An integrated e-Infrastructure for experimental Facilities

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The STFC e-Science Centre has built, in collaboration with STFC scientists, Facilities, and their users, an integrated e-Infrastructure, which enables the automatic capture, management, curation and exploitation of scientific data at scales ranging from Megabytes and minutes to Petabytes and decades. Jointly-agreed data and metadata standards allow data sharing between different facilities and Single-Sign-On facilitates cross-facility access for the users [5],[6]. This e-infrastructure has been deployed at the Diamond Light Source (DLS) and is currently in full operation at station I18 (Microfocus Spectroscopy), with more stations to follow. At ISIS, neutron data collected over the past 23 years of operation has been catalogued and made available to the users and new data will be automatically catalogued on existing instruments from late October 2007 onwards. A closely-related data collection infrastructure for the new Central Laser Facility 'Astra Gemini' project is also under way, with other related deployments planned for ISIS-TS2 and Lab-in-a-Cell. These developments are well integrated into other national and international activities through collaborations with SNS-ORNL, the ILL and the ESRF.

Building upon this infrastructure, scientists are able to analyse, visualise and interact with large volumes of scientific data from their desktop. This technology has facilitated a number of scientific advances, such as:

- Development of a new 3D heart model, to gain better anatomical information for use as the basis for realistic models of cardiac electrical and mechanical activities.
- Prediction of new crystal structures, including a new polymorph of piracetam [1], a drug licensed in the UK for the treatment of cortical myoclonus .
- Establishing how arsenic is taken up and held in the pyrite structure and the factors likely to lead to its release, in order to avoid contamination of drinking water extracted from man-made wells [2].
- Studying the ability of different mineral types to bind dioxin, making it possible to remove it safely from the environment, and how best to immobilise plutonium and high-level radioactive waste [3,4].
- The search for more cost-effective ways to catalytically produce hydrazine from nitrogen by identifying the best transition-metal / ligands combination and geometry for the transition metal catalysts.

The talk will introduce the infrastructure and present initial user responses.

References

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