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## DMSC overview

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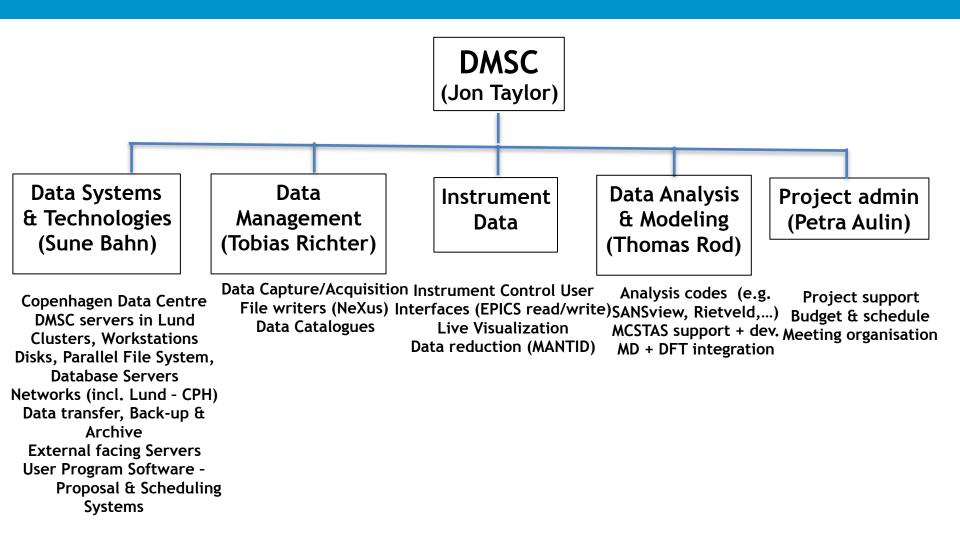
## Centralised scientific computing

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- Lessons learned from other facilities
  - All facilities moving in this direction.
- Single point failures
- Curation of software & data
- Planning & strategy
- User programme efficiency & impact
- Collaborative development

# **DMSC Organization**





## Data Management and Software Centre



Provide world leading scientific software and scientific computing support for neutron scattering at ESS

#### Scientific Software development.

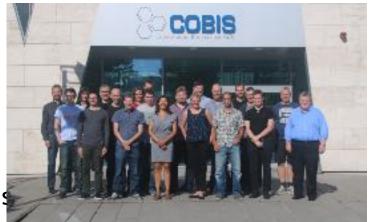
- ➤ The ESS experiment control system
- > Data acquisition software.
- $\succ$  Data correction software.
- Data visualization software.
- Software to model and analyze experimental data s

#### Data centre operations.

- $\succ$  Store & catalogue ESS neutron datasets.
- $\succ$  Provide ESS users remote access to their data
- Compute provisioning for live data correction, visualization and analysis software during and after experiments.

#### User programme support (operations phase)

 $\succ$  Provide support & assistance to ESS users for data treatment and data analysis.



DMSC offices located at COBIS. Copenhagen University north campus

# DMSC high level



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- Development priorities
  - DAQ and detector readout
  - Control
  - Reduction
  - Analysis
- Operational priorities
  - Cluster availability

- Integrated suite of software
- Coupling Control, reduction and analysis
- Sufficient performance to allow real time features
- Provisioning of hardware to support this
  - During and after beam time

# DMSC construction budget

- 20M euro
- Fully allocated
- Hardware provisioning for readout, control, reduction, analysis
- dual location compute infrastructure and link
- Software development
  - Detector readout (Brightness)
  - Data acquisition system
  - Data reduction / Experiment control
  - Data analysis -
    - phenomenological model fitting
  - Data curation

## **Current DMSC activities**

- Cluster operations McStas /MCMPx Geant4
- McStas support / development
- Mantid collaboration
- SASView collaboration
- Brightness funded detector readout
- In-kind at STFC & PSI
- Sine2020 WP10 data treatment software

# Current / Planned in-kind



- Data streaming STFC active
- Data reduction and experiment control STFC active
- Experiment control PSI active
- Data curation PSI active
- Imaging data treatment PSI approved at PSI
- Reflectometry / QENS / Engineering diffraction data treatment FZJ agreed by FZJ

### What is excluded



- Full scope compute solution
- instrument specific data reduction and control
- Modelling and simulation based data analysis
- User office software development

#### Near term data analysis collaborations



- Parteners ISIS & PSI
- Diffraction
  - Partner ILL

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### Software development strategy

- Minimise TD in our chosen frameworks
  - Allow later developments to be less resources intensive.
- · Collaborate with other facilities on common frameworks
- Make the best use of the resources available
- Feature complete core experiment control / DAQ FW
- Minimise unknowns by prototyping
  - WFM, live reduction and analysis pipeline
- Fully functional software for some instrument classes
  - Priority for early instruments
- No development of S/W that is not going to be used
  - Importance of good requirements & specification
  - Importance of good project management no divergence

## What is already decided

- Mantid for reduction and visualisation
- NICOS2 core experiment control
- SASView
- Born again
- Our Inkind partners STFC PSI FZJ

## Scope shifts & core development



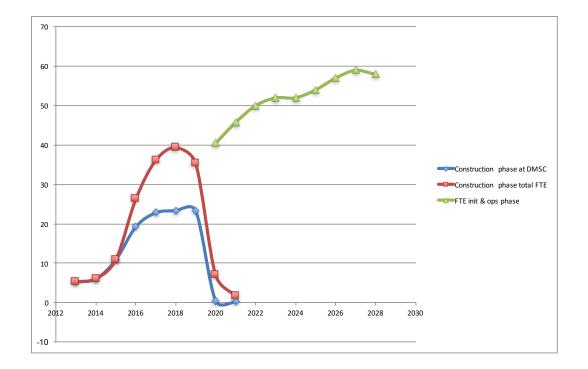
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- Instrument class software discussions
- Instrument specific requirements harvested for core requirements.
  - Edge cases should be known
- Truly instrument specific requirements sent to backlog
- Allow external effort to be usefully utilised
- Develop instrument specific solutions 2020 +
  - From ops funding

### Current staff profile



- Core staff now flat in construction
- Brightness 25py and in-kind 43py bump





## Interface management for Mantid

Mantid



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Collaborative software project at ISIS - ORNL - ESS - ILL

A lot of user requirements

Pre meeting discussions at labs

Harvested in large steering meetings

A very large spreadsheet that is prioritised and allocated resources some integration into Github Communication of progress is an ongoing issue

Weekly management meetings with local PMs



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A single PM for the project to push features and releases

Developers work with instrument scientists on features

Named points of contacts for science groups (ISIS)

Developers attached to specific beam lines (SNS)

Development team in a single location (ISIS)

Development team spread over the science floors (SNS)

#### Requirements



• Who should be the owner

Define completion criteria