

Architecture and Design Aspects in Building Sustainable Large Scale Digital Infrastructures for Research

Abstract—Modern science is data driven, growingly digitalized, and extensively uses High Performance and Data Science Analytics technologies, which require large scale Digital Research Infrastructures (RI) that should support the automation of experiments, data collection, and the handling of vast amounts of experimental data. There is also an increasing demand from all research domains for AI and LLM powered research workflow design and operation, what poses significant challenges to the energy efficiency and sustainability of digital RIs. The paper presents the results and ongoing development in the GreenDIGIT project that is devoted to proposing architecture and technical solutions to make future digital RIs sustainable by achieving energy efficiency and reducing environmental impact while increasing the efficiency of the research workflows. The paper provides an analysis of the sustainability-related standards and regulations to derive/ elicitate the necessary design requirements. The proposed Shared Responsibility Model for Sustainability provides a basis for defining areas of responsibility of the RI Operator and Researcher and necessary architectural and design solutions that need to be embedded in the technical RI design. The presented layered architecture includes both functional components to be implemented in the RI/data center and sustainability aware research development tools.

Keywords—*Research Infrastructure, High Performance Computing and Data Driven Science, Sustainable Research Infrastructure, Shared Responsibility Model for Sustainability, Architecture and Design Principles, Standards and Regulations for Sustainability.*

I. INTRODUCTION

Modern science is data driven, growingly digitalised and extensively uses High Performance Computing (HPC) and Data Science Analytics technologies. It is increasingly powered by digital infrastructures that support the automation of experiments, data collection, and the handling of vast amounts of experimental data. These digital Research Infrastructures (hereafter referred to as RIs or DRIs) are

crucial for advancing scientific discovery in fields such as genomics, climate science, materials research, and artificial intelligence. They provide HPC, cloud resources, and advanced data management systems to support data collection, processing and scientific workflow management. This allows researchers to streamline complex workflows and accelerate the pace of innovation.

An important driver of this growth is the increased use of machine learning (ML) based data processing, which plays a critical role in research across diverse disciplines. Whether it's analyzing large-scale genomic data, processing real-time environmental data, or interpreting experimental results from particle physics, ML models are now central to data-driven research. Furthermore, the recent advances in generative artificial intelligence (AI) and large language models (LLMs) are transforming research workflows by enabling new forms of data generation, hypothesis generation, and automation in scientific writing and analysis.

While these AI-driven approaches offer tremendous potential, they also pose significant challenges to the energy efficiency and sustainability of digital RIs. Large-scale training and inference of ML models, particularly for generative AI and LLMs, require substantial computational resources, often consuming vast amounts of energy. For instance, training a state-of-the-art LLM can result in significant carbon emissions due to the intensive use of GPUs and distributed computing resources. As the research community increasingly relies on these models, addressing their energy consumption has become critical to the sustainability of digital research infrastructures.

In response, there is a growing emphasis on integrating energy efficiency and sustainability principles into the architecture of RIs. Efforts such as energy-efficient experiment scheduling, dynamic resource scaling, and the incorporation of renewable energy sources are being explored to reduce the energy footprint of research

workflows. Additionally, emerging techniques like AI-driven resource management, edge computing, and optimized ML model training are beginning to offer pathways to reduce the environmental impact of advanced AI-based processing.

Despite these developments, current approaches often remain fragmented, addressing only specific aspects of the infrastructure. This paper proposes a comprehensive architecture that embeds energy efficiency and sustainability into the core design of digital research infrastructures, including optimisation techniques tailored for ML, generative AI, and LLM processing. By rethinking the design of computing, storage, and data transfer processes, and integrating emerging energy-saving technologies, we aim to provide a scalable framework that supports the growing computational demands of modern research while minimizing its environmental impact. As research increasingly relies on AI and large-scale data processing, ensuring that these infrastructures are both powerful and sustainable is essential for aligning scientific progress with global sustainability goals.

Europe has well-established practices in building and operating dedicated domain-specific RIs coordinated by ESFRI (European Strategy Forum on Research Infrastructures) [1], which recognises the importance of both environmental research support and improving energy efficiency and reduced environmental impact in the sustainability of future RIs. This aspect is planned to be addressed in the future ESFRI Roadmap 2026 [2].

This paper presents the results and the ongoing development of the EU funded GreenDIGIT project [3], which is committed to proposing architectural, technical and policy solutions to ensure the sustainability of future RIs, in alignment with the ESFRI policy on sustainability. The paper provides analysis of standards and regulations related to sustainability, the Shared Responsibility Model for Sustainability, and discusses a wide range of architectural and design aspects to achieve RI sustainability through the whole lifecycle, including responsibility domain for both RI operators and researchers.

The paper refers to past and recent authors' publications related to the architecture definition for the general Platform RI as a Service (PRIaaS) [4], Sustainable Architecture Design Principles [5] [6] that provide the basis for system and application design, and another paper [7] focused on the experimental research reproducibility and experimental data management, which all provided the necessary background research for defining architecture solutions for RI sustainability.

The paper is organised as follows. Section II provides background information on the global and European initiatives to facilitate the sustainability of the digital RIs. Section III provides an analysis of the existing standards and regulations for energy efficiency and environmental impact and provides mapping to RI and data center functional components. Section IV introduces the proposed Shared Responsibility Model for sustainability and provides a breakdown of expected responsibilities for RI Operator and

Researcher. Section V discusses the architectural and design aspects for sustainable RIs that includes layered architecture and corresponding design suggestions for different architecture components. Section VI discusses the required functionality for the Research Development Environment that should allow sustainability aware research applications development. Conclusion in Section VII summarises the presented technical solutions and outlines the future project developments, inviting the community for discussion and cooperation.

II. GLOBAL AND EUROPEAN INITIATIVES TO FACILITATE SUSTAINABILITY OF RESEARCH INFRASTRUCTURES

A. *Global Initiatives*

Global initiatives aimed at reducing the carbon footprint and promoting sustainability in research infrastructures are growing in number and impact. The most important among them is the United Nations Sustainable Goals (SDGs) [8], which form a global framework for achieving a sustainable future. The SDG goals SDG 9 (Industry, Innovation, and Infrastructure) and SDG 13 (Climate Action) are particularly relevant to research infrastructures:

- SDG 9 emphasizes building resilient infrastructure and fostering innovation, which includes making research infrastructures sustainable by improving energy efficiency, adopting renewable energy, and reducing carbon emissions.
- SDG 13 calls for urgent action to combat climate change, urging research institutions and infrastructures to reduce their carbon footprints through environmentally sustainable practices

The Climate Neutral Data Centre Pact [9], initially proposed as a European initiative, currently become an industry-led initiative to reduce the environmental impact of data centers, including those used by research infrastructures. The key commitments include energy efficiency, use of renewable energy, waste heat reuse, and water and waste management. This initiative directly impacts research infrastructures that rely heavily on data centers for computing, storage, and data processing.

As an interesting move, the famous Top500 list [10] of the most powerful computers started compiling the Green500 list [11] where European supercomputers occupy the top 3 spots in the Green500 edition of June 2024.

The Research Data Alliance (RDA) identified the sustainability of research data infrastructures as an important activity and established the Sustainability Task Force that is focused on reducing the environmental impact of storing, processing, and managing research data [12]. This includes energy-efficient data management, green cloud computing, and open access to environmental data. These efforts are essential for ensuring that scientific and technological advancements can be pursued without exacerbating climate change and environmental degradation. By following global best practices and participating in these initiatives, research infrastructures can significantly contribute to a more sustainable future.

B. European Initiatives

The European Green Deal [13] is the overarching framework for making Europe the first climate-neutral continent by 2050. It sets ambitious targets for reducing greenhouse gas emissions, improving energy efficiency, and adopting renewable energy across all sectors, including research infrastructures.

Horizon Europe [14], the EU's main research and innovation funding program (2021–2027), places sustainability and the reduction of CO₂ emissions as key priorities for research infrastructures. The program funds projects that aim to develop and operate research facilities in a sustainable, low-carbon manner. The GreenDIGIT project [3] is one of the EU funded projects on RI sustainability that sets a number of objectives to make the future European RIs greener.

The European Strategy Forum on Research Infrastructures (ESFRI) plays a central role in promoting the development and sustainability of large-scale research infrastructures across Europe. In the new Roadmap 2026, ESFRI will focus on strengthening the approach of collaborating towards building a robust and sustainable European Research Infrastructure Ecosystem [15].

The European Open Science Cloud (EOSC) initiative, currently supported by the EU EOSC Node [16], aims to create a cloud-based infrastructure that allows researchers to access and share data efficiently across Europe. While focused on data sharing, EOSC will emphasise sustainability in its design and operation that includes energy-efficient data storage, optimized data transfer, sustainable cloud infrastructure to support research process and data analytics.

The EuroHPC Joint Undertaking is a major European initiative aimed at building a world-class supercomputing infrastructure [17]. Since supercomputing facilities are typically highly energy-intensive, EuroHPC intends to set a strong focus on sustainability and reducing the environmental footprint of high-performance computing (HPC) systems.

The EU Code of Conduct for Data Centres Energy Efficiency (EU DC CoC) [18] is a voluntary initiative set up by the Joint Research Centre (JRC) in response to the increasing energy consumption in data centres and the subsequent environmental, economic and energy supply security impact that arises from this. It provides guidelines and best practices to improve energy efficiency in data centers, thereby reducing their CO₂ footprint. The main focus includes Energy-Efficient Design and Operation, Energy Monitoring, Cooling Efficiency, Server Utilization. By following these guidelines, data centers can significantly reduce their energy consumption and environmental impact.

C. GreenDIGIT Project and Focus on Future Green RIs

The GreenDIGIT project is a Horizon Europe funded project that is focused on reducing the environmental impact of Research Infrastructures (RIs) from the generic conceptual point of view by addressing all major factors that define and influence the RI environmental and climate impact. GreenDIGIT was initiated by 4 Digital Research

Infrastructures to address vital needs of the future ESFRI Research Infrastructures and other digital service providers for science in lowering energy consumption and environmental impact:

EGI [19]: Open Ecosystem for Research and Innovation and Advanced Computing Services for Research.

SoBigData [20]: distributed, Pan-European, multi-disciplinary research infrastructure aimed at social mining and Big Data to understand the complexity of our interconnected society.

SLICES [21]: A distributed Research Infrastructure to support large-scale experimental research on Digital Technologies.

EBRAINS [22]: A digital research infrastructure for brain science and brain-inspired technology.

The development in GreenDIGIT is focused on the three interconnected aspects of the DIR design and operation:

- **Energy Efficiency in Digital Infrastructures:** This refers to optimizing digital infrastructures to consume as little energy as possible for a given workload or service. It's about achieving more computational or storage results with less energy input. The outcome will include Architecture definition, Design, and Recommendations.
- **Decarbonization of Digital Infrastructures:** This specifically targets the reduction of carbon emissions associated with the operation and maintenance of digital infrastructures. The outcome will include operation management, monitoring, KPI and metrics definition.
- **Reducing the Environmental Impact of Digital Infrastructures:** This is a more comprehensive consideration of the various ways digital infrastructures might affect the environment, going beyond just energy consumption and carbon emissions. The outcome will include RI lifecycle management, policy and certification, training.

The GreenDIGIT objectives include the whole spectrum of activities that will provide a basis for greening future RIs: **Landscape analysis:** Assess the status and trends of low-impact computing in digital RIs to produce technical and policy recommendations.

Reference architecture and design principles for RI Sustainability, and an actionable model for environmental impact assessment and monitoring, reflecting on the whole RI lifecycle.

New and innovative technologies, methods, and tools for digital service providers within European Research Infrastructures through which they can reduce their energy consumption and overall environmental impact.

Develop and provide technical tools for researchers that assist them in the design, execution and sharing of environmental impact aware digital applications with reproducibility, Open Science and FAIR data management considerations.

Educate and support digital service providers and researchers in the RI communities about good practices on environmental impact conscious lifecycle management and operation of infrastructures and services.

This paper provides information about the recent GreenDIGIT results that may be interesting for the community and will benefit from the wider discussion.

III. STANDARDS AND REGULATIONS FOR SUSTAINABILITY

A. Data Centers and the Challenge of Energy Efficiency

Data centers form the backbone of digital research infrastructures, hosting the computational power, storage, and networking resources that support modern scientific workflows. However, their significant energy demands make them a key contributor to the environmental footprint of research infrastructures. Data centers require large amounts of electricity to power servers, storage devices, and networking equipment, as well as cooling systems to maintain operational efficiency. As a result, reducing the energy consumption and carbon footprint of data centers has become a critical concern in the pursuit of sustainable research infrastructure.

To address these challenges, various international standards and regulations have been developed, focusing on energy efficiency, carbon footprint reduction, and environmental impact mitigation. These standards help organizations implement best practices and monitor key performance indicators (KPIs) for energy management, ensuring compliance with sustainability goals. Below is a summary of the key ISO and European EN standards and regulations that are relevant to data center sustainability.

B. ISO and European EN Standards and Regulations

1) ISO 50001: Energy Management Systems [23]

ISO 50001 provides a framework for organizations to establish, implement, maintain, and improve energy management systems (EnMS). It enables organizations to improve energy performance by developing energy policies, setting measurable objectives, and regularly monitoring energy use. Data centers can benefit from ISO 50001 by integrating energy management practices into their daily operations, allowing them to identify inefficiencies and optimize energy use. This standard also helps data centers reduce their CO₂ emissions through structured energy management. ISO 50001 is complemented with ISO 50002 Energy audits - Requirements with guidance for use [24].

2) ISO 30134: Data Center KPIs [25]

The ISO 30134 series defines key performance indicators (KPIs) to evaluate the energy efficiency of data centers. Some of the most important KPIs in this series include:

- **Power Usage Effectiveness (PUE):** One of the most widely recognized KPIs, PUE measures the ratio of total data center energy consumption to the energy used by the IT equipment alone. A lower PUE indicates better energy efficiency.
- **Renewable Energy Factor (REF):** This KPI measures the proportion of energy used in the data center that comes from renewable sources, such as solar or wind power.

- **Carbon Usage Effectiveness (CUE):** CUE quantifies the total carbon emissions associated with data center operations. It helps organizations track their progress in reducing their carbon footprint.

These KPIs allow data centers to benchmark their energy performance, set targets for improvement, and comply with regulatory requirements for energy efficiency.

3) ISO 14001 Environmental Management Systems [26]

ISO 14001 focuses on environmental management and aims to help organizations minimize their environmental impact, including energy consumption, waste production, and carbon emissions. For data centers, this standard provides a framework for identifying and managing environmental risks, ensuring compliance with environmental laws, and implementing practices that support sustainability, such as energy-efficient cooling systems and responsible e-waste management.

4) EN 50600: Data Center Facilities and Infrastructure [27]

The EN 50600 series of standards is a European framework specifically addressing the design and operation of data centers. It covers various aspects of data center infrastructure, including power distribution, cooling, physical security, and environmental controls. In terms of energy efficiency, EN 50600 provides guidelines on:

- **Energy-efficient cooling systems:** It emphasizes best practices for designing and operating cooling systems to minimize energy consumption.
- **Energy management and monitoring:** EN 50600 promotes the continuous monitoring of energy use and the application of energy-saving techniques throughout the data center lifecycle.

By complying with EN 50600, data centers can ensure that their facilities are designed and operated with energy efficiency in mind, contributing to lower operational costs and reduced carbon emissions.

5) The EU Code of Conduct for Data Centres Energy Efficiency [28] [29]

As mentioned in the previous section, the EU DC CoC aims to promote energy-efficient practices and reduce the environmental impact of data centres across Europe. It provides a set of best practices that data centers can adopt, including:

- **Optimizing IT equipment utilization:** Encouraging the consolidation and virtualization of IT workloads to reduce idle energy consumption.
- **Improving cooling efficiency:** Recommending the use of free cooling and efficient airflow management to reduce cooling energy needs.
- **Renewable energy integration:** Encouraging data centers to source energy from renewable providers.

As an important aspect, the EU DC CoC defines different roles of participants: Operator, Colocation provider. Colocation customer. Managed services provider, Managed services provider in colocation space, and surely researcher or research project as a consumer; and areas of responsibility/management: Physical building, Mechanical and electrical plant, Data floor and air floor, Cabinets and

cabinets, airflow, Metrics and operation measurement points, IT equipment, Operating systems and virtualisation, Software, Operational practices and policies. Participants in the Code of Conduct voluntarily commit to these best practices and report their progress, contributing to the EU's overall energy efficiency and climate goals.

EU DC CoC is complemented with the Commission Delegated Regulation [30], published on 14 March 2024, that provides practical recommendations on methodology and KPI measured and communicated to the European database of data centers twice a year (with the first report required on 15 Sept 2024).

C. Linking Standards and Regulations to Data center and RI functional components

From the implementation and design point of view, it is important to identify the main functional components, services and processes or operations present in a typical data center as a core part of the RI. Figure 1 provides such an illustration and includes data center computing facilities and IT equipment (compute, storage, network), building and environmental facilities (cabinets, cabling, power supply and UPS, cooling, water), operational processes (planning, management, monitoring, data collection, analysis and optimisation, policy).

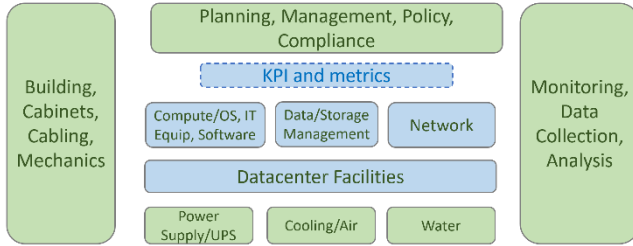


Figure 1. Data center functional components linked to the EU Code of Conduct for Data Centres Energy Efficiency (EU DC CoC) and other related standards.

By linking standards and regulations to functional components of data centers and digital research infrastructures, organizations can systematically implement energy-efficient practices. Collecting and analyzing relevant metrics is critical to benchmarking performance, identifying inefficiencies, and ensuring compliance with international standards. This allows for both reducing energy consumption and operational costs, and also contributing to reducing the carbon footprint of data centers, making them a cornerstone of sustainable research infrastructure.

Referring to data center IT equipment the following metrics are recommended to collect according to ISO 50001, EN 50600, and EU DC CoC:

- Power usage effectiveness (PUE) for both the overall data center and for specific IT components.
- Utilization rates: Track server and storage utilization rates to ensure the hardware is being used efficiently and that energy is not wasted on underutilized or idle resources.
- Processor and server power draw: Measure energy consumption at the component level for processors,

memory, and storage units. This data can help optimize energy usage per workload.

- Energy per operation: For AI and machine learning tasks, measure the energy consumed per inference or training run, particularly for large-scale models like LLMs.

An important element of sustainability related standards is the definition of organisational roles dealing with datacenter operation and related design and management decisions. Refer to the EU DC CoC and section B.5 above for more detailed roles definition) roles of participants. The definition of roles and their responsibility allows efficient stakeholder interaction and independence in their business development.

IV. SHARED RESPONSIBILITY MODEL FOR SUSTAINABILITY

Based on the standards and regulations study and supported by the European RI landscape study, the GreenDIGIT project identified a set of requirements and practices related to both RI operators and researchers that need to be brought in compliance and practical implementation. This is defined in the proposed Shared Responsibility Model for achieving sustainable digital RI operation. It clearly defines the roles and responsibilities of both the RI operator and the researcher in reducing the environmental impact and promoting energy-efficient practices. This model is essential for ensuring that both infrastructure management and research practices contribute to sustainability goals. Figure 2 below illustrates the separate responsibilities of the RI provider or operator and the responsibilities of the researcher or research project together with the functional elements that need to support necessary technical solutions for the proposed Shared Responsibility Model.

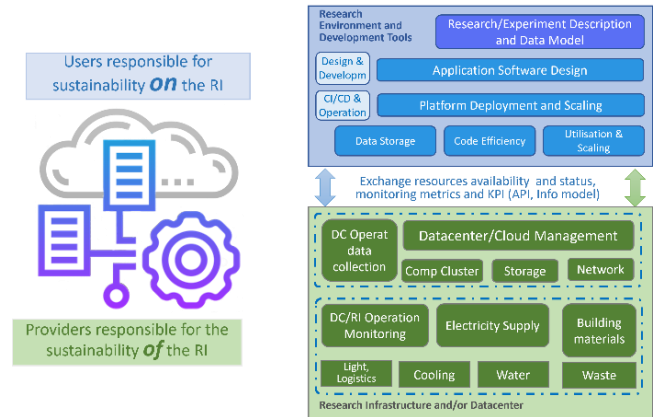


Figure 2. Shared Responsibility Model for Research Infrastructure Sustainability: Sustainability *of* the RI and Sustainability *on* the RI (for research applications)

The following is a suggested breakdown of RI operator and Researcher responsibilities.

RI Operator Responsibilities:

- Energy-efficient infrastructure: The operator is responsible for the underlying infrastructure, including implementing energy-saving technologies such as

energy-efficient cooling, virtualization, and workload management systems. They must ensure the infrastructure meets international sustainability standards and provides researchers with tools to monitor their energy use.

- Resource allocation and scheduling: The operator must offer energy-aware resource allocation systems that dynamically adjust resources according to energy availability, and ensure that computational and data storage tasks are allocated in a way that maximizes energy efficiency.
- Monitoring and feedback: RI operators should provide real-time feedback on energy consumption, offer automated suggestions for energy optimization, and make energy-saving features easily accessible to users.
- Use of renewable energy: Operators should maximize the use of renewable energy sources, communicate availability, and ensure that the infrastructure can efficiently switch between energy sources.

Researcher (and research project) Responsibilities:

- Energy-efficient workflows: Researchers must optimize their workflows by taking advantage of energy-saving features provided by the RI. This includes optimizing data transfers, minimizing resource-intensive operations, and scheduling jobs to align with off-peak energy usage or renewable energy windows.
- Data Management: Researchers should actively manage data storage to minimize energy usage. This includes selecting storage options from different types of data, deleting unnecessary datasets, compressing data, and using energy-efficient storage options.
- Adopt best practices: Researchers need to stay informed about sustainability best practices and incorporate them into their daily workflows, following recommendations and feedback provided by the DRI operator.

Training and Awareness on best practices and technical solutions for sustainability is important for both the operators and researchers. Training and guidelines for energy-efficient practices should facilitate the creation of a culture of sustainability within the research community.

To implement a workable shared responsibility model for sustainable digital research infrastructure operation, the architecture design must include solutions that support real-time monitoring, energy-efficient resource scheduling, feedback systems, sustainable data management, and collaboration tools. These components must empower both the RI operator to manage the infrastructure efficiently and the researcher to optimize their workflows with sustainability in mind. The integration of renewable energy, training, and compliance tracking ensures that all parties are aligned in achieving energy and resource efficiency, contributing to a truly sustainable research ecosystem.

V. DEFINING ARCHITECTURAL DESIGN ASPECTS FOR RI SUSTAINABILITY

A. General System and Software Architecture Design Principles

To address the architecture and design aspects for future sustainable RIs in compliance with the existing standards and regulations, and make the Shared Responsibility Model actionable and workable, the GreenDIGIT is progressing with the defining elements of the “Sustainability by Design” principles based on the best practices in the system and applications/software widely defined by the developer (and DevOps) community.

In this respect, we refer to the ongoing authors’ work on defining the Sustainable/Durable Architecture Design Principles (SADP) and corresponding design patterns introduced in the authors’ previous works [5] [6] and currently being implemented in educational and training materials. SADP summarises the best practices in System and Software Engineering and includes the following architecture design groups:

- General architecture design principles that include layered architecture design for services and mechanisms, including inter-layer interfaces, multi-tier services and infrastructure design, API definition, and stakeholders and roles model defining the main actors and their relationships.
- Service architecture related group that include Service Oriented Architecture (SOA) and Microservices Architecture (MSA), options for cloud native design principles, service lifecycle management model.
- Data management infrastructure and services related group, including information and data models definition supported by metadata definition and management.
- Security and compliance design principles for infrastructure services and applications.
- Project Management and DevOps, including general compliance with the project management principles, models and procedures applied to infrastructure, services, and data handling and analytics.

Sustainable architecture design principles provide recommendations and guidance for the evolutionary approach in designing and implementing complex infrastructure projects. This will create a strong basis for developing the sustainability design principles and necessary design patterns for addressing energy efficiency and reduced environmental of the future RIs through the whole RI lifecycle.

B. Layered RI Architecture for Sustainability Design

Figure 3 illustrates the layered RI architecture that can provide a basis for RI and research applications design for sustainability. The following layers are components of the efficient research ecosystem, including both operated by RI or data center provider and research applications that may be under control of the researcher:

- RI or data center providing compute and storage services that include physical compute, storage, network resources and necessary provisioning functionality,

typically supported by the proprietary and Open Source cloud platforms. Data center should provide KPI and metrics that can be used by upper layer applications. RI and data centers should also provide monitoring, data analytics and optimisation functionality. An overview of the KPI, metrics and required monitoring functionality is provided in details in section III.

- Scientific Workflow and Applications layer provides an environment for executing the domain, project and experiment specific workflow. This also includes a software and execution platform, which can be part of RDE but should not be a focus of the research applications development.
- Research Tools and Portal include both local researcher workplaces supported by SDK/RDE and may also include DevOps (which in the future can include sustainability aspects in DevSustOps) to support effective cooperation of the research project team.
- The upper layer of the Researcher, Organisation or Project is important to include because of continuously required policy based decisions, expertise in designing scientific workflows and research results assessment. To support this, the Research Tools and Portal should provide human readable reports and visualisation of the workflow execution or experiment progress. This is typically provided with the real-time dashboard, with available multiple dashboard platforms for development.

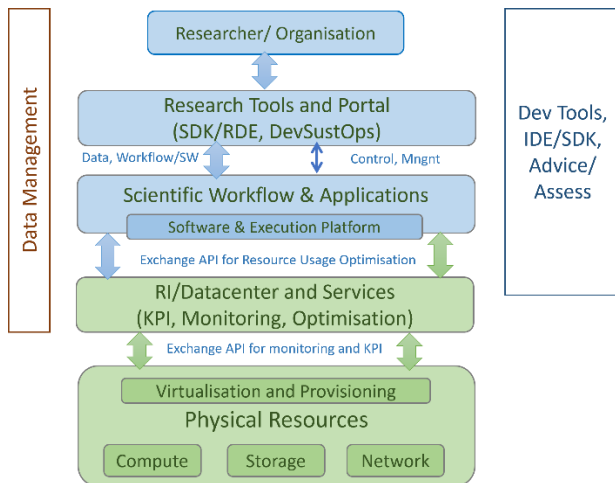


Figure 3. Research Infrastructure layers to address design aspects for sustainability: RI/Data center, and Research workflow and tools.

The sustainability principles must be directly embedded into the architecture and design of digital RIs, data centers, and scientific workflows. This approach ensures that energy efficiency, resource optimisation, and environmental impact minimization are considered from the beginning, rather than being retrofitted into existing systems. To effectively implement Sustainability by Design, several architecture and design aspects must be defined and addressed across hardware, software, operational, and governance layers.

Below are the key considerations:

1. Energy-Efficient Infrastructure Design: At the foundational level, the infrastructure must be designed to

minimise energy consumption while maximising operational efficiency. This includes the choice of hardware, layout, cooling systems, and energy sources.

The key aspects should include: Energy-Efficient Hardware, Modular and Scalable Infrastructure, Sustainable Power Management, Green Energy Integration, and energy-efficient cooling Systems. The design objectives should include minimising idle power consumption, reducing cooling energy costs, maximize renewable energy usage.

An important element of the general infrastructure design is the exchange API and information model that should connect KPI, metrics, metadata and semantics. This is required to ensure effective and reliable/trusted sustainability related information exchange: horizontally between datacenters, RI nodes and operational elements; and vertically between RI architecture layers such as datacenter and scientific applications, workflow management system and user tools.

2. Energy-Aware Software and Applications: Software systems running on the infrastructure must be designed to minimize energy consumption without sacrificing performance or functionality.

Key aspects should include:

- Energy-efficient algorithms: Implement energy-efficient algorithms that minimize computational complexity and avoid unnecessary resource usage. For example, using approximation algorithms or AI/ML models optimized for lower energy usage during training and inference.
- Software optimization for power-aware architectures: Design software that takes advantage of hardware power management features (e.g., DVFS, multi-core processors) to dynamically reduce energy consumption during runtime.
- Energy-aware virtualisation and containerization: Virtualized environments (e.g., VMs, containers) should be energy-aware, allowing for the dynamic scaling of virtual resources based on real-time demand. Implement container orchestration systems (e.g., Kubernetes) that include energy-efficient scheduling policies.
- Intelligent data handling: Minimize data transfers and storage requirements by using techniques such as data compression, deduplication, and caching. Optimize data movement across networks to reduce energy-intensive communication.

Design objectives should include reducing energy consumption at the application and software level, optimising energy usage across virtualised and containerised environments, and minimising computational and storage overhead.

3. Energy-Aware Workflows and Resource Scheduling: Research workflows and resource scheduling systems must be designed to prioritize energy efficiency and resource optimization.

Key aspects should include:

- Energy-efficient workflow scheduling: Implement workflow schedulers that prioritize energy-efficient resources (e.g., low-power nodes, servers powered by

renewable energy) and run workflows during off-peak energy periods or when renewable energy is abundant.

- **Dynamic resource allocation:** Use dynamic resource allocation systems that match resources to the current demand in real-time. This reduces over-provisioning, where unused resources continue to consume energy unnecessarily.
- **Workflow consolidation:** Where possible, consolidate workflows onto fewer, more energy-efficient nodes to reduce idle power consumption across infrastructure components.
- **Flexible execution windows:** Allow for flexible execution windows where researchers can schedule tasks to run during periods of lower energy demand or higher renewable energy availability.

4. Sustainable Data Management: Data handling is a critical part of research infrastructure, and designing for sustainability means reducing the energy impact of data storage, retrieval, and movement.

Key aspects should include:

- **Tiered storage systems:** Use tiered storage that places frequently accessed data in high-performance, energy-efficient storage solutions (e.g., SSDs) and archives infrequently accessed data in energy-efficient, slower storage (e.g., magnetic tape).
- **Data lifecycle management:** Implement data lifecycle policies that automatically archive or delete old data to reduce storage demands and energy consumption.
- **Energy-efficient data transfers:** Optimize data transfer across the network to reduce energy costs, for example by using energy-efficient communication protocols or scheduling data movement during periods of lower energy demand.
- **Data deduplication and compression:** Minimize the storage footprint by implementing data deduplication and compression, reducing both storage and data transfer energy costs.

Design objectives should include reducing the energy consumption of data storage and movement, implementing efficient data retention and archival policies, minimising network energy costs through optimized data transfer.

Other RI design aspects to address include:

- Governance, Policy, and Compliance for sustainability,
- Collaboration, education, and training for sustainable practices,
- Real-time energy monitoring and analytics,
- Renewable energy integration and power management

C. Sustainability Aspects addressed by the major Cloud Services Providers

It is important to mention that sustainability aspects are growingly addressed by the major computing and network vendors and services providers, primarily cloud service providers, and 5G/6G vendors and providers. At least two major cloud providers recently published their “Well-Architected” cloud services design recommendations: Microsoft Azure [31] and AWS [32]. Both frameworks have a similar structure of definition of a number of architecture pillars, where AWS includes a new Sustainability Pillar [33]

for designing sustainable customer applications in the AWS cloud.

Both cloud providers also propose tools for carbon monitoring and assessment, but their concept and services are limited to their area of responsibility as providers; while proposed in GreenDIGIT and described in this paper, the approach intends to involve the researchers in the sustainability of the research ecosystem.

VI. RESEARCHER DEVELOPMENT ENVIRONMENT FOR SUSTAINABILITY

A Researcher Development Environment (RDE) for Sustainability must provide functionality to embed sustainability principles directly into the tools, processes, and workflows that researchers use for their work. The aim is to enable researchers to optimize the use of digital infrastructure, minimize energy consumption, reduce carbon emissions, and align their scientific activities with broader environmental sustainability goals.

RDE for sustainability must include the following functionality:

- **Energy-aware design of research workflows** that optimise the use of computational resources, data storage, and network bandwidth. This may include the following design solutions:
 - Energy-efficient algorithms
 - Dynamic resource scaling
 - Workload consolidation
- **Energy-aware scheduling and optimization** to allow researchers to schedule their tasks, workflows, and experiments based on energy efficiency parameters, such as running computations during periods of low carbon intensity or aligning tasks with renewable energy availability.
- **Sustainable Data Management** is critical for minimising the energy costs associated with data storage, retrieval, and transfer.
- **Integration with sustainable cloud and HPC resources** in a way that prioritises energy efficiency and sustainability. Many cloud providers offer services specifically designed to reduce the carbon footprint of computational workloads.
- **Energy monitoring dashboard** that allows researchers to track the energy consumption of their experiments, data storage, and compute resources.
- **Support sustainability training and awareness programs.**

There are a few Software Development Kits (SDK) for sustainability that are mostly focused on the software development and optimisation of CPU processing and memory. Carbon aware SDK by Green Software Foundation [34] is one of the examples. SDK includes access to various data sources of carbon aware data [35], including WattTime [36], ElectricityMaps [37] including their API based service that provides real-time data on the carbon intensity of electricity used in different regions, and a custom JSON source. Knowledge of carbon aware data is important for the effective development of the carbon aware and optimized research applications.

There are several other services and tools that can be integrated into the application development process and environment to optimize energy consumption, monitor carbon footprints, and support sustainability goals. These tools provide real-time data on carbon intensity, energy consumption, and environmental impact, helping developers and organizations make informed decisions about when and how to run energy-intensive processes. Many of these services offer APIs and integrations that can be embedded into RDE and workflows, DevOps pipelines, and cloud infrastructures.

We can mention the following tools that we found useful:

- Google Cloud Carbon Footprint [38]: A service that helps users measure, track, and report the carbon emissions of their cloud usage and allows Carbon Footprint Tracking, Visualisation of the carbon emissions over time, Emission Reduction Suggestions, cloud API Integration.
- AWS Customer Carbon Footprint Tool [39] that helps AWS users measure the carbon footprint of their cloud infrastructure. It supports tracking the environmental impact of the cloud resources used and encourages the shift towards more sustainable operations. Carbon Emission Reporting, Historical Data, Region-Specific Carbon Data, and Integration with AWS Tools to provide real-time data on the carbon footprint of resources, enabling developers to make energy-conscious decisions.
- Microsoft Sustainability Manager [40] that provides comprehensive, integrated, and automated sustainability management for organizations. It automates manual processes, enabling organisations or projects to more efficiently record, report, and reduce emissions and water or waste impact.

VII. CONCLUSION

This paper presents the results of ongoing GreenDIGIT project development that may be valuable for the research community working on making the research sustainable, more energy efficient, and less environmental impact. This work is based on the authors' long-time experience in designing and developing different infrastructure infrastructures and services in the framework of multiple projects funded by European and national research programs.

The presented paper is intended to provide a basis for discussion among the wide research community by consolidating the whole spectrum of architectural, design and policy activities and developments based on a comprehensive platform or umbrella framework that integrates all stakeholders, tools, and best practices into a unified ecosystem. This platform should allow for continuous development, sharing of knowledge, and collaboration, while also being adaptable to rapidly evolving sustainability standards and technologies.

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