

Abstract of your innovative activity: *(please make sure that you mention the following points)*

The current state of the art facilities cater to a broad user community, the next generation European facilities will have to cater for a much wider community.

The future landscape of users of large scale facilities over the next 10 years will possibly see a reduction in the so called 'career users' and a proportionate increase in users where the Large Scale Facilities (LSF) is a component of a much wider strategic research programme.

The access mechanism of LSF are already aligning to this possible change in use by increasing rapid access and strategic programme access to the facilities.

This change in access and consequent change in user profile presents a unique challenge to LSF to ensure that data analysis and data reduction tools do not need 'apriori' experience of the technique, facility or theoretical models used.

This objective of this proposal is to create a common simple to use interface that allows non 'expert' users of LSF to leverage the breadth of simulation and modelling tools that exist for materials science such that they can generate scientific impact from data collected at neutron and x-ray sources.

One of the objectives of large scale facilities is to increase the efficiency of the data reduction and interpretation chain. This effectively reduces the time between experiment and publication decreasing the "time to market".

It is accepted that:

***Scientific computing enhances understanding of experimental data
One key barrier to publication is analysis and understanding of experimental data.***

It is also clear that that neutron publications that include clear aspects of state of the art modeling and computation physics generate higher citations and thus greater impact.

The simple fact is that large scale facilities must increase the level of and quality of specific data analysis tools and codes. In so doing the facilities will increase the level of published scientific output and thus the scientific impact.

Secondly and of equal importance will be the ability to attract new user communities to neutron / xray science through the provision of simple access to the required tools for researchers to extract the greatest impact from their data.

Only a proportion of the European research community will make use of the tools available at LSF. Furthermore most of the community of LSF users will make use of more than one facility. In order to maximize the impact that this community can make scientifically it is sensible at this time to introduce the idea of common interfaces and frameworks that allow 'common access' to scientific computing across the European landscape of LSF. This pan-europe approach is already underway for access to facilities and data cataloguing, in the pandata and icat frameworks.

This proposal aims to use a similar methodology and apply it the data interpretation and analysis stage of the research workflow creating a synergy of labs working together for a broad common user community

There are clear examples¹ where large facilities collaborating together on software tools really enhance the impact of developments in scientific computing and facility specific software engineering. Importantly the users of one facility are more often than not users of all facilities. This fact generates a clear requirement that all facilities should be involved in software development to deliver to a common user community a common analysis platform / toolkit.

The objective of this proposal is to develop cross facility software that satisfies the current and future user community requirement for easy to access neutron scattering data analysis tools.

1. Develop a comprehensive toolkit that allows direct comparison of simulated and experimental neutron and xray data. Allowing a truly creative approach to generating data analysis workflows.

It is envisioned that a common modelling interface will be created in such a manner as to leverage the capabilities of existing modelling packages. What is novel is the way in which this toolkit will be presented to the users and the modular nature of the workflows that the toolkit will provide

2. Develop such a common API interface to existing data reduction and analysis tools.

It is essential that for a truly modular approach a common api must be specified, planned and implemented. What is novel for this approach will be the collaborative landscape that will be created and fostered.

3. Develop new seamless access tools for neutron and xray data analysis & simulation.

¹ The mantid development.

Data volume from some techniques limits data portability; future data rates and file size will not decrease. To generate a larger community access to data, and analysis tools must be seamless.

Looking forward 10-15 years to the research landscape that will exist both in terms of academic research groups and large facilities it is clear that the current way in which users interact with data collected during experiments, planning such experiments, data analysis workflows and cross technique investigations preclude just an incremental improvement of the current infrastructure. A common pan European will generate greater scientific impact and accelerate the research process.