European Spallation Source (ESS) MANTID Project High Level Road Map.

Summary

ESS intends to develop and use the MANTID project software as a major component of its software suite to ensure a fully functioning software environment for ESS operations in 2019.

This document describes the forward looking strategy of ESS and the Data Management and Software Centre (DMSC) for collaboration with the MANTID Project partners as a member.

Background

The ESS is a multi-national European project to build a 5MW long pulse spallation neutron source in Lund, Sweden. The source will enter commissioning in 2019 with a suite of 16 instruments coming online between 2019 and 2025. The instrument types are listed at http://europeanspallationsource.se/instruments-and-support-facilities

Software development for ESS operations

The scientific computing for the ESS neutron beam instruments and science falls within the remit of the Data Management and Software Centre (DMSC) which is located in Copenhagen Denmark. DMSC is a division within the ESS Science directorate with the organizational structure described in Fig.1

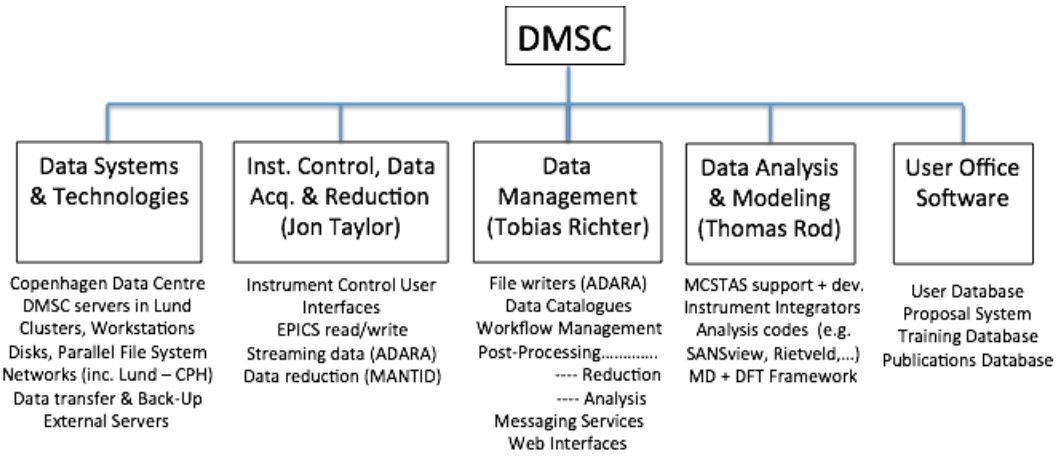


Figure 1 Organizational structure of DMSC

DMSC is responsible for all aspects of scientific computing at ESS.

1. Instrument / Experiment Control software.
2. Data reduction and visualization software.
3. Data streaming, data file creation and archiving.
4. Data analysis, modeling and simulation.

The responsibility to provide instrument control, reduction and visualization falls within the Instrument data group of DMSC.

At this stage the instrument data group at DMSC has a number of high level objectives:

1. Provision of an integrated software environment that on day one integrates instrument / experiment control, data reduction and visualization.
2. Provision of real time data reduction.
3. Provision of real time data visualization.
4. Data reduction and visualization within a parallel, distributed event based instrument architecture.

Project structure and staffing
It has always been the intention of the ESS to leverage the capability of existing software projects and frameworks to guarantee operational success. To this end and with the objectives of DMSC in mind it is clear that development and usage of MANTID at ESS will be resourced and operated in a similar manner as at ISIS and ORNL NDAV.

Our objectives will be realized by creating a single core development team with responsibility to deliver two key projects:

1. Instrument control (IC)
2. Data reduction and visualization (utilizing the MANTID framework)

The core development team is essential for delivery of the integrated software environment required for ESS. Moreover it allows a great deal of flexibility for development in a resource-limited environment.

It is envisaged that the team will be resourced by a mixture of ESS staff and staff working through an in-kind contribution to ESS.

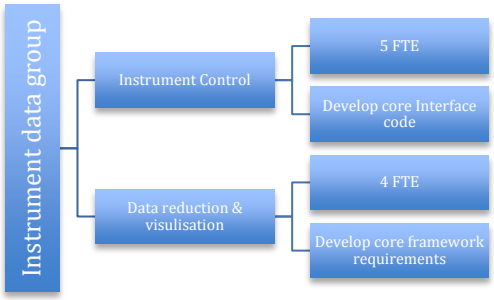
By 2019 DMSC will have a distributed development team of 9 FTEs working in flexibly on the integrated software suite for ESS.

The day one beam lines will each have a dedicated member of staff ensuring that these “pioneering” beam lines are allocated sufficient support for success.
Thus between 2019 and 2021 we will operate in a 1:1 development staff:instrument support mode.

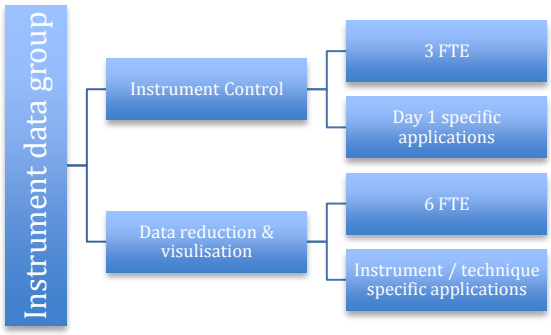
As the number of online instruments increases the staffing of the instrument data group will remain static, thus we will operate in a more usual 1:3 development staff : instrument support mode.

From 2015-2017 we will attempt to maintain a 60:40 split of FTE allocation between the two projects with the bias in favour of instrument control.

In this period the key MANTID development will be core framework based.

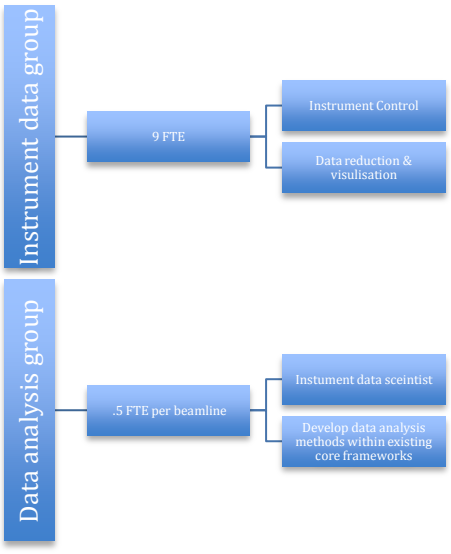


Post 2017 we will reverse the bias towards developing MANTID for specific beam line applications. To allow beam line specific software to be developed



Looking beyond day one to a period when ESS is running a user programme we will continue to maintain a core development team to service ongoing requirements and contribute to the wider MANTID development.

This team will be augmented by beam line data scientists who can service instrument requirements ***for analysis*** that fit within MANTID and also fit within the existing functionality provided by the MANTID Framework.



MANTID Development Roadmap (October 2014)

The development requirements for MANTID as of October 2014 can be split into two broad themes:

1. Core framework requirements.

The core framework requirements for ESS are those that all instruments will use and / or require. It is worth noting that whilst the ESS is a TOF source and as such directly applicable for Mantid, the long pulse and long timeframe will generate unique use cases. For ESS this means a significant amount of resource must be applied to software development to achieve success.

As with other members of the MANTID project this will be performed within the single project manager / distributed development team's organization of the existing project. It is envisaged that many of the ESS specific requirements can be abstracted out for use by other facilities that have similar objectives regarding real time visualization and reduction within an integrated software environment.

Some ESS high level requirements are:

1. ESS specific event mode listener.
2. ESS specific instrument definition files.
3. Framework adaptations to cover instruments with complex motions and motion control requirements.
4. Framework adaptations for specific ESS detector types. B10 voxel detectors
5. MCSTAS integration
6. Development of an API for ESS instrument control software.
7. Integration of the ESS ICAT environment
8. MANTID interfaces for live reduction & visualization servers
9. Development of the MANTID framework to allow distributed instances of MANTID within the ESS compute environment as a requirement to fulfill the objective of real time visualization.

2. Instrument specific requirements as of October 2014.

High level instrument specific requirements at this stage are currently being collected by DMSC, Some of the areas for software development are listed below for instruments that are currently in preliminary engineering design and have been in discussion with DMSC:

Instruments that are in preliminary engineering design as of October 2014:

NMX: Single crystal diffraction, optimized for macromolecular crystallography
Complex motion control and spatial detector configurations

ODIN: Neutron imaging and Tomography.
High data rate and real time visualization of tomographic projections

LOKI: Broadband small angle neutron scattering
High data rate, Tight coupling of data reduction to instrument control to allow single shot and stop flow type experiments to be routinely performed.