

# Mantid user meeting

## Mantid at ESS

# Data Management and Software Centre



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

## **Scientific Software development.**

- Experiment control
- Data acquisition system
- Data reduction, analysis & modelling

## **Data centre operations.**

- Dual location - Lund & Copenhagen
- Data management and curation

## **User programme support**

- Data scientists
- User office software
- Remote access to data and software tools



# Mantid scope at ESS - Priorities



1. Data reduction and correction

2. Data workbench

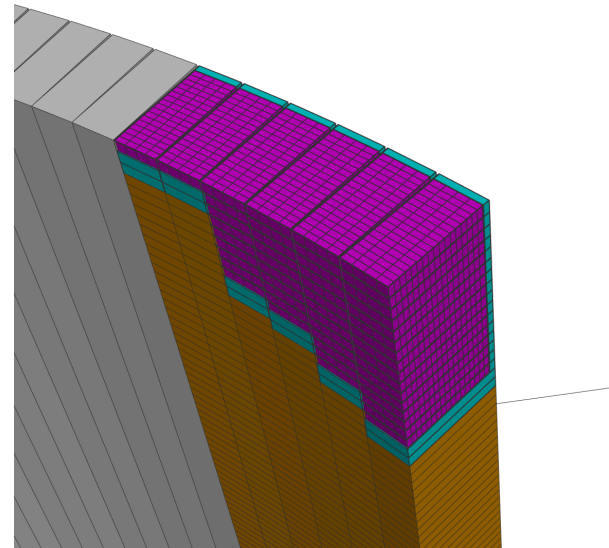
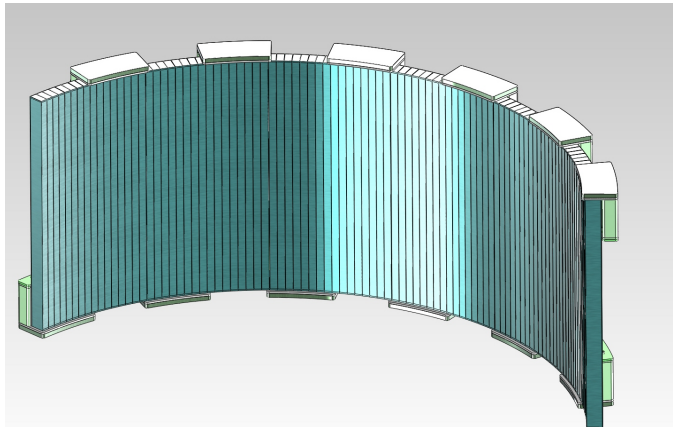
3. Some analysis functionality (QENS)

- ☑ High event rate  $>10^7$
- ☑ Complex detector geometry
- ☑ Software DAQ solution

# Mantid Performance requirements

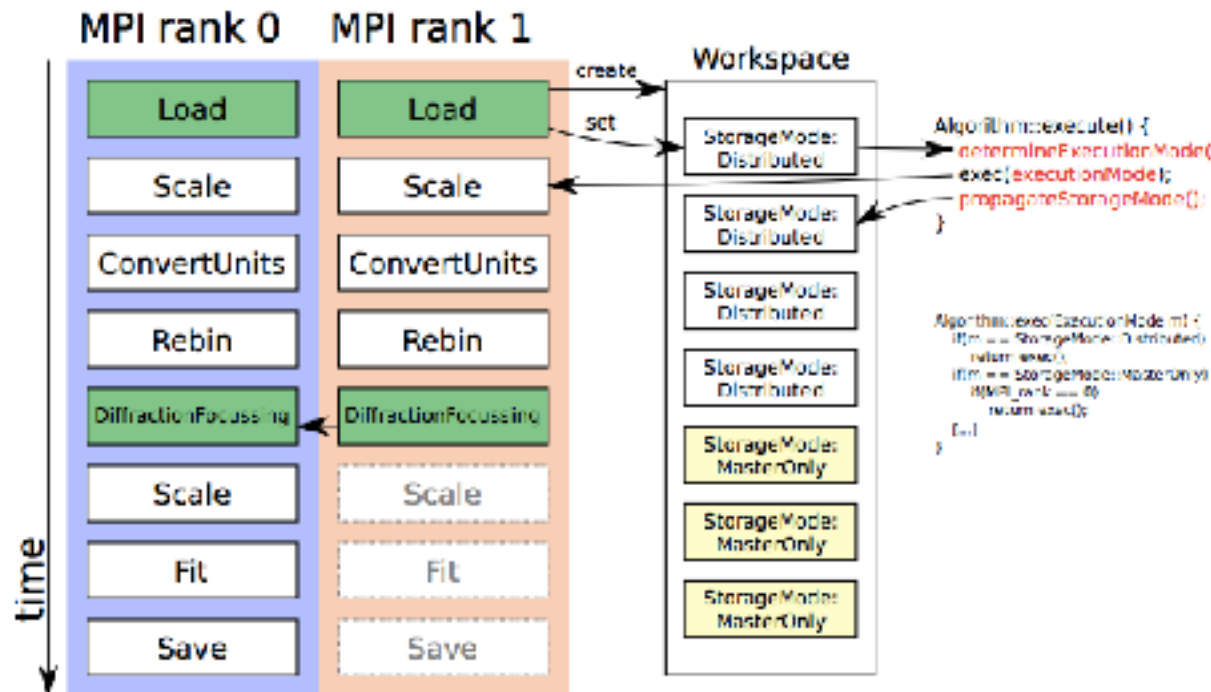
## ► Requirements -

- live data reduction for an event rate of  $> 10^7$
- Filter good events from bad events
- Capability for handling of complex geometries



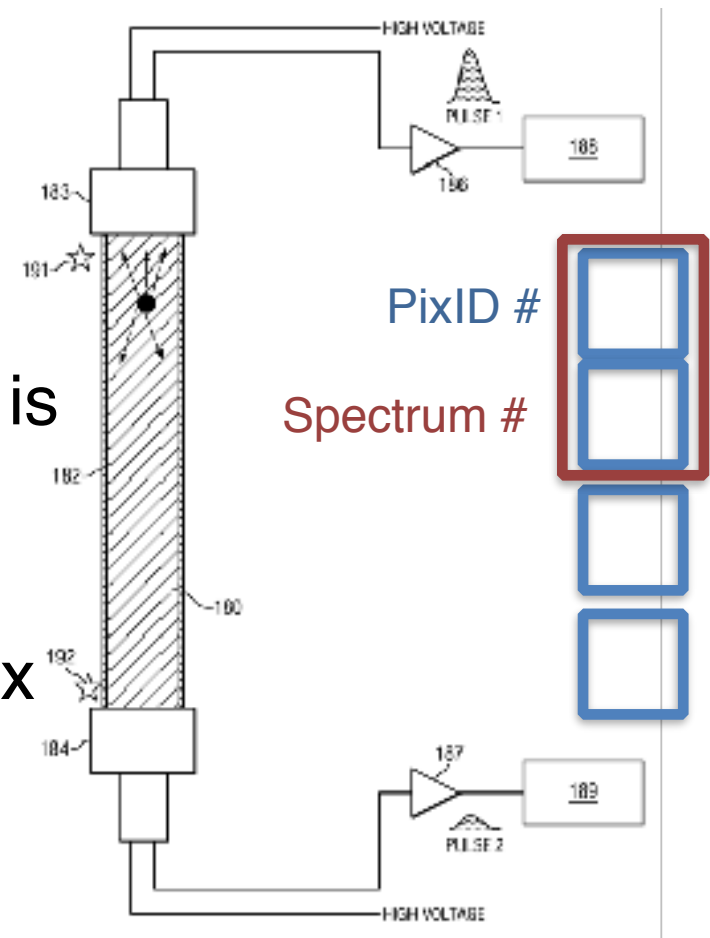
# Towards live data reduction.

- Mantid has
  - Geometry
  - Data types
  - algorithms
- Create a common MPI implementation
- Introduce type safety



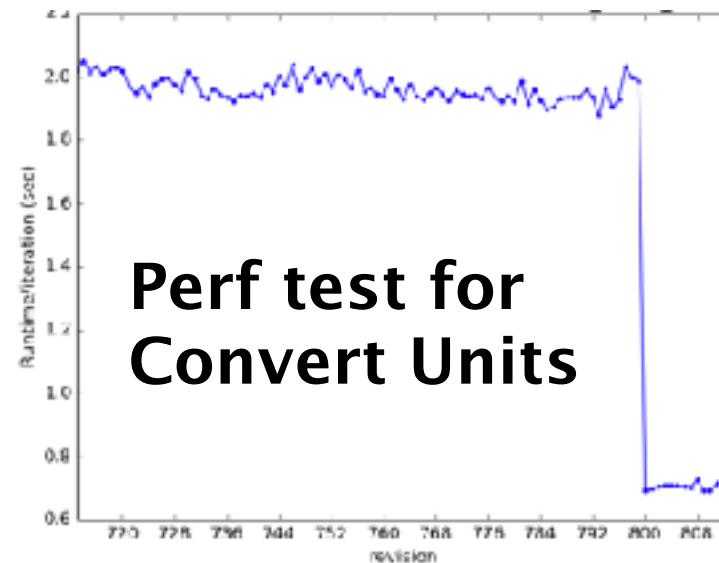
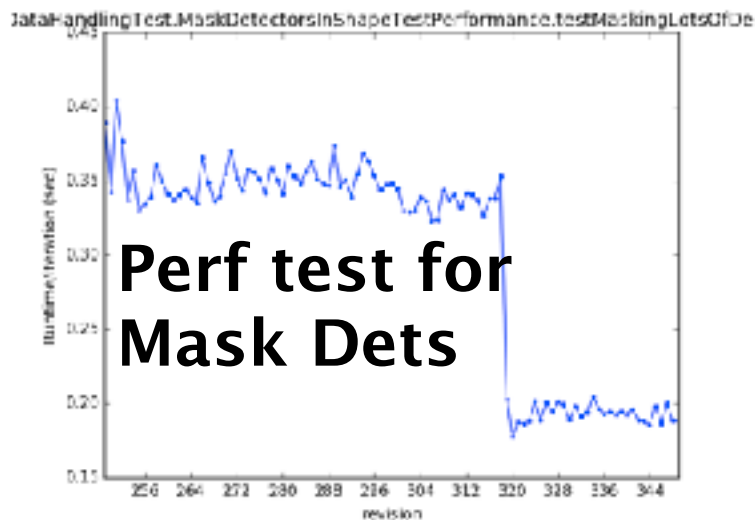
# Instrument 2.0

- Instrument stores geometry and meta data.
- r,t,p spectrum ID map, isMasked...
- Complex detector geometries
- Current Instrument implementation is rate limiting
  - Parameter map is large /complex
  - Organically developed



# Results

- Highlights the cost of refactoring
- Significant improvements across Mantid
- ILL can load interlaced scans from D2B into Matrix
- Direct geometry workflow x2 faster

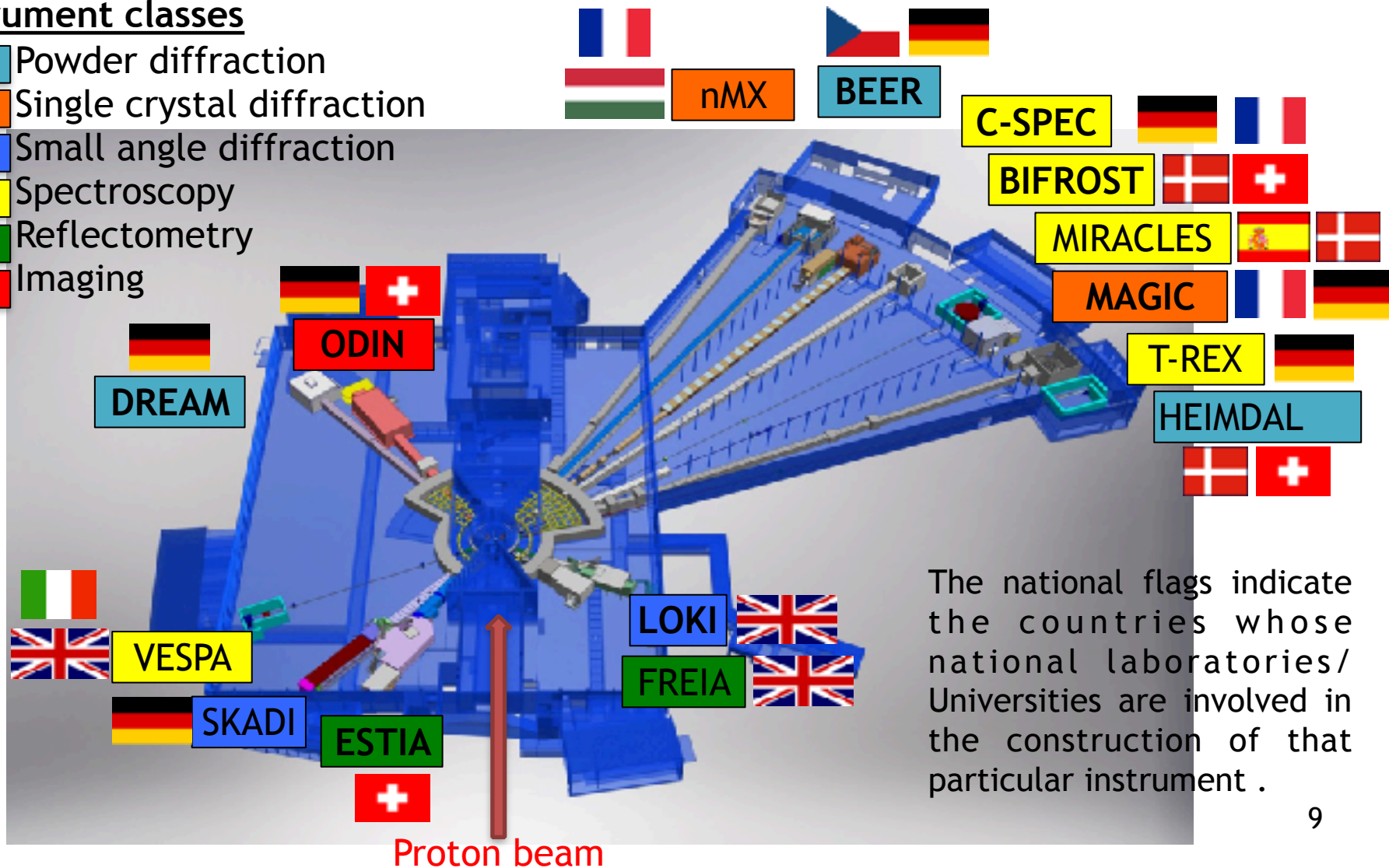




# The ESS Instrument Suite 1-15 (22)

## Instrument classes

- Powder diffraction
- Single crystal diffraction
- Small angle diffraction
- Spectroscopy
- Reflectometry
- Imaging



The national flags indicate the countries whose national laboratories/ Universities are involved in the construction of that particular instrument .

# Stakeholder engagement & science requirements

## Charge:

Outline & agree the core requirements\* for instrument control

Outline & agree the core requirements for data reduction

Outline & agree the core requirements for data analysis

Provide a realistic time line into full operations of diffraction instruments for DMSC.

\*core requirements are provided within the DMSC budget for construction, more with operations funding beginning in 2019.

- DSMC / STAP and Instrument teams
- Reflectometry 21st March
- Diffraction April 7th
- Imaging 26th-27th April
- Spectroscopy 15-16th May
- SANS 1st - 2nd June



Discussing software requirements for the  
@essneutron reflectometers



# Key discussion points

- Key message promote science delivery
- Framework for reflectometry analysis development
- Community gap for PND
- Bragg edge diffraction software for imaging
- **Data management and acquisition for imaging**
- Focus user experience on science domain not instrument / technique
- Rietveld for Inelastic scattering
- Data acquisition modes
- Co-analysis & Batch analysis for SANS

# Summary of instrument software meetings

	<i>1st HC date</i>	<i>DAQ &amp; DM</i>	<i>Control</i>	<i>Reduction</i>	<i>Analysis</i>
<i>Imaging</i>	<i>Q1 2021</i>	<i>Pending discussions</i>		<i>Basic requirements</i>	<i>CT &amp; BE fitting</i>
<i>Spectroscopy Hard condensed matter</i>	<i>Q1 2021</i>	<i>MultiGrid &amp; 3He (BiFrost)</i>	<i>discussed with DMSC / ICS</i>	<i>Basic requirements</i>	<i>Horace &amp; other matlab tools</i>
<i>Spectroscopy soft matter</i>	<i>Q1 2021</i>	<i>MultiGrid &amp; 3He (Miracles)</i>	<i>discussed with DMSC / ICS</i>	<i>Basic requirements</i>	<i>QENS</i>
<i>Mol. Spec.</i>	<i>2024</i>	<i>3He</i>	<i>discussed with DMSC /</i>	<i>Basic requirements</i>	<i>A-Climax +</i>
<i>Diffraction powder</i>	<i>Q2 2021</i>	<i>CDT Jalousies</i>	<i>discussed with DMSC / ICS</i>	<i>requirements discussed</i>	<i>Cannot cover all Fw in 2D</i>
<i>Diffraction xtal</i>	<i>Q1 2022 Magic Q3 2022 NMX</i>	<i>CDT Jalousies &amp; GdGEM</i>	<i>discussed with DMSC / ICS</i>	<i>-</i>	<i>- PND - MX</i>
<i>Sans</i>	<i>Q1 2021 Skadi</i>	<i>LOKI detectors undefined</i>	<i>discussed with DMSC / ICS</i>	<i>requirements discussed</i>	<i>SASview</i>
<i>Reflectometry hard condensed matter</i>	<i>Q1 2021</i>	<i>MultiBlade</i>	<i>discussed with DMSC / ICS</i>	<i>requirements documented</i>	<i>Many tools requires common input &amp; workflow</i>
<i>Reflectometry soft matter</i>	<i>2025</i>	<i>MultiBlade</i>	<i>discussed with DMSC / ICS</i>	<i>requirements documented</i>	<i>Many tools requires common input &amp; workflow</i>

# Headlines

- Cost of refactoring is exceptionally high
  - TD in the FW is unacceptable
- ESS construction requirements are outside of scope of other partners

# Mantid User meeting

## Mantid strategy

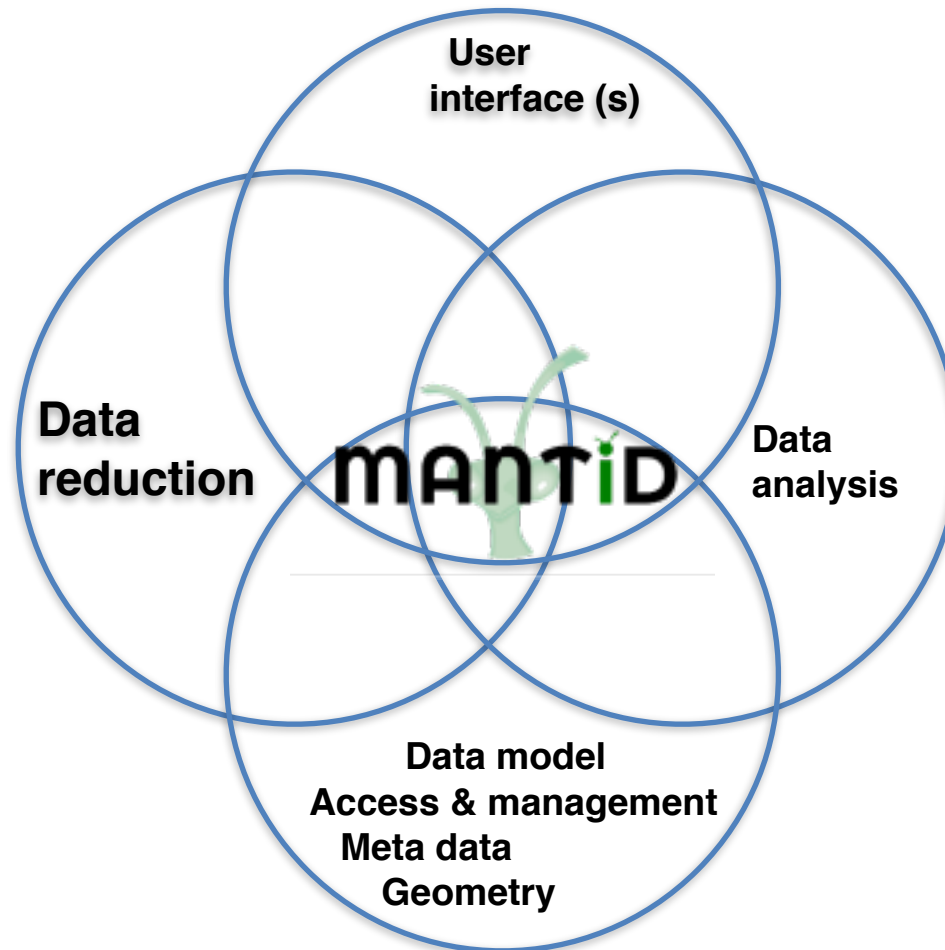
# Mantid: why did it start in 2007

- Mitigate SPOF
  - Centrally resource scientific computing
  - Curation of software and data
  - Increase scientific productivity

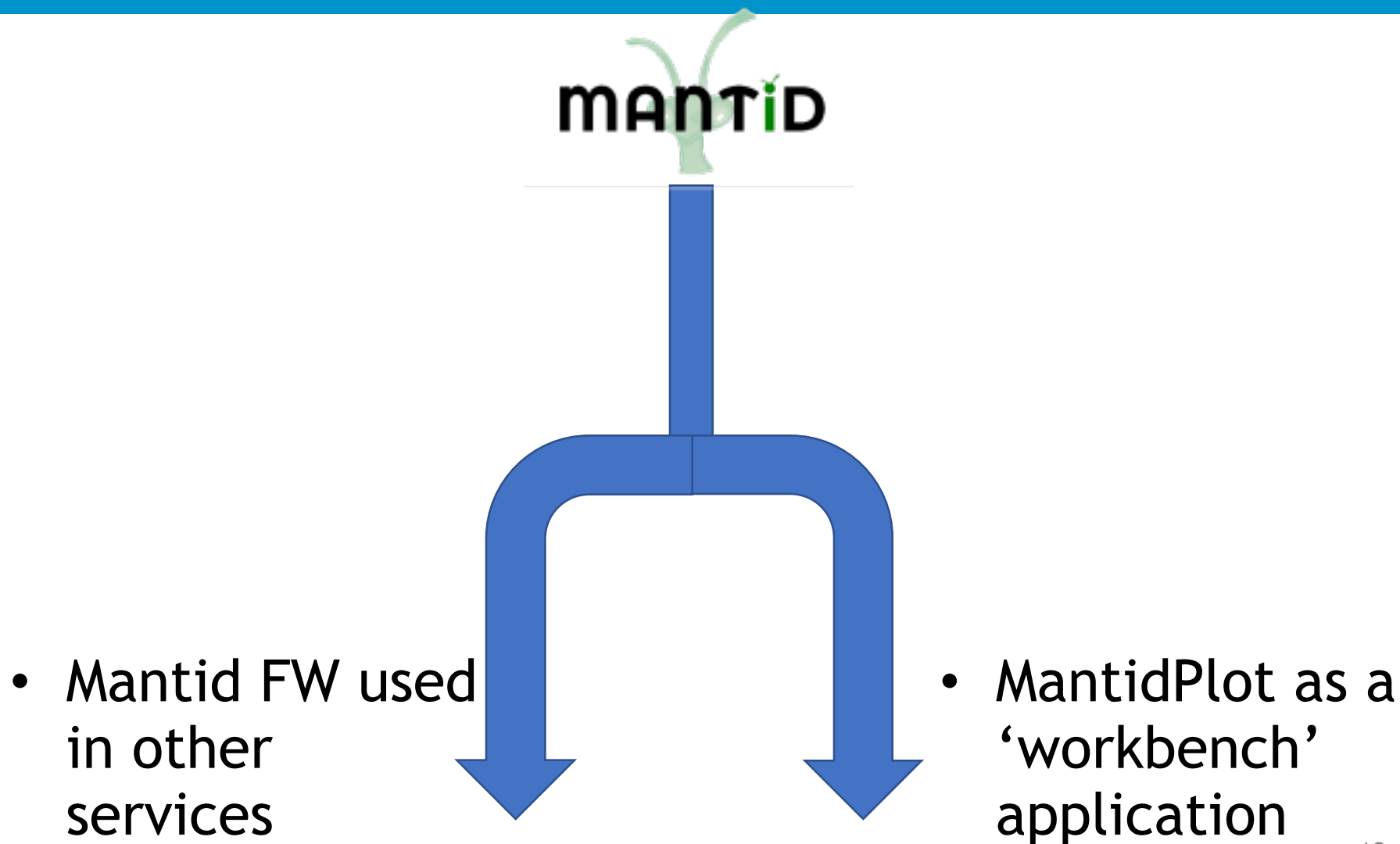
# Project partners





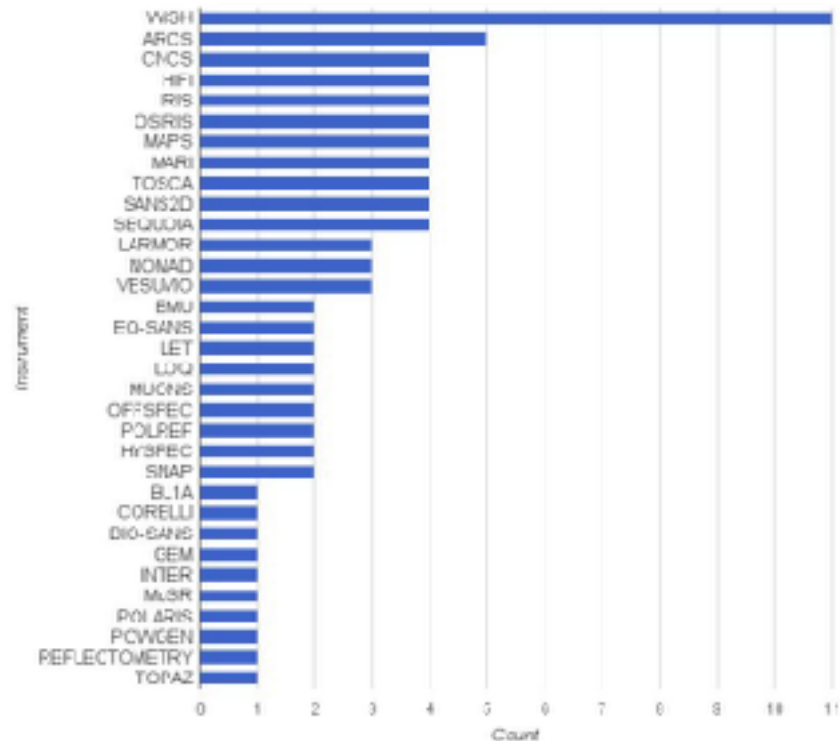


# Two broad modes of usage

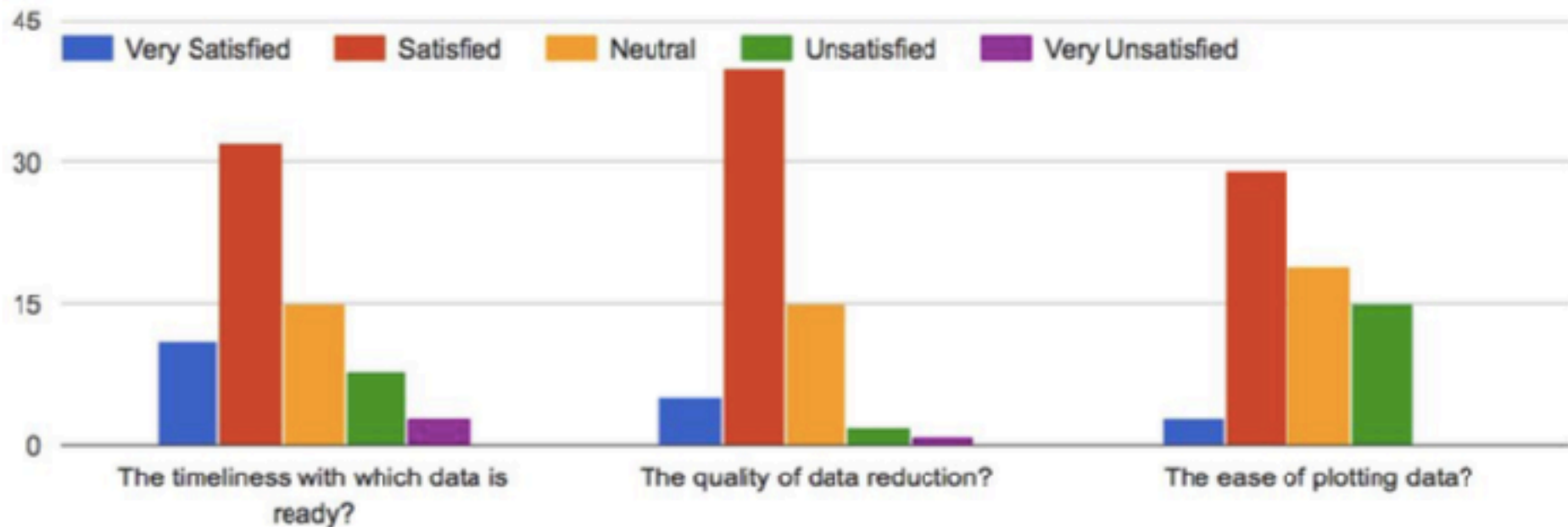


# Mantid project - SSI review

- Two questionnaire based reviews
- Technical
- Collaborative



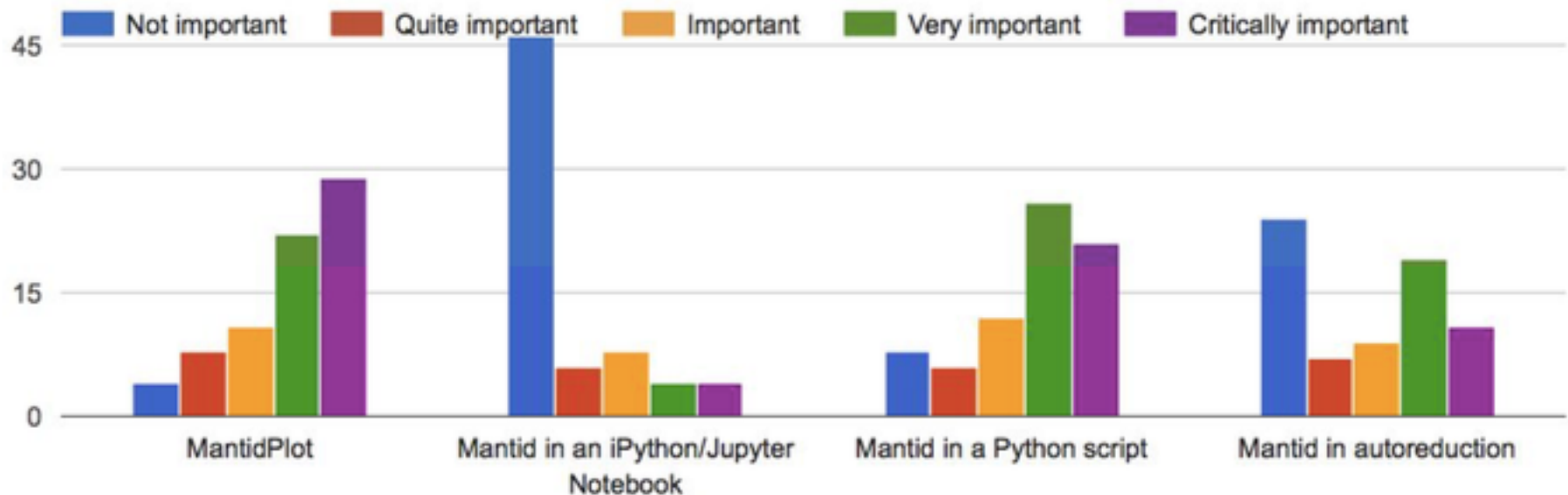
# Results of the collaborative review



**Figure 7.** Satisfaction of respondents with timeliness, quality of data reduction and ease of plotting data

# Importance of a GUI

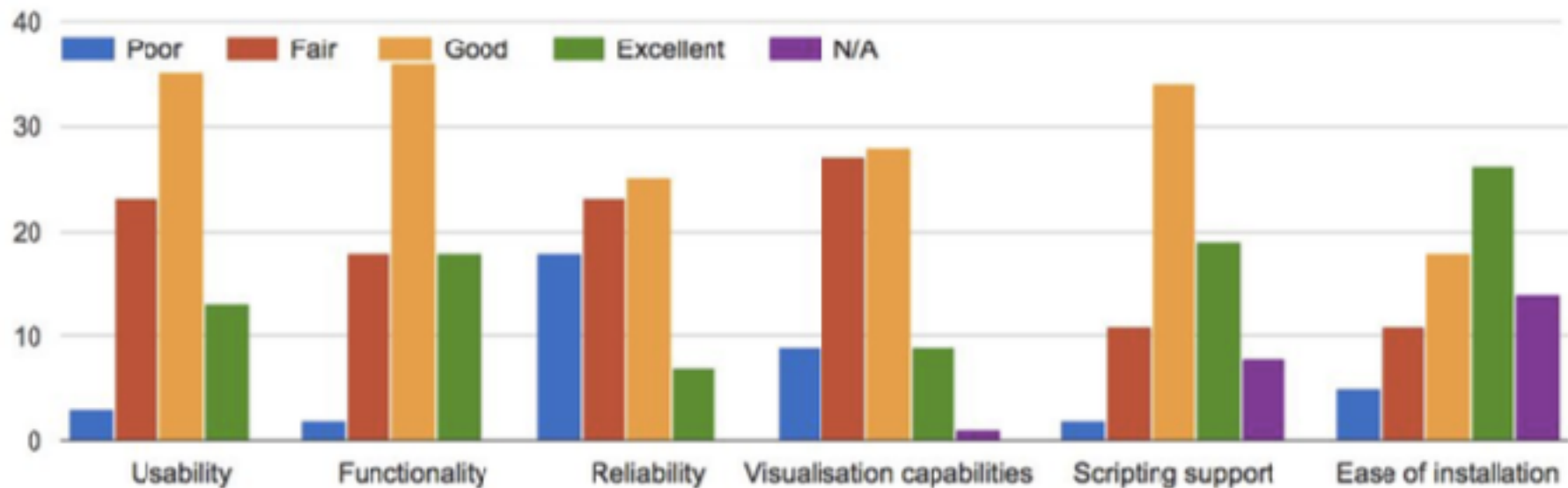
- GUI is critically important



**Figure 11.** How important are the following applications in your work?

# General functionality

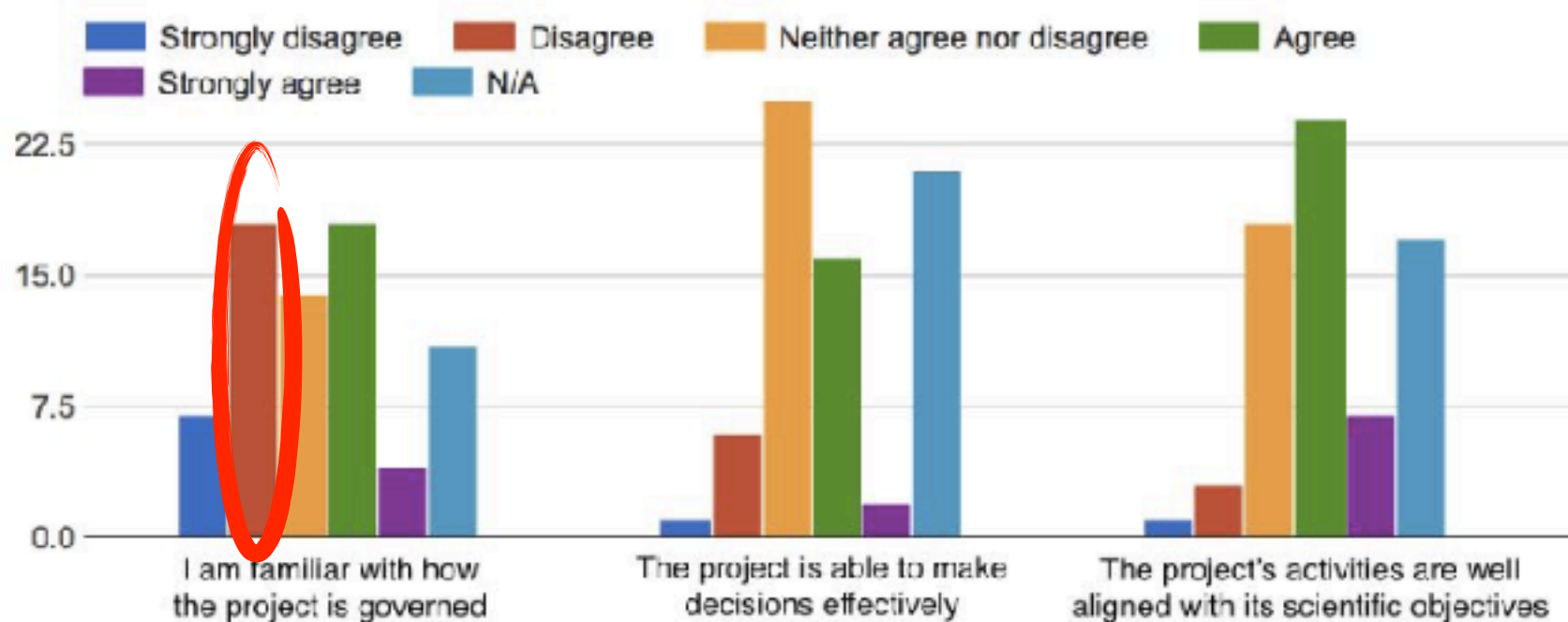
- Reliability
- Usability



**Figure 12.** How would you rate the following aspects of Mantid for your purposes?

# Governance

- 25% of respondents have attended a SSC



**Figure 29.** To what extent do you agree with the following statements?  
(Familiarity with governance, ability to make effective decisions,  
activities well aligned with scientific objectives)

# Headlines

- Stability
- Documentation / Training
- Performance
- improved features
  - plotting
  - UI - cleaner