

Scientific Data Infrastructures: Transforming Science, Education, and Society

Data is everywhere – praktisch bei allen wissenschaftlichen, staatlichen, gesellschaftlichen und wirtschaftlichen Aktivitäten entstehen sie. Die Daten werden erzeugt durch Befragungen, mobile und eingebettete Systeme, Sensoren, Beobachtungssysteme, wissenschaftliche Instrumente, Publikationen, Experimente, Simulationen, Auswertungen und Analysen. Bürger, Wissenschaftler, Forschende und Lehrende kommunizieren durch den Austausch von Daten, Software, Veröffentlichungen, Berichte, Simulationen und Visualisierungen. Darüber hinaus führen die zunehmende Nutzung der visuellen Kommunikation für Unterhaltung und zwischenmenschlichen Beziehungen sowie die rasche Zunahme der sozialen Netzwerke zu riesigen Datenmengen. Daten von Observatorien, Experimenten und Umweltüberwachung sowie aus der Genforschung und dem Gesundheitswesen generieren eine Größenordnung von Daten alle zwei Jahre, die weit über das Mooresche Gesetz hinausgeht – und dabei ist noch kein Ende in Sicht. Wissenschaftliche Publikationen sind Datengrundlage für die weitere wissenschaftliche Arbeit und Publikationen.

Data is everywhere; it is being produced virtually by all scientific, educational, governmental, societal and commerce endeavours. Data is being generated by surveys, mobile and embedded systems, sensors, observing systems, scientific instruments, publications, experiments, simulations, evaluations and analyses. Citizens, scientists and educators alike communicate by sharing data, software, publications, reports, simulations and visualizations. The growing use of visual communications for both entertainment and interpersonal relationships and the rapid increase in social networks are generating huge amounts of data. Data from observatories, experiments and environmental monitoring as well as from genomics and health are generating an order of magnitude more data every two years with no end in sight far surpassing Moore's law. Scientific publications are becoming data for further scientific work and publications.

INTRODUCTION

For data to be useful for scientific research, it is essential that not only it be available, but that it be available in ways that can be searched, analysed, and manipulated across disciplines, domains and national boundaries. To ensure that the data is available for scientific inquiry, it is essential to take a global approach to promote shared usage, interoperability, and discoverability of scientific information resources. This approach should include accepted incentives to share and enable reuse of data and software and adequate funding mechanisms to ensure sustainability. It should help in rationalizing and institutionalizing resources, building trust and widening access and use. In addition to being interoperable, data must be stored, curated, managed. The effective management of digital data requires verifying and reviewing the data to ensure that science is self-correcting and to promote the scientific dialogue which improves the quality of research results and increases the levels of trust. These require-

ments and capabilities can only be met through the establishment of multiple scientific data infrastructures across the globe.

OPEN SCIENCE AND 21ST CENTURY TRENDS

The world wide web is an opportunity to widespread scientific knowledge at unprecedented levels. Science in the 21st century is still about pushing further the frontiers of knowledge and about understanding how nature works through rational and objective methods. It is still about sharing and discussing results with peers to verify and ensure scientific work of the highest quality. It is still about innovating and creating the foundations of socio-economic development by exploiting new knowledge and about spreading it by making it accessible through education and development of new skills.

At the same time, 21st century science harbours emerging features that challenge the way researchers work. The same happens for educators, students and even curious citizens. The volume, diversity and complexity of research data collected and processed every minute confront us with new challenges. Large, more or less formal, *n*-way networks of interest groups are formed even as we write and work on relevant scientific issues, re-emphasising the open attitude that originally stood behind the scientific enterprise.

Whether it be scientific results, the data that feed into them, the pieces of software that sit beneath them, or the educational resources that help us teach and learn, we must recognize that opening science broadens scientific disciplines, transforms knowledge territories, and encourages cross-disciplinary research. Opening science implies opening the supporting infrastructures to a large community of users, making research dissemination effective through open channels and, last but not least, opening minds, cultures and established practices. Opening science in the Internet era has more chances to succeed if done in the perspective of building the capacity to modernise research and education.

RESEARCH INFRASTRUCTURES

Research Infrastructures (RI) are pillars for the advancement of scientific discovery. Some very advanced research is not possible without highly specialised and



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open science

novel instrumentation. Research Infrastructures offer scope for world-leading research; often this requires large investments. They offer services of broad interest to research and education and are test beds for new technologies, innovative methods with impact on socio-economic development.

Large Research Infrastructures (LRI) offer unique conditions for scientific experimentation and are used by several research teams of users with highly advanced research projects. Their large size implies that individual groups cannot operate them on their own. The levels of investment are such that long-term plans for their scientific objectives, funding and exploitation are essential at design phase and throughout their economic life-cycle. As infrastructures providing services to users they have to care for a continuous, reliable and dependable operation.

Information and Communication Infrastructures (ICI) have been steadily growing in importance in the RI context. Modern RIs being designed to start operation in the next decades will be extremely well wired to ensure high-speed connectivity. They will be surrounded by high performance computation infrastructures. They will be very large data factories.

Scientific instruments like the LHC (Large Hadron Collider) already generate tens of petabytes per year that must be served to thousands of scientists; planned survey telescopes like the LSST (Large Synoptic Survey Telescope) will generate hundreds of times this much data to be analysed by astronomers, computers, and school kids around the planet; DNA sequencers at campuses and research facilities are already generating terabytes of data per day and provide new research opportunities in medical research and innovative health services; sociologists are able to analyse millions of tweets per day to track and map national moods and trends; sensor and environmental networks provide prodigious amounts of data that are being used for weather predictions and climate modelling as well as for modelling pandemics; cities are providing access to public data that can be used for transportation, construction, and evacuation planning; and, industry and commerce use data effectively to manage everything from just-in-time manufacturing to operations to supply-chain management. Data has quickly become the new currency for science, education, government and commerce. And when this data is coupled with innovative information technologies, it transforms science, business, government and education; it also impacts the very fabric of society.

INFORMATION AND COMMUNICATION INFRASTRUCTURES

Information and communication technologies (networking, high-performance computing platforms and research data) bring a new dimension to RIs. They become more and more served by unprecedented connectivity, processing, storage and preservation capacity. The overall combination of services has a great potential to modernise research and education in an economically sustainable way. In this context the emphasis must be on the reliability, continuity and persistence of the services not on the technologies as such and therefore it is better to refer to Information and Communication Infrastructures (ICI)¹ rather than to information and communication technologies.

The Internet emerged in the context of research and education; by now, we know that it is actually transforming society. The world wide web, first viewed as a *«vague but exciting»*² idea, and was initially conceived with the limited aim of enabling scientific collaborations between large numbers of scientists at CERN. The goal of ICI is to deliver highly reliable, widely accessible basic capabilities and services supporting the full range of scientific work.³ This is anything but trivial to achieve. Several barriers (described in [3] as *base-level tensions*) have to be overcome, or at least lowered, in order to achieve the goal in a sustainable way.

Barriers differ in nature and origin. For instance, it is difficult to reconcile funding cycles with the variable time scales of technological evolution. Another difficulty is to achieve global interoperability when the ICI are composed of distributed parts requiring *«local»* developments and optimisation. Other obstacles relate to tensions between top-down planning versus more chaotic developments, with a strong bottom-up drive, triggering incremental changes in complex systems.

Ultimately, the development of infrastructure is influenced by social, economic, and technological dimensions. It requires interaction and engagement of different stakeholders to take their share of responsibility and contribute to lead the way. The process to find the right balance between standardisation and invention, control and freedom, performance and cost, public and private, international and local is a key element of infrastructure development.⁴ As stated in [3] *«complications challenge simple notions of infrastructure building as a planned, orderly, and mechanical act. They also suggest that boundaries between technical and social solutions are mobile, in both directions: the path between the technological and the social is not static and there is no one correct mapping»*.

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SCIENTIFIC DATA INFRASTRUCTURE

Research data have become an important asset in the modern processes of discovery. More and more data are produced as a result of our continuously improving ability to measure with precision, to analyse in more depth and to process data on scales never contemplated before. New research data are also produced by processing existing data through large scale simulations. In fact, scientific modelling is shaping up as the third great scientific revolution after observation (e.g. Aristotle), and experimentation (Boyle).

All fields of knowledge rely on data, lots of data that are complex and diverse and no »size fits all«. There are specificities and cultural variations in different scientific domains but all of them face the same challenge of acquiring the capacity and the skills to seize the opportunities that information and communication infrastructures provide.

The required scientific data infrastructures are made of environments supporting advanced data acquisition, connectivity, storage, curation, management, integration, mining and visualisation and computing and information processing services and communication networks beyond the scope of a single institution.

Essential attributes of global data infrastructures include viability, flexibility, participation, reliability, security and openness. Making it happen requires the involvement of researchers, universities, research laboratories, standardization bodies, governments, funders, citizens and industry.

The complexity of the data enterprise, especially when coupled with how data is transforming science and engineering, raises an equally wide range of complex challenges that need to be addressed. While many of the challenges are technical (data creation, storage, preservation, accessibility, software), other challenges necessarily include political dimensions (access, standards, international coordination) and still others are social (education, training, work force development). All these challenges need to be addressed to support modern scientific inquiry and its various functions within society.

It is important to point out that although the larger research community has been addressing many of these issues and challenges, the sharing and exchange of data at the international level remains minimal. Part of this is due to the complexity of the problems to be addressed; part is due to lack of international agreements around interoperability standards; part is also due to the fact that this is a new way to do science which, in turn, is in the process of transforming the very institutions, organizations, and agencies that support scientific inquiry.

Another major problem is related to the fact that scientific data inquiry is an ecosystem; as a result, there is sometimes a belief and desire to understand each of its components, and consequently the entire ecosystem before data can be effectively shared. Lastly, there is also a parallel tendency and desire in the research community to wait until a uniform or international standard for data interoperability is approved before establishing global data infrastructures. The end result, as noted, is that international exchange of data across geographic regions and disciplines is minimal even though there is a recognized need and agreement that it needs to happen.

TIMES OF CHANGE

The presence and role of libraries in our familiar research environment warrants some pondering, as it points to structural transformations that are similar in importance to the ones we are beginning to witness in our own times. When, in the 17th century, the world of experimentation began to add itself to the older world of observation, the means to communicate science also changed. Experimentations, by their very nature, implicitly challenged any person becoming aware of them to repeat them in order to check the results. Communicating experiments required much shorter documents than the treatises of old: thus was born the scientific article. Reading an article forced the reader into the role of a witness to the experiment. Either the reader accepted it or not; if not, the reader had no other recourse but to repeat and verify the experiment.

In such a context, libraries came to play a number of crucial roles for the development of science. First, they became the archive, the memory, of choice. This also facilitated scientific paternity or attribution. But it also provided the ground on which one could mount a criticism of any part of science at any time. In a very real sense, the experimental nature of science also called for the setting up of a kind of scientific jurisprudence to which everyone was supposed to refer to in doing science. Not knowing previous work could no longer be accepted or even excused.

In our times, modelling is increasingly viewed as a third way for the production of scientific knowledge, and for a richer encounter with reality. This requires forms of publication which, through the use of data and algorithms, permit to produce not one interpretation of experiments and observations, but a whole array of such interpretations. Selecting various fractions of the data and working on them with various calculated models are ways to communicate scientific work that are growing in importance.

**scientific data inquiry
is an ecosystem**

**essential attributes of
global data infrastructures**

**libraries play crucial roles
for the development of
science**

Like the previous revolution (experimentation), the advent of modelling strongly suggests that deep changes in scientific communication are looming. This means that we have to rethink the traditional role of libraries in entirely new ways: libraries will not just preserve, classify and care for static pieces of printed paper; they will also look over data and algorithmic tools. Furthermore, these new roles will be exclusively digital, thus requiring new and complex skills. But, at the same time, observing how libraries will respond, theoretically and practically, to these challenges will be very instructive in showing how this new triad – facts, algorithms, interpretations – evolves, expands, networks, etc.

BRIEF INTRODUCTION TO EUROPEAN POLICY FRAMEWORK

The European policy framework related with open data was updated in 2011 with the proposed amendment of the PSI Directive 2003/98/EC on re-use of public sector information⁵ and the adoption, in July 2012, of the scientific data package.⁶ The INSPIRE Directive⁷ (2007) is another key piece of the policy framework addressing spatial and geographical information.

The policy framework definition follows the inter-institutional discussions seeking to ensure coordination with the EU Member States and the European Parliament, and it is making very good progress. Neelie Kroes, Vice-President of the European Commission and responsible for the Digital Agenda for Europe, announced in April 2013 that the European Union (EU) Member States had approved the text for the new PSI Directive governing the re-use of public sector information, otherwise known as Open Government Data.⁸

The different parts of the policy framework serve different purposes, characteristics and contexts in which data is produced and used. Borders between the different parts are sometimes blurred, for example, public sector information can be used in the context of research (for instance in the field of social sciences and humanities); data collected primarily for research activities can be relevant to governments (for instance for agricultural development, environmental monitoring, etc.). On the whole, the different streams of the policy framework rest on a general principle, that of removing access barriers to data, in order to improve transparency and trust.

From the PSI directive text we quote,

»Public bodies produce, collect or hold a wealth of information and content, ranging from statistical, economic or environmental data to archival material, collections of books or works of art. The digital revolution has significantly increased the value of this resource for inno-

vative products or services based on data as raw material«.

Therefore removing unnecessary access barriers releases socio-economic value on a large scale.

From the same text but referring to the package on scientific information (resulting from publicly funded research) we quote,

»The Commission's objective in the area of scientific information is to maximise the benefits of information technologies (internet, supercomputing networks, data mining) for better access to and easier reuse of scientific knowledge. »Open access« policies pursue the goal of making scientific articles and research data freely accessible to the reader on the web. The Commission intends to take steps to promote access to and preservation of scientific information, including publications and data of research projects funded by the Union budget. The Commission's objectives in this area are very closely aligned with those of the PSI Directive in the sense that both aim to make public information more widely available in Europe for access and re-use«.

This is the basis for the open science strategy: by opening research data – in compliance with legitimate commercial interests and issues like ethics and privacy – scientists, scholars, etc. take advantage of new ways to do research while making use of high-performance computing and high-speed connectivity.

The above policy frameworks (for public sector and for scientific information) put the emphasis on reusability and »readiness of accessibility« meaning more than the mere absence of a restriction of access to the public. Re-use of data can be made difficult because of lack of information about its existence, its availability, or its format. Mechanisms to discover data are an important component of data infrastructures. If the user is not certain about the terms of re-use or the encoding formats the re-use of data becomes difficult or expensive. Mechanisms to annotate and curate data with fit-for-purpose metadata are also important. Barriers such as the above would mean that public data cannot be readily accessible.

RESEARCH DATA ALLIANCE: A GLOBAL CONTEXT OF DATA-INTENSIVE RESEARCH AND INFRASTRUCTURES

The grand challenges of the 21st century transcend borders, and science will be increasingly global. Data-driven science is made of global collaborations⁹ and researchers have an active role in the worlds' production of knowledge. Research data itself is global. Clear examples are agricultural data, biodiversity data, oceanographic data etc.

The recent White House executive order entitled »Making Open and Machine Readable the New Default for Government Information«¹⁰ translates into action the US commitment to the open exchange of appropriate government data. It highlights the importance of robust consensus on international standards and the strategic work that the Research Data Alliance (RDA)¹¹ is set out to perform enabling data exchange on a global scale.

The initial phase of RDA has been supported by the collaboration between the European Commission, the US National Science Foundation and the Australian Ministry of Research. RDA is being set-up to bring a diversity of stakeholders together and improve interactions between users and technology and service providers. It is important to stress that these interactions are essential to the bottom-up path for global interoperability across geographic and disciplinary boundaries. In this regard, fundamental lessons drawn from Internet history should not be forgotten.

RDA is a community-led initiative; all those who want to participate in RDA and shape the way the global data infrastructure operates are welcome to join and take the lead. It is focused on the real needs of the research communities and will seek links with industry. It aims at being the place where practitioners stop discussing about the ideal solution and /or the complete set of standards and start implementing practical solutions and share data.

RESPONDING TO THE G8+O6 GROUP OF SENIOR OFFICIALS ON RESEARCH INFRASTRUCTURES

The Group of Senior Officials (GSO) on Global Research Infrastructures has been working under the G8¹² auspices since March 2011 seeking better exchange of information and international cooperation on research infrastructures. The GSO has worked and has met three times in extended configurations with outreach countries (Brazil, China, India, Mexico, South Africa and Australia). One of the three working groups established by the GSO worked on identifying the basic elements that should be considered in developing global data infrastructures:

Creation (generation) of research data: diversity is likely to remain a dominant feature of scientific information. *Preservation*: the need to find cost-effective solutions for preserving the value of data to make it available, to use, reuse and recombine it in order to support the creation of knowledge.

Access: all research builds on earlier work, therefore fuller and wider access to scientific data will help avoid reinvention and accelerate innovation.

Computing: scientific software, models and algorithms embed valuable information and knowledge. This includes the software and models that were used for generating, processing and correlating data so that the reproducibility and accuracy of the data can be verified.

Culture: efficient support to global e-science and research communities requires the development of world-class e-Infrastructures capable of new »participative« collaboration paradigms. There are also social and behavioural aspects to be addressed like the clash of cultures between different disciplines, legacy frameworks and the need to rethink organisational models. *International Coordination*: it will not be possible to achieve an integrated data infrastructure if each country or region acts alone. It will be necessary to develop a new generation of advanced infrastructure services and tools to find data, integrate data sets or manage the scientific workflow. Interoperability, for example, requires adherence to technical standards but also reciprocal agreements between governments. Policies for access, preservation, security, have to be compliant with legal frameworks in different jurisdictions.

As conclusion of the last meeting in March 2013, the GSO supported the need to work together at global level to develop a »Global Collaborative Data and Knowledge Infrastructure« and welcomed the efforts to set up the Research Data Alliance.

While interoperability at the level of storage, connectivity and computation is relatively well established, achieving interoperability at the level of data interoperability is a far harder challenge.

The paragraphs below describe principles put forward by the Data Working Group to the GSO as guidance for establishing cost-effective global interoperable data infrastructures widening access and ensuring long-term preservation.

Discoverable

Scientific data sets, even though valuable and available, will see little or no use if they cannot be easily found using conventional search method. These data sets must be accessible to web crawlers and have adequate description information to allow the searcher to understand the content, specialized formats, or languages. Making data easier to find and more readily discoverable will enable efficient use of the data sets, reduce costs for research and development, and increase innovation. Examples of approaches that can improve discoverability include implementation of appropriate persistent identifier frameworks, adoption of descriptive metadata standards, and the use of appropriate data formats and taxonomies.

Research Data Alliance (RDA)

Global Collaborative Data and Knowledge Infrastructure

fuller and wider access to scientific data

Accessible

Publicly funded scientific research data should be made openly available with as few restrictions as possible. Ethical, legal or commercial constraints may be imposed on the use of research data to ensure that the research process is not damaged by inappropriate release of data. Normal research practice regarding the citing of sources should be observed – namely, that secondary users of research data must acknowledge the source of the data and have to give credit for any intellectual contribution made in collecting and organising the data. Users of data may be required to sign up to terms of use or licenses associated with particular data, for example, regarding consent or the protection of privacy of human subjects, preservation of intellectual property, or agreeing to an embargo approach. Once alternative systems are in place to adequately acknowledge the contribution of data providers, it should be possible to reduce or remove embargo periods and other restrictions to accelerate data driven knowledge creation and innovation.

Understandable

Scientific data sets must be understandable in order to be effectively used. A set of numbers, texts, pictures or even videos alone cannot be understandable without additional context, semantics, data analysis tools, and algorithms. Observational and sensor data must be accompanied with the documentation about the location, time, and method of observation. A set of rules must be established to ensure the integrity and provenance of the data including data quality, curation and preservation. Although English has become the de facto common language in many fields of research, translation among data collections is essential and translation between disciplines will become ever more important as inter-disciplinary research efforts and international collaboration continues to grow.

Manageable

In order for research data to be managed in an efficient and effective manner, data management policies and plans must exist for all data at both project and institutional levels. Making research data available in a form in which it can be effectively used by others requires considerable and continued efforts over and above those which are necessary to undertake the primary research itself. Data management policies and plans must make it clear who is responsible for maintaining the availability of data and how the associated costs are to be met including issues associated with curation, storage and services. Plans and processes must be in place that will take into consideration

the full range of potential uses for the data in a cross disciplinary context as well as the requirement for data with acknowledged long term value to be preserved and remain usable for future research. Coordination of provision of technology and data services so as to make effective use of common technology and avoid duplication of effort will be instrumental in ensuring an efficient data infrastructure.

People

A global approach requires a highly skilled and adaptable workforce and culture that is able to capture the available data and make it available to those that are able to use it appropriately. There is a need for specialised data custodians who can work across complex data sets and with diverse data protocols. Some of the specialist skills required are not yet fully reflected in existing qualifications and training programs and there is a need to develop suitable programs of training to meet this need. There is also a need to change the culture of research data management within the research community. In addition to the specialised skills required, there will need to be broad-based training provided as part of research training programs to ensure that researchers understand the need for, and benefits of, data sharing and the principles by which this will happen.

CONCLUSIONS

There is no viable way to design a scientific data infrastructure with a top-down approach. Very much in the same way that it is not imaginable to design the Internet top-down. The Internet has grown into an infrastructure through open communication mechanisms, global collaborations and practical solutions to problems («rough consensus and running code»). The Research Data Alliance is an important response, led by the community, to achieve the vision of Open Science through Open Infrastructures.

Scientific data infrastructures that promote access also enhance capabilities for measuring impact. Many nations and institutions are investing in digital scientific data and data infrastructure recognizing the potential value in catalyzing discovery, innovation, education, and entrepreneurship. Responsible management requires the ability reliably to measure the impact of those investments. Facilitating the ability to measure return-on-investment, including implementing incentive schemes for researchers, is critical to this effort.

Open scientific data e-Infrastructures increase scope, depth and economies of scale of the scientific enterprise; they are catalysts of new and unexpected solutions to emerge by global and multidisciplinary

nary research. They bridge the gap between scientists and the citizen and are enablers of trust in the scientific process. In particular, as the issue of replicability becomes ever more important, it becomes obvious how the teaching of young scientists could be much enhanced by training them with open data while allowing them to test the quality of the interpretations proposed in peer-reviewed scientific publications. This would also be an excellent way to train scientists, at least partially, in developing nations, despite a chronic lack of laboratory facilities.

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Note: *Carlos Morais Pires* views are his and do not commit the European Commission.

¹ e-Infrastructures or cyber-infrastructure are terms used by the European Commission and National Science Foundation.

² <http://info.cern.ch/Proposal.html>

³ Understanding Infrastructure: Dynamics, Tensions and Design – final report of the workshop on »History & Theory of Infrastructure: Lessons for New Scientific Cyberinfrastructures, Jan 2007.

⁴ European Commission. »Riding the Wave: How Europe can gain from the rising tide of scientific data.« October 2010. <http://cordis.europa.eu/fp7/ict/e-infrastructure/docs/hlg-sdi-report.pdf>

⁵ http://europa.eu/rapid/press-release_MEMO-11-891_en.htm?locale=en and http://ec.europa.eu/information_society/policy/psi/docs/pdfs/directive_proposal/2012/en.pdf

⁶ COM(2012) 401 final, Brussels, 17.7.2012: Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and the Committee of the Regions – Towards better access to scientific information: Boosting the benefits of public investments in research and C(2012) 4890 final, Brussels, 17.7.2012: Commission Recommendation on access to and preservation of scientific information (http://ec.europa.eu/research/science-society/document_library/pdf_06/era-communication-towards-better-access-to-scientific-information_en.pdf).

⁷ <http://inspire.jrc.ec.europa.eu/>

⁸ www.lapsi-project.eu/what for more info.

⁹ »Scientists are collaborating across borders to an unprecedented degree, broadening opportunities in Big Science and Big Data projects and helping bridge the gulf between nations« – from Scientific American Magazine December 2012, www.scientificamerican.com/report.cfm?id=state-of-worlds-science-2012

¹⁰ www.whitehouse.gov/the-press-office/2013/05/09/executive-order-making-open-and-machine-readable-new-default-government

¹¹ <http://rd-alliance.org/>

¹² <http://en.wikipedia.org/wiki/G8>

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