problems. However the TBL originator has, in his words, recalled the concept because it is not functioning as intended (Elkington 2018).

3.2.2 Organisational Transformation

Woiwode et al. (2021) discuss the role of "inner transitions", also cited in the IPCC 6th Assessment Report (Denton et al. 2022). This work draws on discussions of leverage points Abson et al. (2017), Chan et al. (2020), and Fischer and Riechers (2019) in the broader sustainability literature, and specifically on the suggestion which suggests that the most efficient means of achieving significant change in sustainability is through re-thinking our intentions and mindset. IPBES (2019) identify the need for transformative change, which they define as a "fundamental, system-wide reorganization across technological, economic and social factors, including paradigms, goals and values."

3.2.3 Barriers between Commercial and National Capability Services

Differing business models between commercial and research digital infrastructures create interoperability barriers for users.

The commercial services providing cloud hosting for businesses and private customers are driving the industry and individual perceptions of digital services. In contrast, services funded by research agencies remain the focus for innovation and delivery of specialist services which are co-designed with scientific research communities.

It is tempting to start with a comparison of digital services provided by commercial versus research infrastructures, but attention needs to be paid to the nature of the contract with users and the constraints imposed by the basic paradigms of the global scientific enterprise to advance human knowledge.

Paradoxically, commercial services have, in the field of cloud services, moved ahead faster than National Capability services in providing easy and open access with minimal barriers through "freemium" services. The PANGEO project has (PANGEO Team) trialed some free services for the research community, but funding to maintain the services is limited to the duration of a research contract.

While research services are free to the user, they clearly have their costs. If we look a little deeper, we see similarities. The first level is "free and open" services, available to anyone at no fee. This includes both freemium services from commercial providers and open access services from UKRI DRI facilities, such as data access. The remaining services could be defined as having "qualified access". In the commercial world, you qualify by paying, while in the UKRI DRI world users generally qualify by some form of review process or institutional membership.

The complementary roles of free and premium services in the"freemium" business model are discussed by Kumar (2014). Kumar identifies the marketing value of free services: it is not just the fact that the free-service users may migrate to premium, they also serve as a magnet to bring in new users. In this case, the free service is part of a marketing activity which offers users a gift in order to generate goodwill and interest. The balance between the level of service which is provided for free and the services attracting fees is adjusted to optimise the in-flow of paying users.

The division between open access and qualified access services in UKRI DRI facilities has a different underlying logic. The open services are designed to disseminate knowledge as widely as possible. Here, the level of services provided is not determined by user decisions to transfer but rather by a balance between funds spent on research and funds spent on the dissemination of digital research outputs.

Within the UK academic sector, access to compute services has traditionally been restricted both by institutional membership and by a review process. The compute services have been separately managed and have had distinct funding streams.

One of the factors which has led to the collapse of the boundary between academic repositories and compute services has been the growth in volume of the data collections handled by repositories.

Drawing comparison between shareholders of commercial companies and funding agency support for UKRI DRI may appear fanciful at first sight, but there are similarities in the role played.

3.2.4 Reduction of allocated embodied carbon through end-of-life management

The embodied carbon, the carbon or carbon equivalent pollution emitted during the construction of a device or building, is a significant component of the overall footprint of ICT equipment in general, including data centres and user devices.

An analysis of recent (2021) life cycle assessment data of three main vendors of HPC servers, Fujitsu, Dell and HPE yields the following figures for the relative amount of CO2 offset as a result of recycling of the servers.

Dell the report (Dell 2021) is for the PowerEdge series of servers, 4 years use, assuming average energy mix for Europe. The usage estimate is 1700kWh/y; the embodied carbon estimates for the R6515 and R6525 models are 1300 kg CO2e and 1700 kg CO2e respectively (without usage or EoL). The following list gives the carbon footprint savings associated with recycling, the overall footprint and the saving as a percentage:

- R6515: 105 kg CO2e on 3605 kg CO2e, 3%
- R6525: 172 kg CO2e on 5672 kg CO2e, 3%

Excluding the use phase (i.e. assuming all energy is zeroCO_2), recycling would offset 8% for the R6515 and 10% for the R6525.

HPE the data (HPE 2021) are for the HPE ProLiant MicroServer Gen10 Plus, 4 years use, assuming average energy mix for Europe. The usage estimate is 1400kWh/y; the embodied carbon estimate is 500 kgCO2eq (without usage or EoL). HPE mentions that ”95% of the components is recycled” but does explicitly mention of any reduction in overall footprint. Instead they report 9 kgCO2e for End of Life. Assuming that this 9kg is purely the embedded carbon in the remaining 5% (i.e. the most optimistic scenario), then it would mean that without recycling it would have been 171 kgCO2e. With that assumption, recycling would offset 6.4% of the CO2. Excluding the use phase (i.e. assuming all energy is 0-CO2), recycling would offset 25%

- HPE ProLiant MicroServer Gen 10 Plus 171 kg CO2e on 2671 kg CO2e, 6.4%

Fujitsu : the report (Fujitsu 2021) is for the ESPRIMO P9010 desktop, 5 years use, assuming energy mix for Germany and Norway

- Germany: 35 kgCO2e on 710 kgCO2e, 5% (Germany)
- Norway: 35 kgCO2e on 445 kgCO2e, 7.9% (Norway)

Excluding the use phase (i.e. assuming all energy is carbon neutral), recycling would offset 10%.

Microsoft, Google and HP have initiatives to reuse and recycle datacentre components and devices (Swinhoe 2022). HPE in particular reports that at its Technology Renewal Centre, out of four million devices processed in 2018, 89% was sold on. This shows that reuse can be a viable commercial option.

This has a positive effect on emissions from manufacturing but it is not clear if it also has a positive effect on emissions from usage as that would only be the case if the devices are used as replacements. If they are used to perform additional work, there will be a net rise in emissions from usage.

3.2.5 Electricity Generation and Storage

The costs of power storage are projected to fall. IRENA (2017) suggest a fall of 54-61% for Lithium Ion batteries between 2016 and 2030.

IRENA (2020) show that renewable power now dominates new generation capacity world-wide.

While renewable energy supplies are often considered as carbon-neutral, a close look reveals that they do have non-zero footprints (Pehl et al. 2017, e.g.).

The transmission of power also incurs a footprint. Harrison et al. (2010) calculate a CO2e footprint of 11 g/kWh for the national transmission network. 85% of this is associated with the footprint of power which is lost during transmission. The footprint of this component will diminish in line with the falling footprint of the transmitted power. The remaining 15%, around 1.5 g/kWh is dominated by SF_6.

On-site generation of electricity for emergency back-up power supply of machine rooms generally uses small diesel generators. These can be replaced with battery systems, including the possibility of site-wide systems, or modified to use biodiesel. Biodiesel is not carbon neutral, but the Climate Change Committee fuel supply carbon budget, CCC (2020), estimates that the carbon intensity of biodiesel will drop from a 2020 value of 28 g/kWh CO2e in 2020 to 3 g/kWh by 2050, compared with 270 g/kWh CO2e for standard diesel (BEIS 2022).

3.2.5.1 Risks

For power supply we may consider three risks: displacement, burden and finance. These map onto three broadly distinct methods of allocating carbon footprint discussed above (2.6).

Burden : Purchase causes increased local demand which results in more local emissions. Risk mitigation by (1) use of batteries to reduce burden and (2) offsets through land-use change and biological carbon uptake.

Displacement : Purchase of power supply may appear sustainable, but causes displacement effects which result in carbon emissions elsewhere. Impact is estimated as national been carbon intensity of generation. Risk mitigation by (1) careful choice of contracts and (2) offsets by displacement (investment in generation capacity).

Finance : The impact of volatile oil and gas prices on the cost of energy. Risk mitigation by (1) choice of contracts to minimise dependency on fossil fuel and (2) engagement in activities to accelerate the transition to renewable energy generation.

3.2.6 Landscape of Exascale DRI Research

Heldens et al. (2020) conduct a data driven literature survey, based on article with titles matching “exascale” or “extreme scale systems/compute” to provide insight into the important themes of exascale computing research. An automated analysis of relationships was used to extract key themes and topics which they condensed the results to 8 topics:

- Energy/Power
- Fault Tolerance/Resilience
- Data Storage
- Network interconnect
- Computer Architecture
- System Software
- Parallel Programming
- Scientific Computing

3.2.7 Text analysis of a literature survey

The following search found 1,344 results in Web of Science:

```
(TI=(((energy efficiency) OR green OR sustainable)
    AND (computing or (data centre) or (digital infrastructure))))
AND PY=(2010-2022)
```

Visualised with VOSviewer, picking out common terms (Eck and Waltman 2021; Nees Jan van Eck and Ludo Waltman) in Figure 3.1.

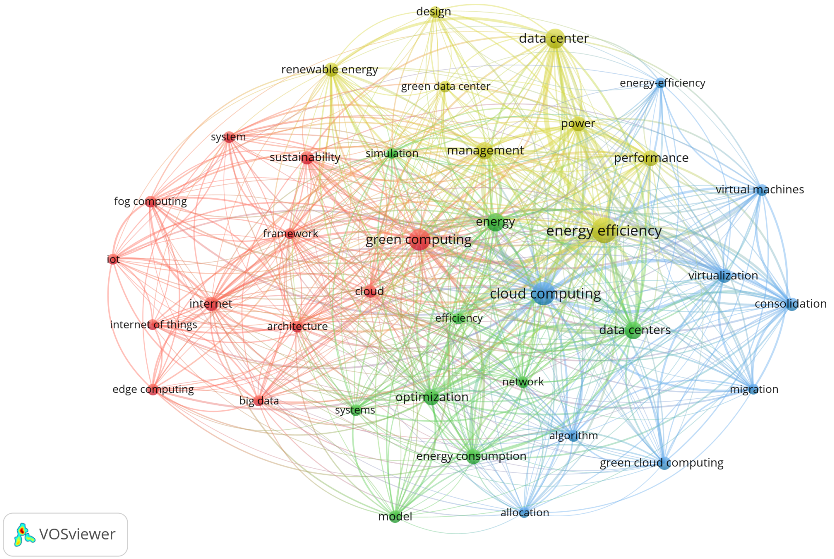
3.3 Machine room and hardware

R. Rahmani, I. Moser, and Seyedmahmoudian (2018) discuss the components of a machine room and supporting infrastructure relevant to the power consumption, including:

- Supporting infrastructure: backup generator and/or power storage.
- Power supply: Uninterruptible Power Supply (UPS) and Power Distribution Unit (PDU).
- Cooling systems
- IT equipment : server farm.

Rostirolla et al. (2022) review the potential for integrating renewable energy supply into data centre operations investigating solutions to the flexibility challenge on power and IT to tackle generation intermittency.

Figure 3.1: Display of common phrases clustered by proximity in abstracts. The clusters show areas of activity



Koronen, Åhman, and Nilsson (2020) review technological issues around data centre efficiency (looking at the broader commercial sector) and the European policy context.

Abbas et al. (2021) provide an analysis of the efficiency of different cooling system architectures (note that their Figure 1 has a value for US Data Center power usage which appears to be based on projections by Whitney and Kennedy (2012) which are double more recent estimates by Shehabi, S. J. Smith, et al. (2018)).

3.4 Machine architecture and operation.

3.4.1 Chip and transistor technology

Disruptive chip and transistor technology changes have the potential to radically reduce the energy intensity of computation.

3.4.1.1 New to general purpose computing

General Purpose Computing on GPUs Graphical Processing Units (GPUs) were designed to manipulate images. They evolved from graphics cards which were used to deal efficiently with common instructions needed for manipulating information on computer terminals. As the power and flexibility of GPUs grew they started being used for other tasks which could exploit their efficiency at applying transformations to a matrix of values. For many problems, however, the overhead of transferring data to and from GPUs is a bottleneck which limits performance (e.g. Mittal and Vetter 2015). Mittal et al. also survey the software available to support use of heterogeneous architectures.

Field Programmable Gate Array (FPGA) chips provide another route to substantial energy savings for a range of applications, though that range does appear limited at present.

Among other applications, FPGAs are being used for genome sequencing (e.g. Dandass et al. 2008; Salamat and Simunic 2020) and light etection and ranging systems (Leoni et al. 2021). Q. Jia and Zhou (2016) report on substantial performance gains and energy savings using the high-level OpenCL language to solve 1 and 2-dimensional stencil problems.

3.4.1.2 New on specialist infrastructures

Peta-scale computing on a chip New technologies such as the Graphcore Intelligent Processing Unit (IPU) and Cerebras CS-1/2 Wafer Scale Engine (WFE - CEREBRAS 2022) are breaking new ground. The computational power etched in a single chip is increased to the point at which complex real-world problems can be solved. The latest of these, the Cerebras CS-2 boasts an incredible 850,000 cores and a Petaflop rating. However, like GPUs, these machines pose challenges for the software developer.

The Cerebras CS-2 is available for use commercially at $60,000 per week or to academic communities via EPCC and LLNL (Russell 2021; Thomas 2020). The services are targeting Artificial Intelligence applications. CEREBRAS 2022 provide benchmarks: the CS-2 supports a memory bandwidth of 20 PB/s on 23kW. Rocki 2020 benchmark a stencil code on the CS-1, achieved 0.86 PFlops at 20kW in mixed 32/16 bit precision mode. At 1 TFlops per Watt this is an impressive result, though potential differences in benchmarking approach need to be considered when comparing with the Jia et al. result for the IPU cited above. This is the processor performance and should not be confused with the server performance (see Shao et al. 2022, and §3.1.2). The CS-2 is one of many devices targeting the growing demand for Approximate computing (Mittal 2016; Reuther et al. 2020; SRC 2021).

Louw and McIntosh-Smith 2020 discuss the potential for running complex simulations on a single Graphcore IPU with 1216 cores and 256KiB memory per core. Their paper deals only with codes which fit entirely in the c. 30MB total memory, avoiding the bottleneck of shifting information between IPUs. Z. Jia et al. 2019 provide detailed benchmarking. Unlike GPUs, which operate on a Single Instruction Multiple Data (SIMD) basis, IPUs and the WFE allow independent execution on each core, so that complex operations can be completed fully on-chip. Jia et al. record 31 TFlops in single precision benchmarks, running on power consumption of 250W. This equates to around 100 32-bit Gflops per Watt, which is slightly behind the MN-3 MN-Core Server which tops the Green 500 list on 14th March, 2022, with 29.7 64-bit Gflops per Watt. There is a distinction, however, as the high reliance on GPUs reduces the versatility of the MN-3 machine compared to the IPU approach.

Application-specific integrated circuits (ASICs) customized for a particular use, rather than intended for general-purpose use,are finding use in high-throughput digital signal processing (SRC 2021).

3.4.1.3 Emerging Technologies

The Ballistic Deflection Transistor (BDT) is a potentially disruptive innovation which provides a new switching technology with higher response rate and lower power consumption than existing devices. The BDT design is some distance from implementation in computing devices, but has potential to become significant. Margala, H. Wu, and Sobolewski (2015) and H. Wang et al. (2018) describe how a BDT might be used to create a THz amplifier.

Quantum computing has long been seen as bringing a major paradigm shift to computing. The approach relies on the way in which an observation of a superposition of states will throw the system into a specific state. Shor's algorithm (Wikipedia contributors 2022) describes a problem for which the quantum computing approach appears to have a decisive advantage. The advantage of quantum computing over conventional computing will only be realised if the qubit capacity of quantum computers can increase faster than the logarithm of the switching rate of conventional machines, and it is unclear if this can happen.

Y. Wu et al. (2021) claim quantum supremacy with a 66 qubit machine (called "Zuchongzhi" after a Chinese astronomer) running a benchmarking task. They estimate that their task, which took 1.2 hours on Zuchongzhi would take 8 years on a powerful conventional supercomputer.

In 2021 IBM announced the first 100 qubit computer (Ball 2021), but Egan et al. (2021) cautions that it is not yet clear how many qubits are needed to perform useful calculations.

There is exploratory work in other areas, including valleytronics (e.g. Nebel 2013), spintronics (e.g. Wolf et al. 2001) and biocomputing (e.g. Nicolau et al. 2016).

Summary As mentioned by Rocki et al, the significance of the Cerebras CS-2 is not just the impressive machine performance, but the demonstration of a new approach to computer architecture which opens out many new possibilities.

3.4.2 Wide-area Load Sharing

Google (2020a) and Radovanovic (2020) reports on their success in aligning compute load with carbon-free energy to reduce the overall footprint.

Rasoul Rahmani, Irene Moser, and Cricenti (2022) present a case study based on three green data centres with local renewable energy supplies.

3.4.2.1 Batteries

Many organisations are now using batteries to reduce their electricity demand at times of peak cost and carbon load. Energy Superhub Oxford is the first group in the UK to launch a large-scale grid-connected storage facility (Energy Superhub Oxford 2022).

BloombergNEF (2021) describe energy market scenarios which meet the global 2050 net zero target and emphasise the critical role of batteries for power storage, with a projected 176-fold increase between 2030 and 2040.

UKRI is also investing in a battery storage facility at RAL and investing into research and demonstration activities into a wider range of storage technologies.

There are many drivers of battery technology which are attracting substantial investment. New technologies offer significant advantages over Lithium Ion batteries, which currently dominate the sector, in specific areas (e.g. Aluminium air batteries have a much greater energy density, iron flow batteries have a much lower material cost). A sample are listed here:

- Electric flight and the decarbonisation of air transport: first battery powered commercial flights are expected within a few years using Lithium Ion batteries, but are expected to require new technologies with higher energy density by mass in order to achieve real commercial viability.

- Grid scale storage, particularly to store energy generated by solar power for use at night and to increase supply at times of peak demand, reducing the need for flexible fossil fuel power generation.

- Institutional scale storage, allowing power to be drawn from the grid at times of low cost and used flexibly. The institutional scale storage is similar to grid scale storage, but can be designed to match institutional demand requirements and avoid power losses of delivering from grid scale storage back into the network. This can be done in collaboration with the national grid.

- Embedded wearable power supplies (Vališevskis et al. 2021) for use in medical monitoring. The separation of the electrolyte and the electrodes (the electrolyte is applied only when the battery needs to be activated) makes storage time virtually infinite.

Dinesh et al. (2018) discuss the current status of iron-flow batteries and review the pros and cons of a range of different battery technologies. The aluminium air battery, a non-rechargeable technology which offers high energy densities, is discussed in detail by Mori (2020). The high energy density of aluminium air batteries make them an attractive prospect for electric vehicles, but the cost of the materials used in electrodes remains prohibitive.

3.5 Embodied Carbon in Computer Hardware

Malmodin and Lundén (2018) estimate that, for US server rooms, as much as 15% of the carbon footprint is associated with the manufacture of equipment. For user devices the embodied carbon, the carbon pollution associated with the manufacture of a device, is generally greater than the carbon emissions during use (e.g. Jattke et al. 2020).

Some information on the embodied carbon is provided by the Product Attribute to Impact Algorithm (PAIA) which is used by a number of suppliers (e.g. DELL 2022). Note that the PAIA reports apply to typical consumer configurations options, such as additional memory or SSD drives, can have a substantial impact. The PAIA assessment is designed as a practical tool and is not considered as reliable as a full Life-cycle assessment (LCA). A full LCA of one server (DELL 2019) reveals that for this particular server the SSD drive dominates. Gibb (2022) shows that the relevant drive has 4 packages each consisting or 16 stacked “dies” (individual chips). Further details are not readily available.

The LCA calculation for IT equipment is difficult because of the depth and diversity of the supply chain feeding the manufacture of user devices. For example, BASF (2021) describes the methodology used by BASF to establish the Product Carbon Footprint (PCF) of chemicals and components.

An interesting consequence of the high embodied carbon of a SSD is that a HDD running on renewable energy could have a lower life-cycle carbon footprint than a SSD, despite using more energy. It is possible that the production of SSD and other integrated circuits will make up an increasingly high proportion of digital research infrastructure carbon footprint if, as expected, the UK electricity supply decarbonises faster than the supply in the countries responsible for the manufacture of our equipment.

Some further discussion on the role of embodied carbon is provided by:

- The problems of the supply chain footprint is widely recognised. Microsoft (2022) detail plans to engage with suppliers to commit to carbon reduction activities by enabling and incentivizing them.
- Google (2020c) also report on working with suppliers, but put greater emphasis on the circular economy (see also §2.8), working with the Ellen MacArthur Foundation (Google 2020b).
- Boyd (2012) discuss the role of fugitive emissions of PFCs (Per-fluorinated compounds) in the manufacture of integrated circuits.
- Taiariol et al. (2001) provide a LCA for a single chip.

It is clear that there is significant uncertainty in the precise value of embodied carbon, but also clear that it is a substantial element of the overall UKRI DRI footprint. Section 1.6 above recommends three lines of action to improve quantification, support steps to reduce carbon intensity of production and enhance reuse of materials through the circular economy.

3.6 Consolidation of services and low-impact clients

Whitney and Delforge (2014) and Whitney and Kennedy (2012) report on the potential for substantial efficiency gains through consolidation of services into multi-use facilities which can achieve a consistent high utilisation factor (UF).

User devices are a potentially significant element in the UKRI DRI footprint. It may be that the user devices are serving multiple purposes and linking to the UKRI DRI does not add materially to the requirements or to the associated carbon footprint. However, as working practises evolves, it is necessary to consider what options can support the transition to Net Zero, and what aspects of UKRI DRI design can influence the requirements imposed on user devices.

The terminology of "fat", "thin" and "zero" clients refers to use devices with varying specification. The "fat" client is a high-specification laptop or desktop PC capable of running a broad range of applications and handling large volumes of user data. The "thin" client will run a limited set of applications, but still includes a conventional operating system and local file storage. The "zero" client takes this one step further, eliminating the support for user data files and for the conventional laptop/PC operating system. The zero client requires more work to be done by the data centre servers as the client can only act as a dumb terminal with the capability to establish a secure internet connection. The terminology is qualitative and a thin client in 2022 may have the capabilities of a fat client from 2010. Some also use the term "ultra-thin" to refer to a device located in the growing gap between "thin" and "zero" clients.

Farthing, Langner, and Trenbath (2018) suggest that the extra work done in the data centre can mean a higher net power demand during use for thin clients as compared with fat clients, but do not look at the issue of embodied energy which can dominate the user devise footprint. Uni. Pennsylvania (2016) suggest that the extended lifetime of thin clients, among other factors, gives them a considerably lower annualised lifetime carbon footprint than desktop or laptops. The DELL WYSE 7030 zero client, for instance, has a PAIA embodied carbon estimate of just 46 kg.

3.7 Effective Computation: making each simulation count

There are many challenges around evaluating and improving the effectiveness of research use of complex computing resources. Our project will investigating these issues through a range of activities starting in June to September 2022 (Townsend 2022). The following sections provide a sample of published work.

3.7.1 Specialist libraries, languages and standards

As discussed in §3.4.1, there are many novel machine hardware configurations which offer substantial advantages for applications which are suited to their performance characteristics.

The Message Passing Interface (MPI 4.0 Standard) is a message-passing library interface specification (see also MPI Forum). MPI is implemented on many platforms and can be considered (e.g. Chunduri et al. 2018). MPI is used in conjunction with $C++$ and FORTRAN codes and supports parallel operations which each have independent data. The OpenMPI project provides an open-source implementation of MPI.

An Amazon Web Service (AWS) benchmark study (Turner, Ashton, and Tourpe (2020) shows that a hybrid approach, combining OpenMP and MPI delivers optimal results for Computational Fluid Dynamics (CFD) problems on the AWS P3 service).

OpenMP oversees the OpenMP API specification (MP 5.2 Standard) which covers user-directed parallelization, wherein the programmer explicitly specifies the actions to be taken by the compiler and runtime system in order to execute the program in parallel.

OpenACC provide directives-based programming model for high performance computing in addition to providing training, education and supporting standards development. IN the OpenACC programming model, tasks are coded in standard C++ with added directives.

The CUDA language provides a more powerful and specific language for GPUs, which gives some performance advantages.

OpenCL is an open standard for cross-platform, parallel programming of diverse accelerators found in supercomputers, cloud servers, personal computers, mobile devices and embedded platforms. A python wrapper is provided by PyOpenCL. SYCL is a cross-platform abstraction layer building on the underlying concepts of OpenCL.

3.7.2 Leveraging AI

Artificial intelligence is having a growing impact on many areas of computing. Three recent studies are provided here as examples:

- Silva, Heaney, and Pain (2021) demonstrate data assimilation on a low order system.
- Ayala et al. (2021) emulate a climate model simulation.
- Sun et al. (2020) discuss the use of machine learning to model performance of MPI codes.

3.7.3 Guidance and application benchmarks

There is a huge range of work on application benchmarks, reflecting the wide range of application architectures. A sample is listed here:

- The commercial CFD solver ”zCFD” (zCFD) has been used for benchmarking studies, showing potential for exploiting GPU accelerators. Appa, Turner, and Ashton (2021) benchmark simulations of flow around an aircraft using Reynolds averaged Navier-Stokes (RANS) equations an identify substantial savings when the code is ported to GPUs.
- Cardoso and Bicudo (2011) compare GPU and CPU for a lattice gauge theory problem.

- Caldwell et al. (2021) benchmark impact hydrocodes (applications analysing the fluid flow which results from a high energy ballistic impact).
- Navarro, Hitschfeld-Kahler, and Mateu (2014) survey the use of GPUs in parallel computing architectures.
- Lee et al. (2010) discuss the factors which can lead to the benefits of GPUs being exaggerated.
- Ryu and Kwon (2018) discuss further the potential for GPUs.
- The Department of Energy Exascale Project (ECP) provides benchmarks via the Center for Efficient Exascale Discretizations (CEED).
- SPEC (SPEC) is a non-profit organisation defining a range of benchmarks.
- Lannelongue, Grealey, Bateman, et al. (2021) provide 10 simple rules for efficient computing which are targeted at computational biology, but most have a more general applicability.
- Georgiou, Rizou, and Spinellis (2019) review software techniques and tools and conclude with recommendations in four areas:
    1. Selection of configurations and parameters.
    2. Limited investigation on diverse programming languages.
    3. Appropriate data structure selection.
    4. Interoperability, usability, and precision for tooling support.
- CodeCarbon provide power monitoring tools for AI platforms.
- Hubblo 2022 provide consultancy and open source software to assess, monitor and reduce the environmental impacts of digital technologies of organizations, including the Scaphandre power monitoring tool for hypervisors. Power API provide a range of middleware tools to monitor power usage in a Kubernetes environment.
- EAR for HPC power metrics.

3.8 Procuring low carbon power

Willis (2020) reviews electricity supply issues for the Climate Change Committee (CCC) and discusses the rising use of Power Purchase Agreements (PPAs) both to manage costs and to achieve greater influence over the generation mix used and the level of investment in renewable power generation achieved by the supplier. O'Flynn et al. (2021) describe use of a PPA by Uni. Surrey to achieve Net Zero goals.

3.9 Carbon Capture and Offsetting

3.9.1 Why we need to remove carbon from the atmosphere

IPCC projections imply that there will be a need to bring atmospheric carbon dioxide levels down in order to stabilise the climate. There are a number of approaches possible. Direct industrial extraction of carbon dioxide from the atmosphere is problematic. There are many strands of research, pilot and demonstration projects, and operational services. There are significant open questions about technology, the feasibility of scaling and the potential side effects of large scale adoption of any of these processes.

There is a fundamental constraint imposed by the laws of physics which make it clear that the energy needed to take carbon out of the atmosphere is significant. Sanz-Pérez et al. (2016) suggest 30kJ mol^{-1} as a theoretical minimum value of the work required to extract CO_2 from the atmosphere. BEIS (2022) give 9.05kWh as the energy content of a litre of petrol (average biofuel blend) which will release 2.19 kg of CO_2, or 50 mols. Given the figures above, the minimum energy required to extract the gaseous CO_2 from burning 1 litre of petrol would be 1500kJ, or 0.4kWh. Note that this does not cover storage.

There are however, doubts about carbon capture (§3.9.3) and about the scale of capture that will be possible by 2040.

3.9.2 Classes of carbon capture

Biological Carbon Sequestration (BCS) refers to storage of carbon in biological systems. This is a natural process, and already happens at scale. There are difficulties in establishing additionality and persistence, making this a good intermediate step, but weak as a long term solution. There are three major strands of BCS work:

- **Biochar generation through pyrolysis**. This is a well-known process which is already taking place at scale. Advocates, such as Mohan and Kung (Takachar), see greater biochar production as addressing multiple sustainability issues. Biochar offers potential for extraction and storage in agricultural soils with a residency of centuries (J. Wang, Xiong, and Kuzyakov 2016). Biochar can be used both for long term storage and as a catalyst of enhanced biosphere activity leading to additional replenishment of ecosystem reservoirs. CarbonFuture (2022) and Puro (2022) offer biochar projects at €350 per tonne upwards. The case for biochar is put succinctly by Levitan (2010):

  > If we got ourselves into this climate mess by digging up and burning coal, maybe we can fix it by creating some more coal and putting it back into the ground.

  The biochar approach depends on available biological feed-stocks. Fawzy et al. (2021) estimate global capacity at 0.3-2GT $year^{-1}$ by 2050, which would amount to around 5% of current emissions.

- Bio-energy Carbon Capture and Storage, in which biomass is burnt to generate electricity and the resulting CO_2 is captured for storage. The energy release through full combustion is clearly greater than that obtained by pyrolysis for biochar production, but the challenge is then lack of complete carbon capture and the cost of transporting and storing CO_2.

- Replenishment of Ecosystem Reservoirs, many of which have been substantially depleted. Arguably, this is needed to repair damage done through land-use change and cannot be counted again as an offset of carbon emissions generated from combustion of deposits laid down millions of years ago. Costs of carbon offsetting through ecosystem capture and storage are relatively modest (see table 2.5). The CCC issued a "Carbon Offsets call for evidence" in early 2022 and will be reporting on the outcomes later in the year (CCC 2022). Broekhoff et al. (2019) provide a review and advice on the use of offsets, noting that many schemes require projects to maintain a buffer to deal with offset reversals caused by, for instance, fires consuming trees. Broekhoff et al. report that the concept of a temporary offset credit which expires after 30 years, introduced in the Clean Development Mechanism has been difficult to implement. A strongly critical view is provided by Watt (2021) in the form of a psycho-analytical ideology critique of the continuing support for carbon offsetting despite its many failures. The Watt analysis draws attention to real problems, but appears to ignore multiple benefits of well managed offset programs described by Broekhoff et al.

- Carbon Capture Use and Storage (CCUS) (Schweitzer et al. 2021; UNECE 2022) refers to the "process of capturing carbon dioxide (CO2) emissions from fossil power generation and industrial processes for storage deep underground or re-use systems which keep CO_2". This is viewed as a bridging technology, paving the way to CCS systems. Many pilot projects have failed (N. Wang, Akimoto, and Nemet 2021) and the sector does not appear likely to attract significant funding without a substantial increase in the carbon price. Despite this, Agency (2021b) describe a net zero scenario based on a rapid scale up of the sector by 2030 to 2Gt annual capacity from "almost nothing" in 2021 (40 Mt Agency 2021a). Many of these prototype projects are based on capturing $CO_2$from fossil fuel extraction processes and so have no potential for contributing directly to offsetting emissions resulting from the combustion of fossil fuel.

  Direct Air Capture (DAC) refers to capture from ambient air. Cost estimates for DAC range from \$30 to \$1000 per tonne of carbon (Sanz-Pérez et al. 2016). From a strategy perspective the absence of a clear pathway to implementing the technology at scale is important. Climeworks (2022) launched a commercial offering in 2021, with a price (April 2022) of £900 per tonne of CO_2 extracted from the atmosphere and stored in rock. This is an important demonstration and practical implementation, with a capacity of 4000 tonnes per year. Fawzy et al. (2021), IEA (2022), and McQueen et al. (2021) suggest that the cost of CCS is likely to fall as the technology scales, but it is unclear at this point whether the technology will attract large scale investment at a carbon price which far exceeds most mitigation costs.

- In the Exhaust Carbon Capture process CO_2 is captured from the waste gasses of an industrial process. This is a mitigation process, reducing existing emissions, but does not directly contribute to compensating for emissions elsewhere. It has been promoted as a step on the road to developing a full scale carbon capture and storage infrastructure, exploiting the high concentrations of CO_2 in some waste gas streams to develop technology. Many proof-of-concept CCUS projects use Exhaust Carbon Capture.

Supplier	Price per tonne of CO_2
Forest Carbon	£22.50
My Carbon Plan	£6.5
Carbon Neutral Britain	£5.60

Table 3.3: A selection of UK CO_2 offsetting suppliers

3.9.3 Doubts about Carbon Capture and Offsetting

Carbon offsetting through biological systems is a special case of Payment for Ecosystem Services (PES). PES provides, according to advocates, "*a transparent system for the additional provision of environmental services through conditional payments to voluntary providers*" (Tacconi 2012).

Kolinjivadi et al. (2017) argue that the PES approach of putting a price on ecosystem services is fundamentally flawed because it neglects the "*complex, non-linear and intertwining reality of both human society and biophysical nature*". Muradian et al. (2013) discuss the traps of the "*compensation logic*" which, according to Muradian et al. underlies the concept of PES and the carbon market.

Compensate (2021) recommend improved criteria and report that 90% of schemes fail.

Tarnoczi (2017) discuss carbon offset risk using data from the carbon market of Alberta, Canada, building on an earlier analysis of the Californian market (Saines and Forrister 2013).

3.9.4 Reducing Emissions from Deforestation and forest Degradation

Parrotta et al. (2022) report on the impact of the REDD+ program (see REDD+ Platform), a vehicle to provide technical and financial support for effort in developing countries to reduce emissions and enhance removals of greenhouse gases through a variety of forest management options. They find that REDD+ plays an important but limited role in climate change mitigation. There is not yet sufficient evidence to reliably evaluate questions around permanence of emission reductions and leakage (the risk that actions taken to limit emissions reductions in one geographical area cause enhanced emissions elsewhere).

3.10 The plus side of the digital research infrastructure carbon account

There are well-founded expectations that digitally enabled research will expand in scale and significance. Increasing importance of numerical simulation; increasing fidelity and flexibility; ability to reduce cost of physical experimentation; accelerate design (e.g. Wilkinson et al. 2020b).

Hopper et al. (2020) and NOC (2021) discuss the positive role that the digital infrastructure in general can play in reducing the carbon footprint of activities by shifting emphasis from physical to virtual investigation.

3.11 Net Zero: What holds us back?

There has been a broad societal commitment to the idea of curbing emissions for some time, but emissions have continued to climb. One possible barrier lies in the gap between conscious intent and decisions influenced by the subconscious (implicit bias Beattie and McGuire 2012, 2016), sometimes referred to as a cognitive barrier (Weber 2017). There can also be conscious decisions based on the perception that others hold greater responsibility. Watt (2021) discusses the desire to accept unrealistic promises.

Whitmarsh et al. (2020, 2021) discuss the factors that prevent individuals from converting an awareness of the carbon footprint of flying into substantial behavioural change. The actual amount of travel by researchers appears to be determined more by social and structural reasons than by attitudes to climate change. The reasons given for travel include a belief in superior quality of face-to-face interactions.

Bache et al. (2015) look at the "pathologies of democratic competition" in the context of local government response to the Climate Change Act (UK Government 2008).

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On behalf of the UKRI Net Zero DRI Scoping Project team.

Methodology

A1 Procedural

A1.1 Literature Survey

An exploratory approach has been taken to develop the literature survey. The topic areas defined in the project work plan, as modified on the basis of feedback by the assessment panel and Steering Committee, have been taken as the basis for literature searches. Key results and themes are drawn out from the search results.

Objective analysis of keywords using the Nees Jan van Eck and Ludo Waltman application and search results from Web of Science is also used to obtain an overview of topics addressed within subject areas and to analyse clusters of activity.

A1.2 Drafts and Review

- Zero order draft : limited review
- First order draft : limited review
- Draft Final: open review

A1.3 Grey Literature

Where possible, this report uses peer reviewed literature. In many areas, however, important information is published through grey literature. This includes authoritative reports from, for instance, the Climate Change Committee or the International Energy Authority, reports by research consortia or consultancies, and even news articles.

We follow the IPCC (e.g. Editorial 2011) in accepting grey literature but taking care to use it with caution and also to be clear about the nature of the information being used. In particular, press releases can give a reliable indication of the ambition and aspiration of organisations, and that is an important indicator of the direction of development in a fast moving industry, but should not be used as the basis of detailed technical analysis. Some organisations, such as the IEA, have rigorous systems for gathering information and their reports can be considered to be as reliable as peer-reviewed literature.

In this report, grey literature will be assigned one of the following categories:

- Authoritative: produced by an authoritative organisation with transparent procedures or containing sufficient evidence of an internal review process (e.g. through community engagement);
- Authoritative Opinion: produced by an individual or individuals placed in a position of trust in an organisation with a reputation for academic independence.
- Commercial: produced by a commercial organisation.
- Opinion: treated as representing the opinion of the authors.

The category assigned will be displayed in the bibliography, as in the following example, which is an editorial from the Nature Climate Change journal:

> Editorial (Aug. 2011). "Evolving the IPCC". In: *Nature Climate Change*. Authoritative Opinion. URL: `https://www.nature.com/articles/nclimate1189.pdf?origin=ppub` (cit. on p. 80).

A1.4 Bibliography Review

One or more technical reviewers will be engaged to perform a systematic review of all sources cited in the bibliography, checking the categorisation of grey literature, the consistency of attributed information with the source and validity of links provided.

It has not been possible to complete this secondary check for the interim report, but a more systematic review will be put in place for the final review.

A2 Technical

A2.1 Units of Measure

The international scientific community has gone through a long process of defining and adopting units of measure which have a universal meaning which is independent of the quantity being measured. This approach is not yet universal, and a notable exception is widespread in the climate impacts and climate policy community with quantities such as as the carbon intensity of power generation being expressed in pseudo-units of gCO_2-eq / kWh. While this approach is clearly understood by all concerned, it is likely to create problems if used in a database designed for automated processing in which software expects units to follow SI. Exceptions to handle non-SI units can easily be added in local software tools, but interoperability is impaired. Since interoperability is a key element of enhancing efficiency in order to minimise waste through duplication and barriers to re-use, we here adopt SI. This means that "a carbon intensity of 6 gCO_2-eq / kWh" will be expressed as "a CO_2-equivalent intensity of 6 g / kWh". Where the timescale over which equivalence is determined needs to be expressed explicitly, the form "a 100-year CO_2-equivalent intensity of 6 g / kWh". In this report, when the time scale is not given, it is assumed to be 100 years.

Glossary

API Application Programming Interface (API) is a type of software. Application refers to any software with a distinct function and interface is a contract of service between two applications. 51

Approximate computing Approximate computing is an emerging paradigm for energy-efficient and/or high-performance design which includes a plethora of computation techniques that return a possibly inaccurate result rather than a guaranteed accurate result, and that can be used for applications where an approximate result is sufficient for its purpose. 68

Benchmarking Benchmarking is usually associated with assessing performance characteristics of computer hardware, for example, the floating point operation performance of a CPU, but there are circumstances when the technique is also applicable to software. Software benchmarks are, for example, run against compilers or database management systems (DBMS). Benchmarks provide a method of comparing the performance of various subsystems across different chip/system architectures. 68, 73

Biodiesel Biodiesel is a form of diesel fuel derived from plants or animals. 65

C++ C++ is a general-purpose programming language. It is extension of the C programming language with classes. 73

Carbon intensity The emission rate of a given pollutant (carbon dioxide in this instance) relative to the intensity of a specific activity, or an industrial production process; for example grams of carbon dioxide released per megajoule of energy produced, or the ratio of greenhouse gas emissions produced to gross domestic product (GDP). See also Carbon Intensity API. 19, 38, 47

Catena A connected series of related things. 17

CFD Computational Fluid Dynamics: modeling physical phenomena involving fluid flow through computational solutions. 73

Circular economy The circular economy, which promotes the elimination of waste and the continual safe use of natural resources. 71

Clean Development Mechanism The Clean Development Mechanism (CDM), defined in Article 12 of the Kyoto Protocol, allows a country with an emission-reduction or emission-limitation commitment under the Kyoto Protocol (Annex B Party) to implement an emission-reduction project in developing countries. Such projects can earn saleable certified emission reduction (CER) credits, each equivalent to one tonne of CO2, which can be counted towards meeting Kyoto targets. 76

cyberinfrastructure From cyber, which means relating to computers/information technology and the word infrastructure, which is a organisational structure or facility. Cyberinfrastructure is referring to information technology systems with very powerful and advanced capabilities. 34, 35

DCMS UK Department for Digital, Culture, Media and Sport. 34

Department of Energy US Department of Energy. 74

Ecosystem Services Ecosystem Services are the direct and indirect contributions ecosystems (known as natural capital) provide for human wellbeing and quality of life. This can be in a practical sense, providing food and water and regulating the climate, as well as cultural aspects such as reducing stress and anxiety. 77

Embodied carbon In the building industry, embodied carbon refers to the greenhouse gas emissions arising from the manufacturing, transportation, installation, maintenance, and disposal of building materials. More generally, embodied carbon is the amount of carbon pollution emitted during the creation and disposal of a device (sometimes referred to as “Embedded Carbon”). 20, 63, 71

False equivalences This is when equivalence is drawn between two subjects based on flawed or false reasoning. The colloquial equivalent of this term is the expression ”comparing apples and oranges”. 61

Freemium Freemium, a portmanteau of the words ”free” and ”premium,” is a business model in which a company offers basic or limited features to users at no cost and then charges a premium for supplemental or advanced features. 63

Greenwash Publicity material which, knowingly or otherwise, misleads people about the environmental sustainability of an organisations products or business model. 62

GWP The Global Warming Potential (GWP) allows the comparisons of the global warming impacts of different gases. Specifically, it is a measure of how much energy the emissions of 1 ton of a gas will absorb over a given period of time, relative to the emissions of 1 ton of carbon dioxide. 45

HDD A Hard Disk Drive is a electro-mechanical data storage device (WikipediA). 71

Horizon 2020 Horizon 2020 was the EU's research and innovation funding programme from 2014-2020 with a budget of nearly €80 billion, the predecessor of Horizon Europe. 51

HPC High Performance Computing (HPC) generally refers to processing complex calculations at high speeds across multiple servers in parallel (Red Hat 2021) . 1, 5, 55

Implicit bias In social identity theory, an implicit bias or implicit stereotype, is the pre-reflective attribution of particular qualities by an individual to a member of some social out group. 78

IT "Information technology is a broad term that involves the use of technology to communicate, transfer data and process information" Comptia (2022). 44, 47, 71

John Houghton Sir John Theodore Houghton CBE FRS FLSW (30 December 1931 – 15 April 2020) led the first three Intergovernmental Panel on Climate Change (IPCC) reports. He was co-chair of the IPCC scientific assessment working group which shared the Nobel Peace Prize in 2007 with Al Gore.. 12

Julie's Bicycle This is a not-for-profit that aims to mobilise the arts and culture to take action on the climate and ecological crisis. 19

Kubernetes Kubernetes, also known as K8s, is an open-source system for automating deployment, scaling, and management of containerized applications. Google originally designed Kubernetes, but the Cloud Native Computing Foundation now maintains the project. 74

Lattice gauge theory Lattice gauge theory is a formulation of quantum field theory with gauge symmetries on a discrete space-time lattice which can be solved by computation. 73

LCA Life Cycle Assessment: Compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle. An LCA identifies the main contributors (materials, energy sources, etc.) to key environmental impacts throughout the products entire life cycle. 50, 71

LCIA Life Cycle Inventory Analysis (LCIA) is a part of the Life Cycle Assessment (LCA) and is a thorough procedure accounting for the environmental loads during the product's life cycle. 50

location-based The location-based approach to carbon accounting of scope 2 emissions (e.g. from purchased electricity) reflects the average emissions intensity of the grid based on the location where the energy is consumed. 36

market-based The market-based approach to carbon accounting of scope 2 emissions (e.g. from purchased electricity) is based on electricity bought via contractual instruments such as power purchase agreements (PPAs). 36

MPI Message Passing Interface: a standardized and portable message-passing standard designed to function on parallel computing architectures. 72, 73

NC3Rs The National Centre for the Replacement, Refinement and Reduction of Animals in Research. This is a UK based scientific organisation dedicated to helping the research community to use the 3Rs in technologies and approaches. 19

Net Zero Challenge The challenge of achieving global neutrality in carbon emissions as the first step on a journey to stabilising climate and reversing the increase in dangerous climate extremes. Although net zero is well defined at the global level, there is controversy at the national level and an open and anarchic field at the organisational level. 14

Non-Departmental Public Body A Non-Departmental Public Body (NDPB) is a body which has a role in the processes of national government, but is not a government department or part of one, and which accordingly operates to a greater or lesser extent at arm's length from ministers (Cabinet Office 2006). 36

PCF The Product Carbon Footprint (PCF) sums up the total greenhouse gas emissions generated by a product over the different stages of its life cycle. 71

PFC Per-flourinated compounds: organic substances in which all of the hydrogen atoms of the hydrocarbon backbones are substituted with fluorine atoms. Potentially released in integrated circuit manufacture. 44, 45

PFlops Petaflop is a unit to measure a computer's processing speed. It is a quadrillion (10^{15}) floating point operations per second (FLOPS). 19, 68

PPA A **Power Purchase Agreement** is an agreement through which a company contracts an electricity generator (such as a company running a wind or solar farm) to supply it with electricity over an extended period of time, typically 10 to 20 years. 74, 85

PUE Power Usage Effectiveness is a ratio that describes how energy efficient a computer data centre is. In other words, PUE is equal to the ratio of total energy used by a computer data centre facility to the energy delivered to computing equipment. 53

qubit A quantum bit, the basic unit of quantum information in quantum computing. 69

Rebound effect "The reduction in expected gains from new technologies that increase the efficiency of resource use, because of behavioral or other systemic responses" (Wikipedia 2022a). 5, 18, 38, 48

REDD+ REDD+ (reducing emissions from deforestation and forest degradation; conservation of forest carbon stocks; sustainable management of forests; and enhancement of forest carbon stocks) is a framework created by the UNFCCC Conference of the Parties (COP) to guide activities in the forest sector that reduces emissions from deforestation and forest degradation, as well as the sustainable management of forests and the conservation and enhancement of forest carbon stocks in developing countries. 77

Responsive mode Responsive mode Research Council funding is a stream designed to support ideas generated in the scientific community. 34

SF_6 Sulfur hexafluoride or sulphur hexafluoride (British spelling) is an extremely potent and persistent greenhouse gas that is primarily used by the electricity industry as an electrical insulator and arc suppressant to keep networks running safely and reliably.. 37, 44, 45, 65

SI The International System of Units, known by the international abbreviation SI, is the modern form of the metric system and the world's most widely used system of measurement. 81

Speculative Execution An optimization technique where a computer system performs some task that may not be needed. 57

SSD A solid-state drive (SSD) is a solid-state storage device that uses integrated circuit assemblies to store data persistently (WikipediA). 71

TFlops Teraflop is a unit to measure a computer's processing speed. It is a trillion (10^{12}) floating point operations per second (FLOPS). 68

unavoided emissions Some limited emissions of CO_2 may remain unavoided, such as those emitted through the shipping of goods. 1, 25, 30

UNFCCC United Nations Framework Convention on Climate Change. 115

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