Instrument Independent Reduction and Analysis at ISIS and SNS

Nick Draper

Teswww.mantidproject.org

Tessella
Technology & Consulting

SNS
SPALLATION NEUTRON SOURCE

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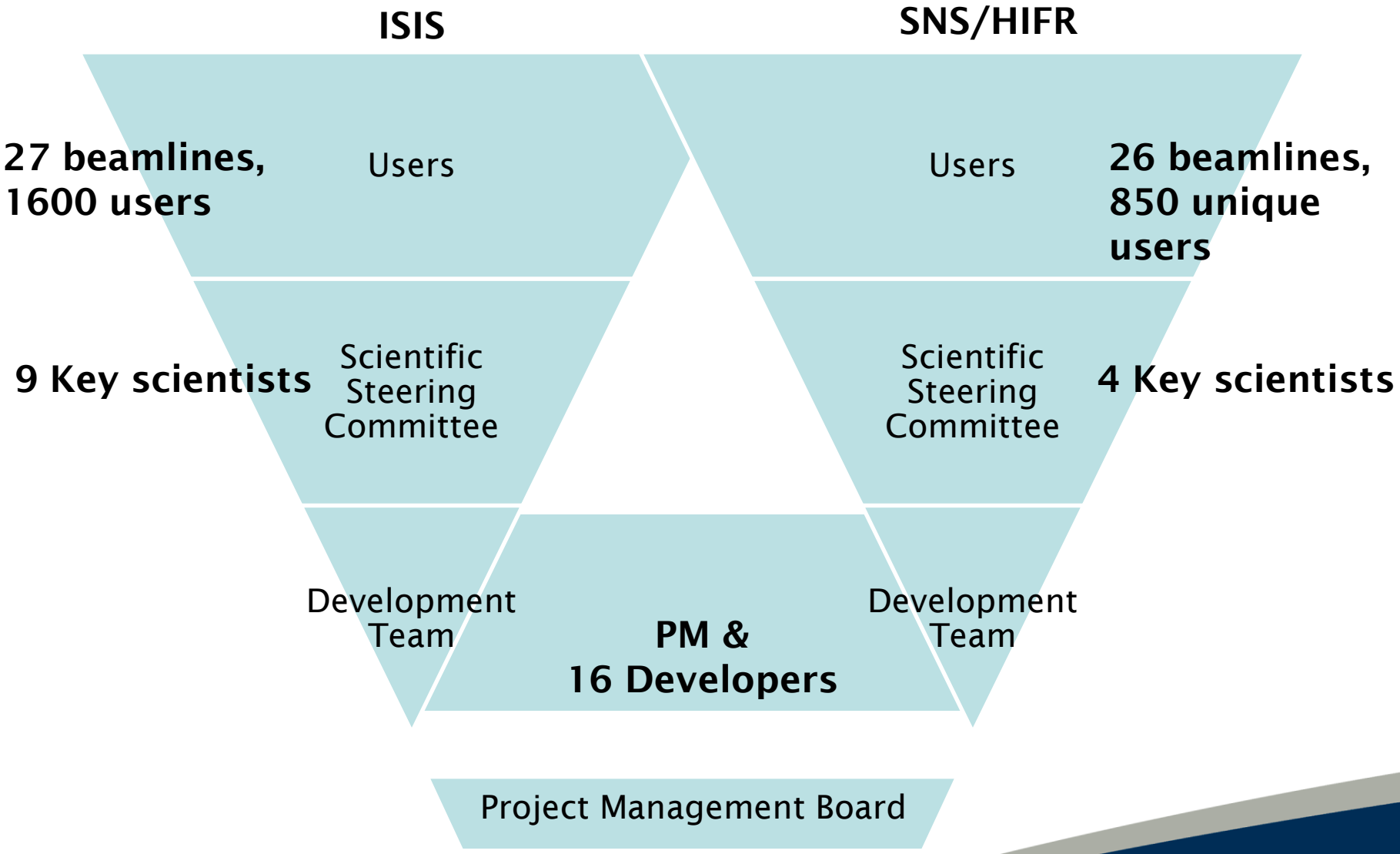
ISIS

Project Organisation



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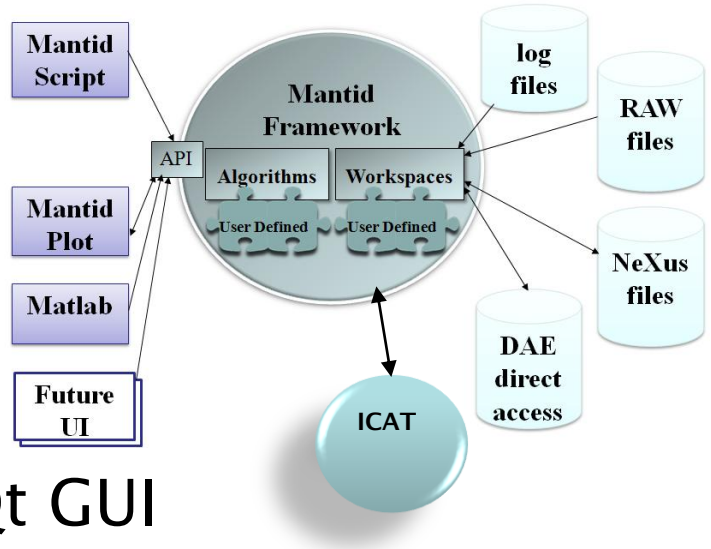
How we do it Technically

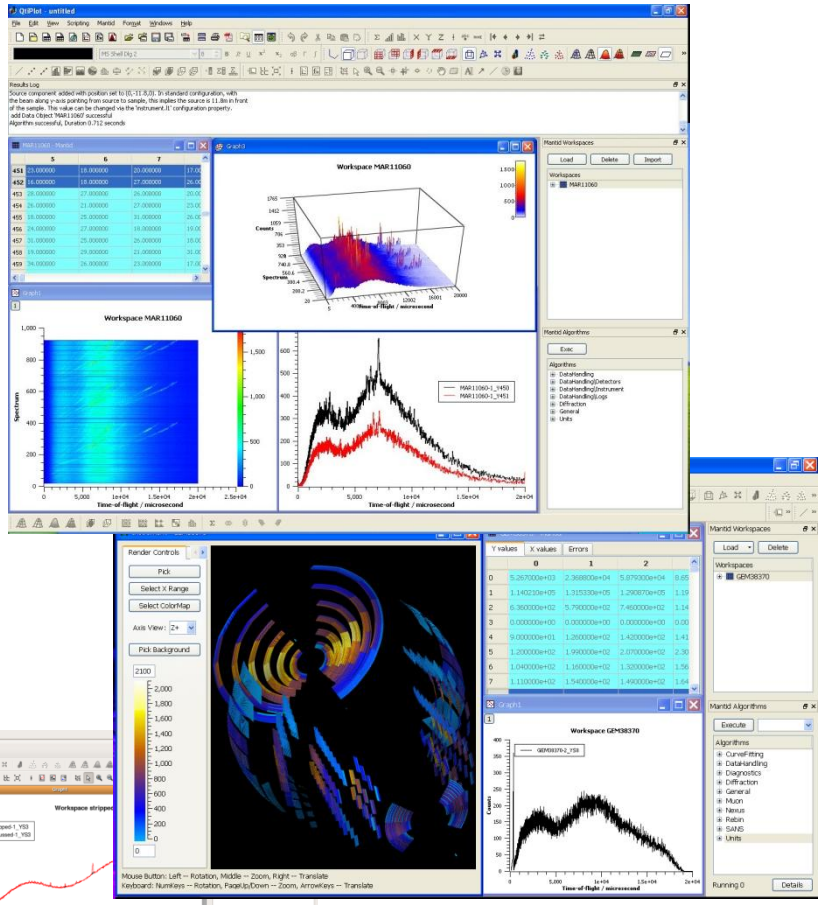
- Organisation
  - Open source
  - Continuous integration
  - Automated build, test & deploy
  - Distributed team

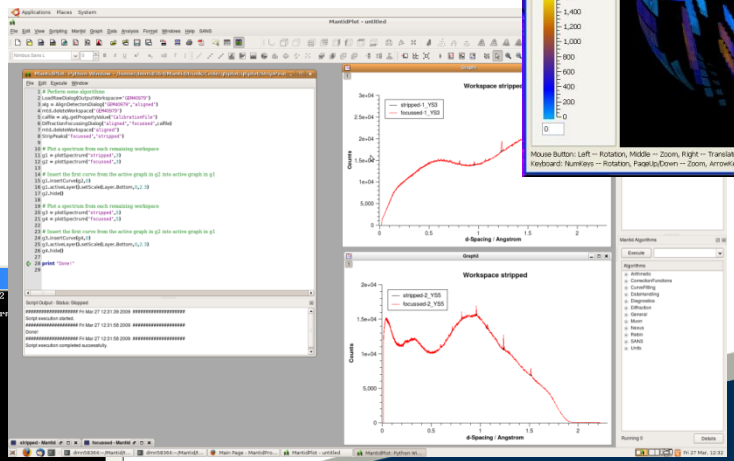


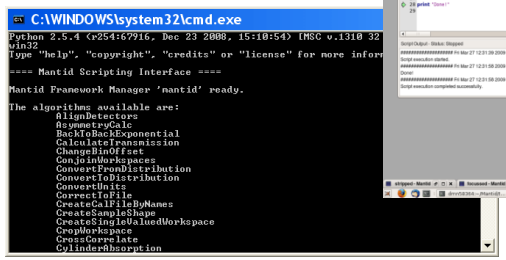
- C++ Framework
  - Win, Linux, Mac
  - Memory Management
  - Performance optimisation
    - OpenMP
  - Common Interfaces
  - Plug in Mechanism
- Qt GUI
  - Extended from QtiPlot
- Python Scripting
  - Using Boost Python
  - Powerful and extensive coverage
  - Integration with NumPy

User interfaces

- MantidPlot
  - 1, 2 and 3D plotting
  - Interactive Instrument view
  - Ad hoc analysis
  - Specific User interfaces
  - Integrated scripting
  - Extendable with plugins
- MantidScript
  - Pure command line support







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Rollout

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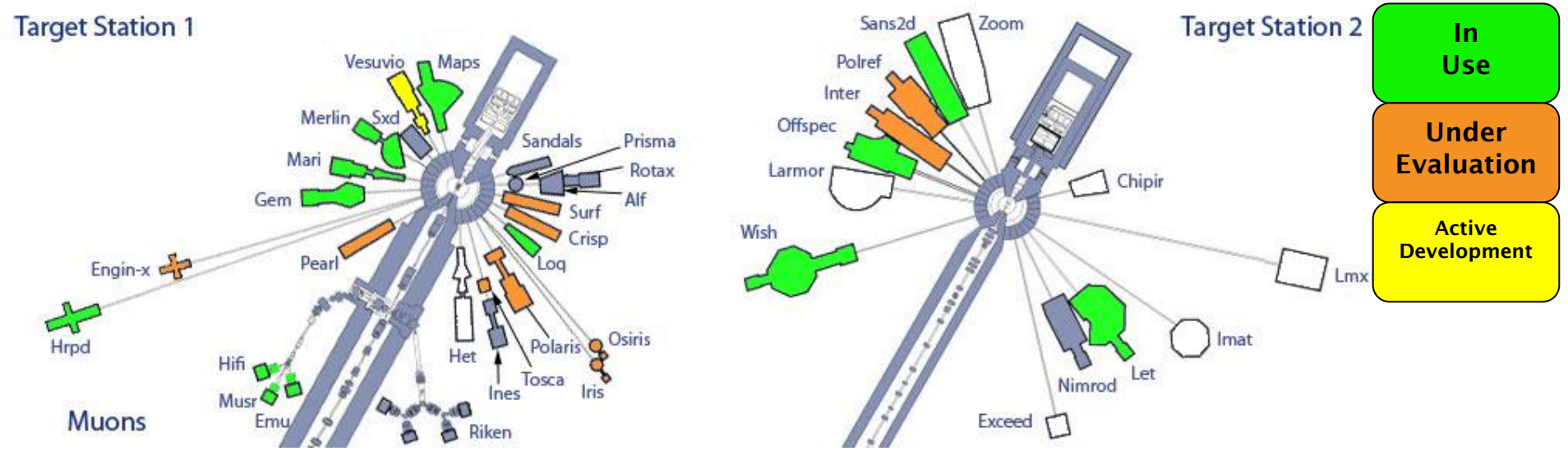
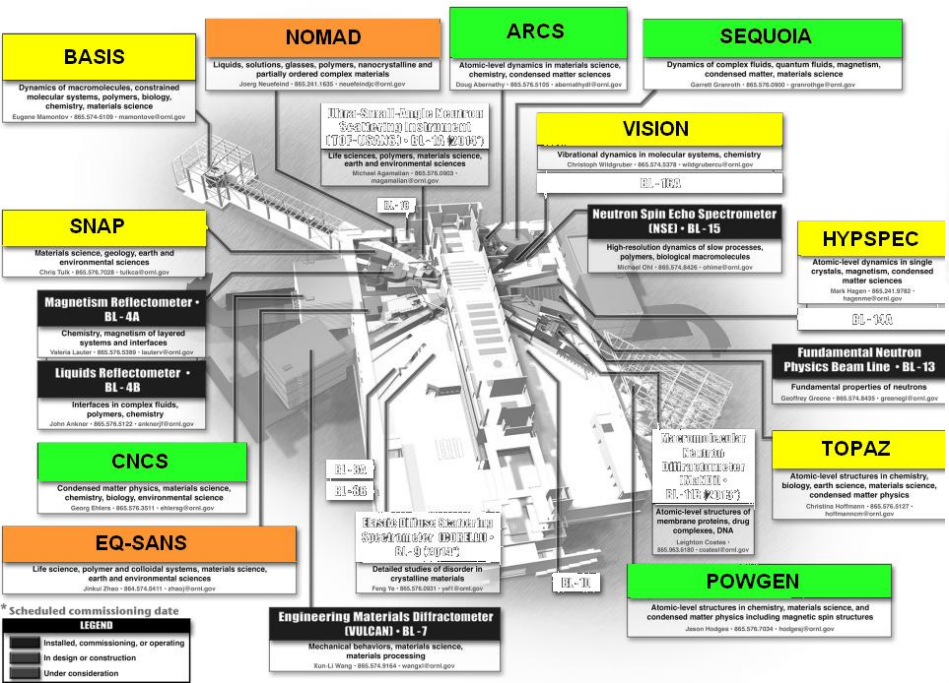
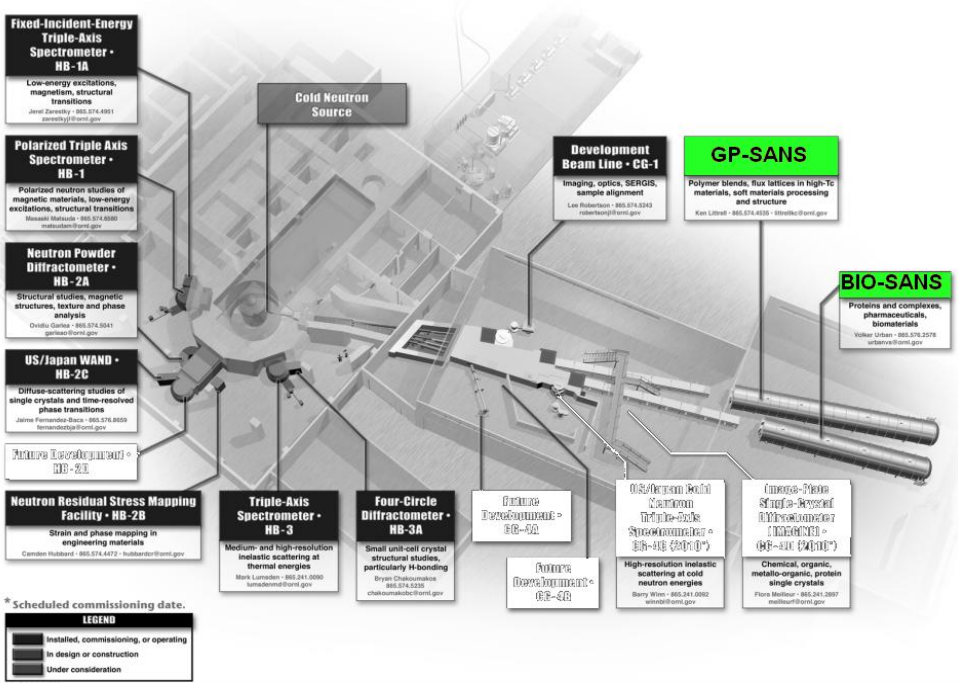


SNS



HFIR

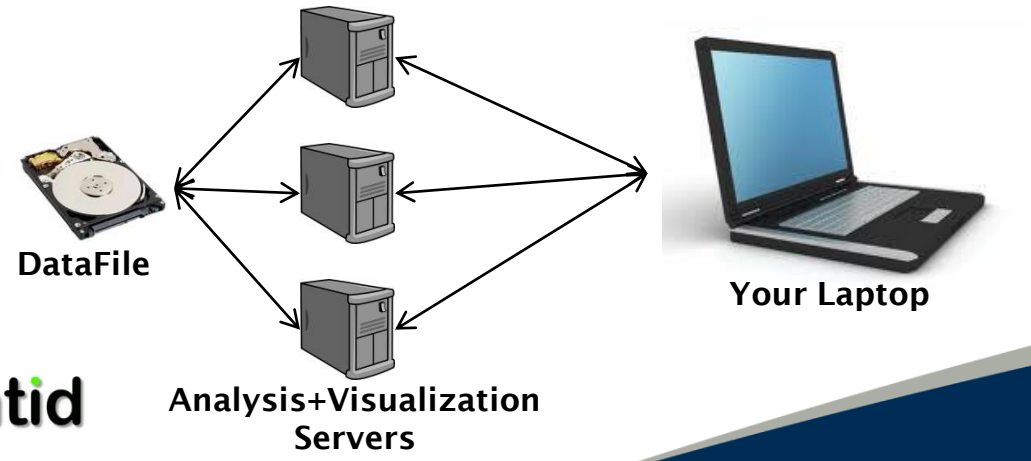


Other possible collaborations

- ILL
  - Pilot starting to evaluate and improve support for Triple Axis apectrometers
- Julich & Helmholtz association
  - Considering piloting Mantid and possible becoming a full partner
- ESS
  - Planning to use Mantid for data reduction
  - Initial steps will increase Mantid – McStas integration

VATES - Advanced visualisation & analysis

- Problem
  - Large 100GB datasets
  - 4+ dimensions
    - Q(x,y,z), ω, temp, field, etc.
- Solution
  - Distributed Parallel visualization
    - Paraview
  - On the fly parallel data rebinning



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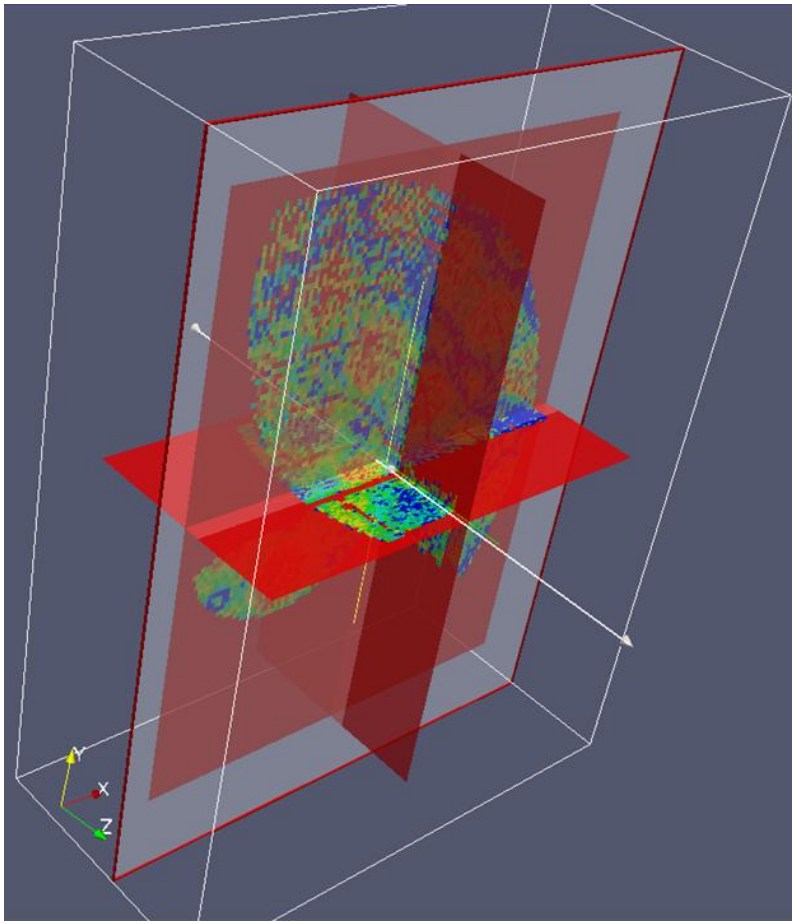
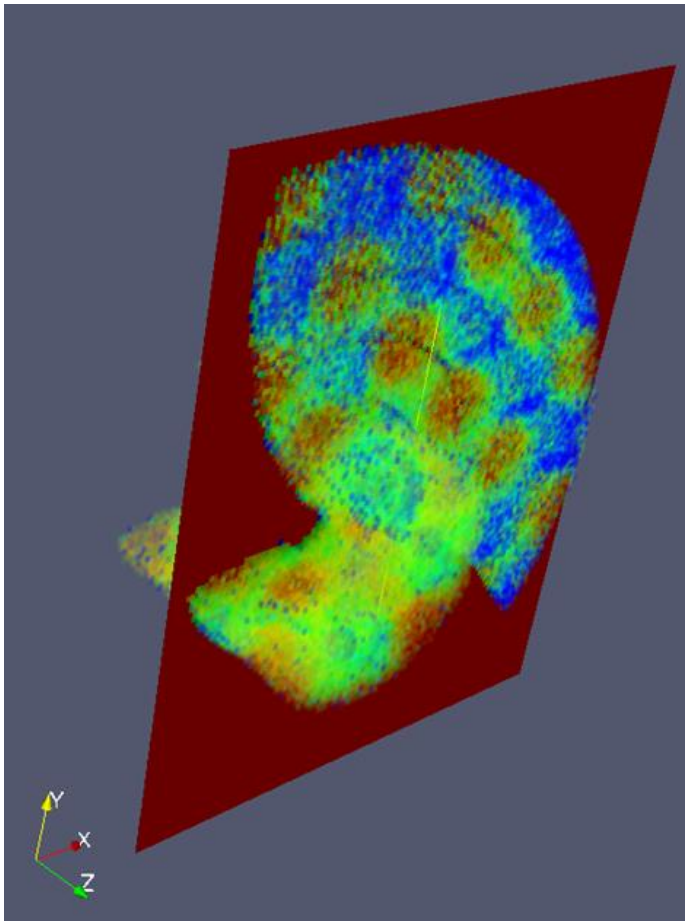
Multidimensional data visualisation





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Mantid & Danse

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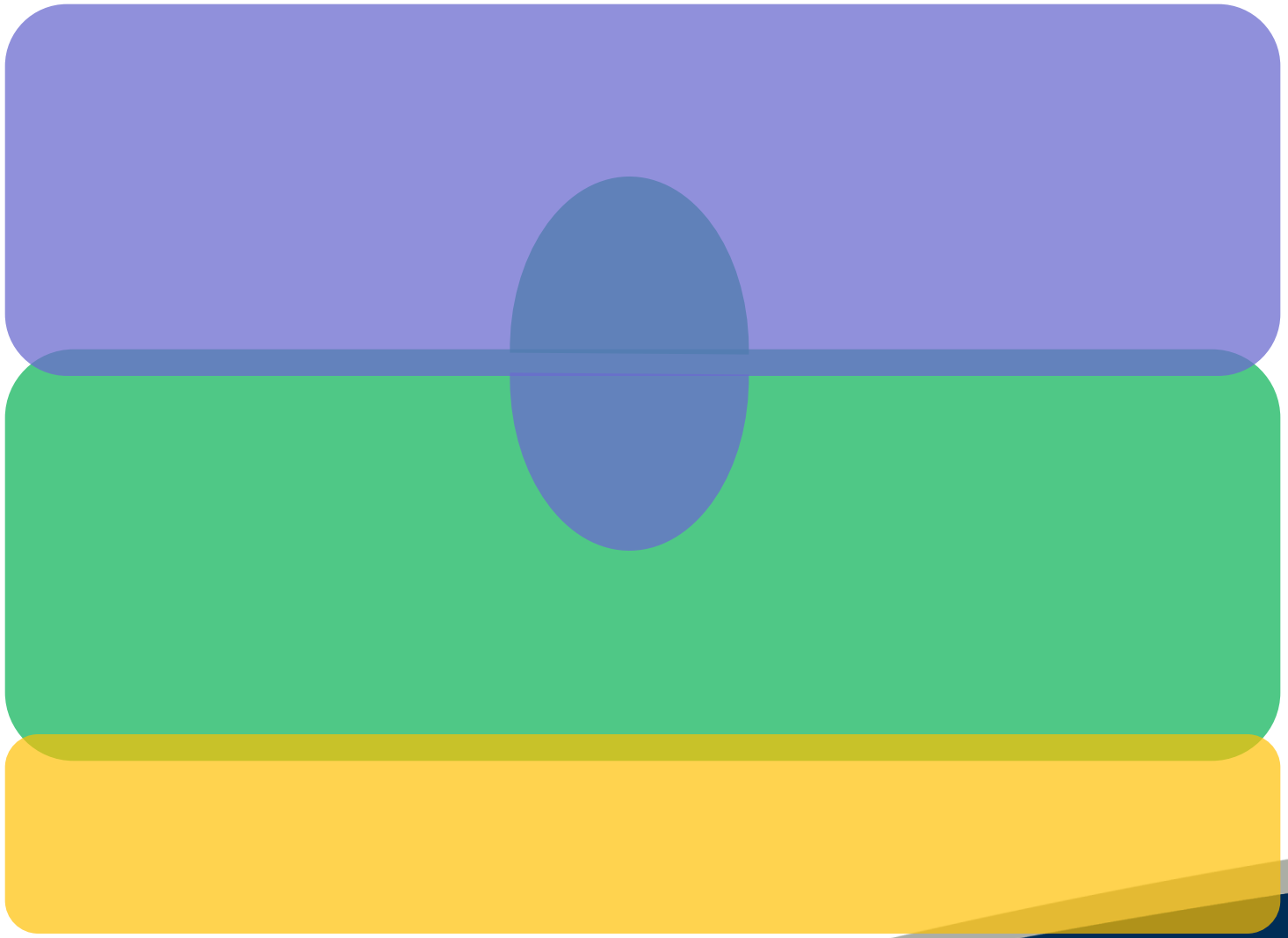
Mantid – Danse Scope



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Integration Possibilities

- Control Scope
  - Maintenance
    - We cannot do everything
  - Installer/ pre requisite bloat
    - Harder to install for users and maintain for us
    - Places restrictions on DANSE
- Provide a good user experience
  - Usage
  - Installation
- Maximise reuse – effort
- Start Simple!

Mantid SANS Requirements

- Provide a comprehensive SANS model fitting solution
- Provide an extensible library of models
  - Some cab be integrated from FISH
- Support complex constraint functions

DANSE SANS software

- SANS Models
  - Library of 50+ models
  - Originally from NIST
  - Thoroughly tested
  - Accessible via C++ and Python
- SANSView
  - Fitting package in 1D and 2D
  - Constrained fitting
  - “slicing tools”
  - P(r) inversion, SLD calculation

Mantid DANSE SANS plan

- Integrate with SANSView
  - File Transfer for SANSView
    - via CanSAS1S and Nexus formats
  - Reading NIST raw data into Mantid
    - Improve file integration
    - Speed up testing
  - Launch SANSView from Mantid
    - Identifying file to load
    - SANSView must be easy to install on Win, Mac and Linux
  - Integrating SANS models into Mantid
    - From both DANSE and FISH
    - Using a thin translation layer if possible

Mantid DANSE SANS plan

- Integrating SANS models into Mantid
  - From both DANSE and FISH
  - Using a thin translation layer if possible
- Add a P(r) inversion algorithm to Mantid
  - Using the underlying DANSE package
- Integrating the SANSView Calculators & Data Processors into Mantid
  - Scattering Length Density
  - Sector averaging
  - Box summing
  - All use PeriodicTable (already in use in Mantid)

Reflectometry

- DANSE SANS software
  - Reflectometry Models
  - GARefl
    - Simultaneous model fitting for multiple data sets
- Mantid DANSE SANS plan
  - Provide an easy to use user interface
    - Easy to install
  - Launch from within Mantid

Inelastic

- VNF
  - Produce Event based Nexus file output
    - Can be read into Mantid
- Mystic, Pathos
    - To be considered for VATES distributed computing
    - Need to be careful about too many C++ - Python switches
- Third Party Bindings
  - Gulp, VASP, Quantum Expresso
    - Could be of direct use in VATES

Diffraction

- PDFFit / PDFGUI
  - Integrate at a file level
  - Initially via PDFgetN, later direct
- SrRietveld
  - Batch processing of reduced data
    - Already possible in Fullprof directly
  - More interesting:
    - Extract out data from the refinement of multiple datasets
    - Plotting using run meta data
      - » Trend plotting and fitting
      - » Display of 2D and 3D engineering stress maps