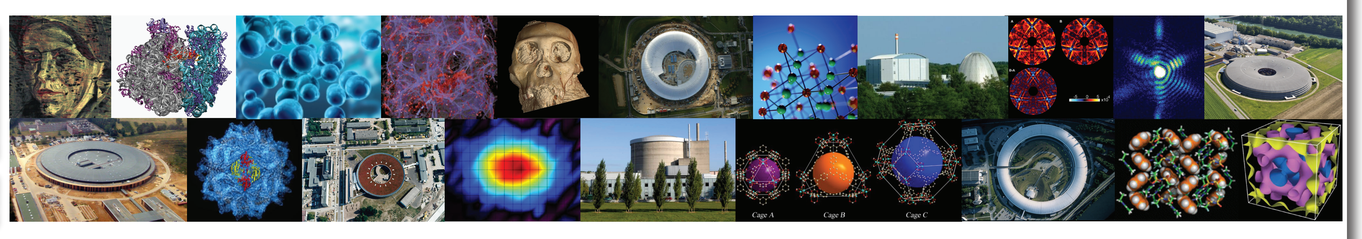
Open Data Infrastructure

Building blocks of the PaNdata Open Data Infrastructure



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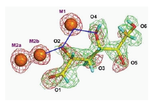
Abstract

PaNdata is a long term co-operation of European Neutron and Photon Research Infrastructures. Within the FP7 framework PaNdata has launched two projects. PaNdata Europe, which was successfully completed in 2011, laid the basis for a common data management framework with the development of common policies on data lifecycles, user and software. PaNdata ODI has started end of 2011 and aims to provide a federated, sustainable data infrastructure across the participating facilities, to establish a common authentication and authorization system, to accelerate data analysis and to provide tools to link between experimental data, the analysis pathway and the scientific publications related to the experiment.

PaNdata

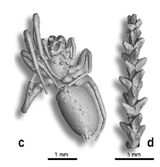
The PaNdata consortium involves thirteen major world class European Research Infrastructures. Most of these ERIs operate several lightsources (like e.g. DESY, ELETTRA) and/or a combination of Neutron and Photon Science facilities (like for example PSI, HZB or ILL and ESRF), providing hundreds of highly advanced scientific instruments, and ultimately serving several ten-thousands of users from a wide range of scientific disciplines. Neutron and Photon diffraction can exploit complementary aspects of physical and natural sciences. Although being quite different in various aspects, the basic principles are often quite similar. PaNdata intends to fully exploit the synergies arising from common approaches ranging from application development to user management. PaNdata aims to offer the user communities an infrastructure to fully exploit the complementarity within in unified environment, and at the same time facilitate user, data and resource management for the research infrastructures. PaNdata supports the movements towards Open Data by enabling users to rapidly analyse data, easily share information and results, and track and manage the process from the proposal to the scientific publication.

Science and Users



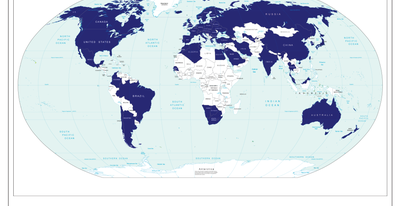
1) Difference neutron scattering (green) and electron density (red) maps. Source: epn-campus.eu

Neutron and x-ray scattering experiments for example can provide very different, complementary information of a protein structure, which has been recognized already 40 years ago. While x-ray diffraction provides a detailed view of the tertiary structure of a protein, it usually fails to locate hydrogen atoms. To fully understand the catalytic mechanism of an enzyme, the knowledge about the position and relocation of hydrogen atoms during catalysis is absolutely crucial. Neutron scattering can provide such information, however the joint refinement of neutron and x-ray data is often hampered by lack of standards, appropriate tools and accessibility of scientific data. In the long term PaNdata aims to create an open data infrastructure to provide access to all experimental data created at any of the participating facilities, thereby promoting collaborative research, distributed analysis, complementary use of data from different experiments and facilities. This will allow providing open access to unique, curated data, like the paleontological samples shown in (2). X-rays now make it possible for palaeontologists to study opaque amber, previously inaccessible using classical microscopy techniques. Scientists from the University of Rennes (France) and the ESRF found 356 animal inclusions, dating from 100 million years ago, in two kilograms of opaque amber from mid-Cretaceous sites of Charentes (France). Long term, open accessibility of such precious data is hence absolutely essential for comparative analysis to gain new insights into the evolution of species.

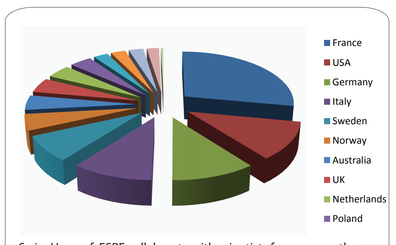


2) Examples of 3D reconstructions of organisms embedded in opaque amber. Credits: M. Lak, P. Tafforeau, D. Néraudeau (ESRF Grenoble and UMR CNRS Rennes).

The majority of the research groups using neutron or x-ray sources visit more than just one facility, with varying group members and projects. In addition, users are commonly involved in small or large and volatile collaborations. Collaborating scientists might need access to data as well, though the have never been involved in an experiment and are hence not a priori known to the facilities. On the other hand, the process from proposal submission to radiation protection regulations require unique and persistent identification of a user/person. Collaborations and user are spread over all 5 continents. A solution for authentication/ authorization needs to be easily accessible from everyone and simple enough to be usable on a very infrequent basis.

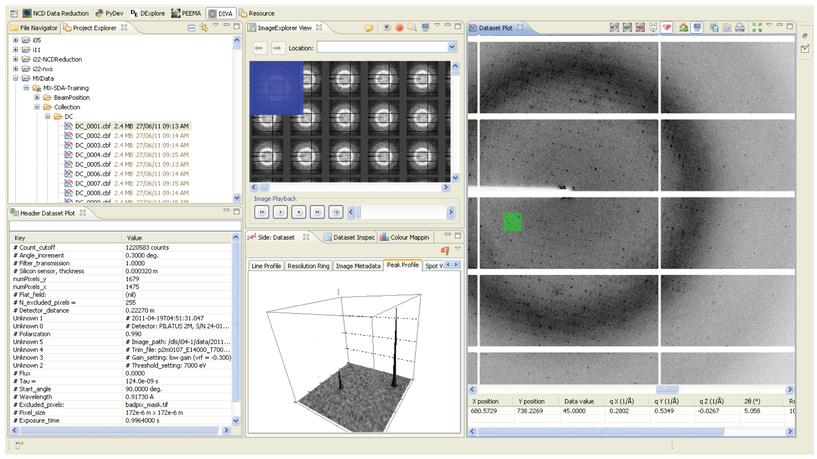


Geographical location of the user communities home institutions

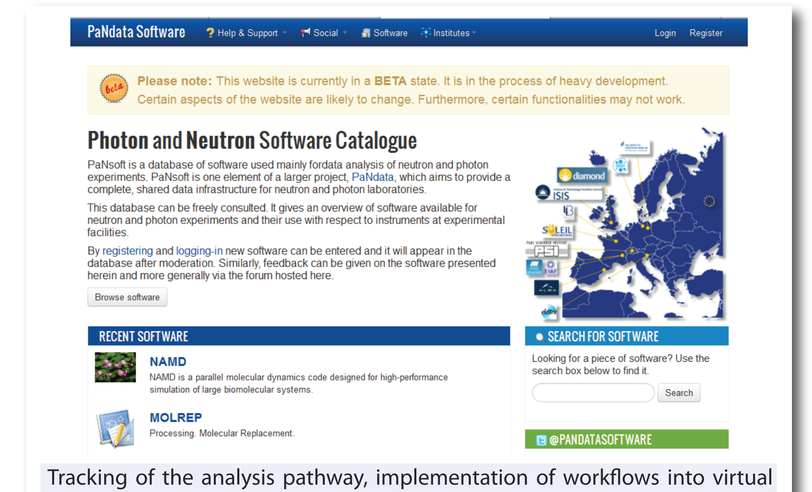


Swiss Users of ESRF collaborate with scientists from many other countries world wide

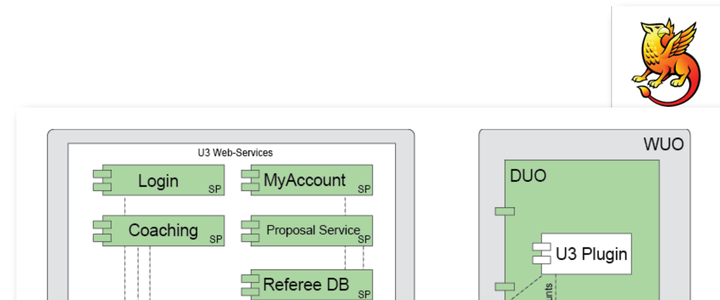
Infrastructure Building Blocks



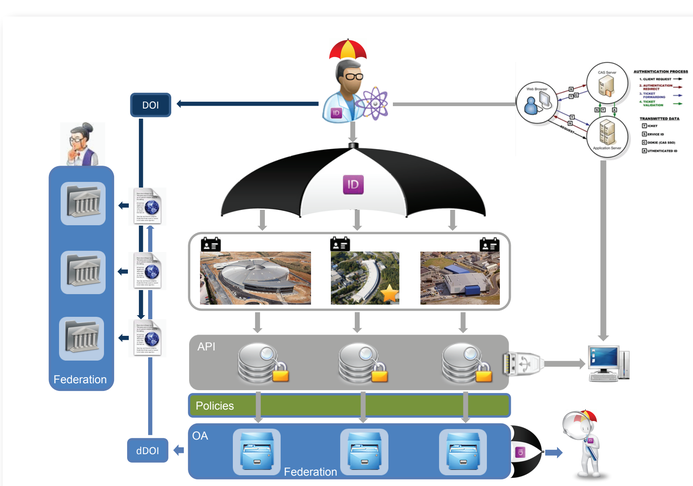
Virtual labs integrate the different building block into a virtual a research environment. DawnScience is for example an application integrating NeXus capabilities with advanced workflows and interfaces to explore the ICAT data catalogue DAWN



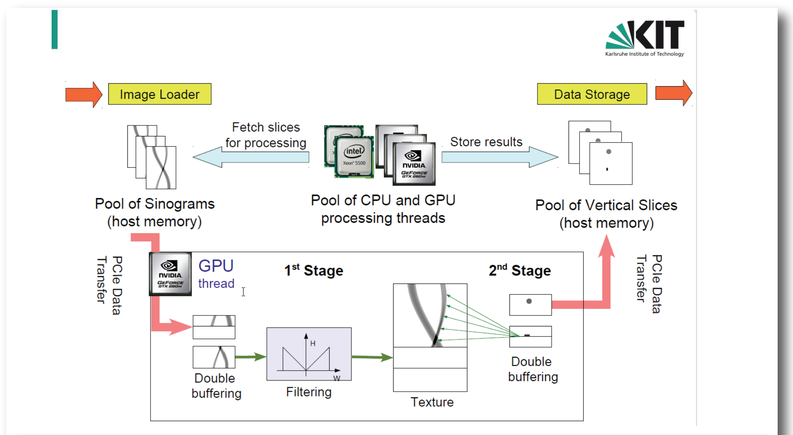
Tracking of the analysis pathway, implementation of workflows into virtual labs and mining data repositories greatly benefit from the common software data catalogue.



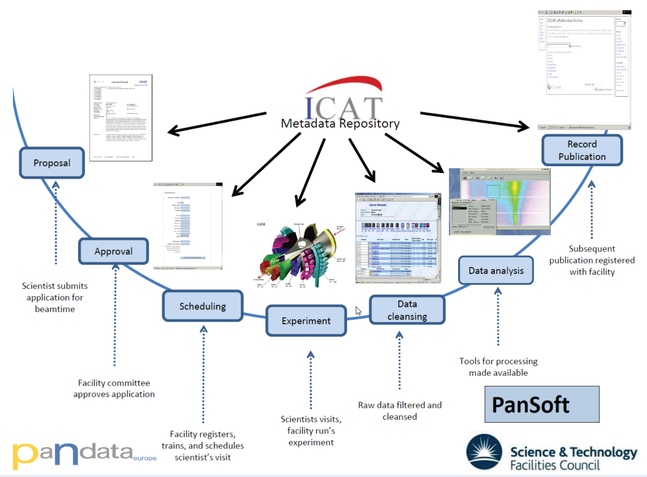
The whole process from proposal submission, running an experiment, accessing data and publication requires unique and persistent identification of the scientist. The Umbrella project provides tools to support the process in a unique way across the facilities.



Federation of resources and services is a crucial element to provide scientists with a panEuropean research environment, including a common AAI infrastructure, the federation of data catalogues as well as affiliation and publication databases.



Rapid data analysis and visualization is crucial to tune experiments in real time. In co-operation with projects like PNI-HDRI, GPGPU and multi-core acceleration of tomographic reconstructions is a particular successful development. Integration into virtual labs can tremendously enhance the scientific outcome.



The data catalogue is the core of the data infrastructure. ICAT provides the tools and services supporting the whole process from proposal submission to publication; data analysis and workflows; data ingestion, curation and provenance.

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