

**TITLE and type of activity (Networking, Joint Research development):
Virtual research environment for treating N & X data including
simulations**

Leading beneficiary: ESS (Thomas Holm Rod; Data Analysis Group Leader, European Spallation Source)

Partners: ILL, ESS, etc

EINFRA-9 Virtual Research Environments

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

What Mark and I have been discussing so far is a proposal centered around making it possible to perform co-analysis of data from different sources, e.g. from neutron scattering techniques or x-rays but also from computational methods like DFT and classical MD.

Topics that could be addressed in such a proposal would be:

- Remote user access to raw as well as processed data acquired at different facilities;
- the possibility for users to process and re-reduce data remotely;
- user access to the computer power necessary for generating theoretical data (e.g. MD simulations) that can be included in the data analysis ;
- standardised file and data formats;
- development of a platform and application programming interface (API) that makes it possible to combine different data analysis tools;
- development of automated workflows;
- implementation of a software development environment that can be shared between different facilities/corporations allowing for joint development and the use of best practices to ensure long-term maintenance;
- development and implementation of a policy/agreement for how to perform joint developments.

I believe that many of the components required for this have been developed already or is under development in existing projects like PaNData. Thus, I see that the main goal of this proposal would be to reuse these components and make them available to users and developers in a form where they are maintainable and user friendly to use, can be used remotely for instance through a web based GUI and with a well documented API so that external developers for instance at universities can make their own methods available for other users at the research

infrastructures. I believe that such a proposal matches the requirements listed in the call very well.

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