MANTID

The Mantid Project

The challenges of delivering flexible HPC for novice end users

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SOS18

ISIS

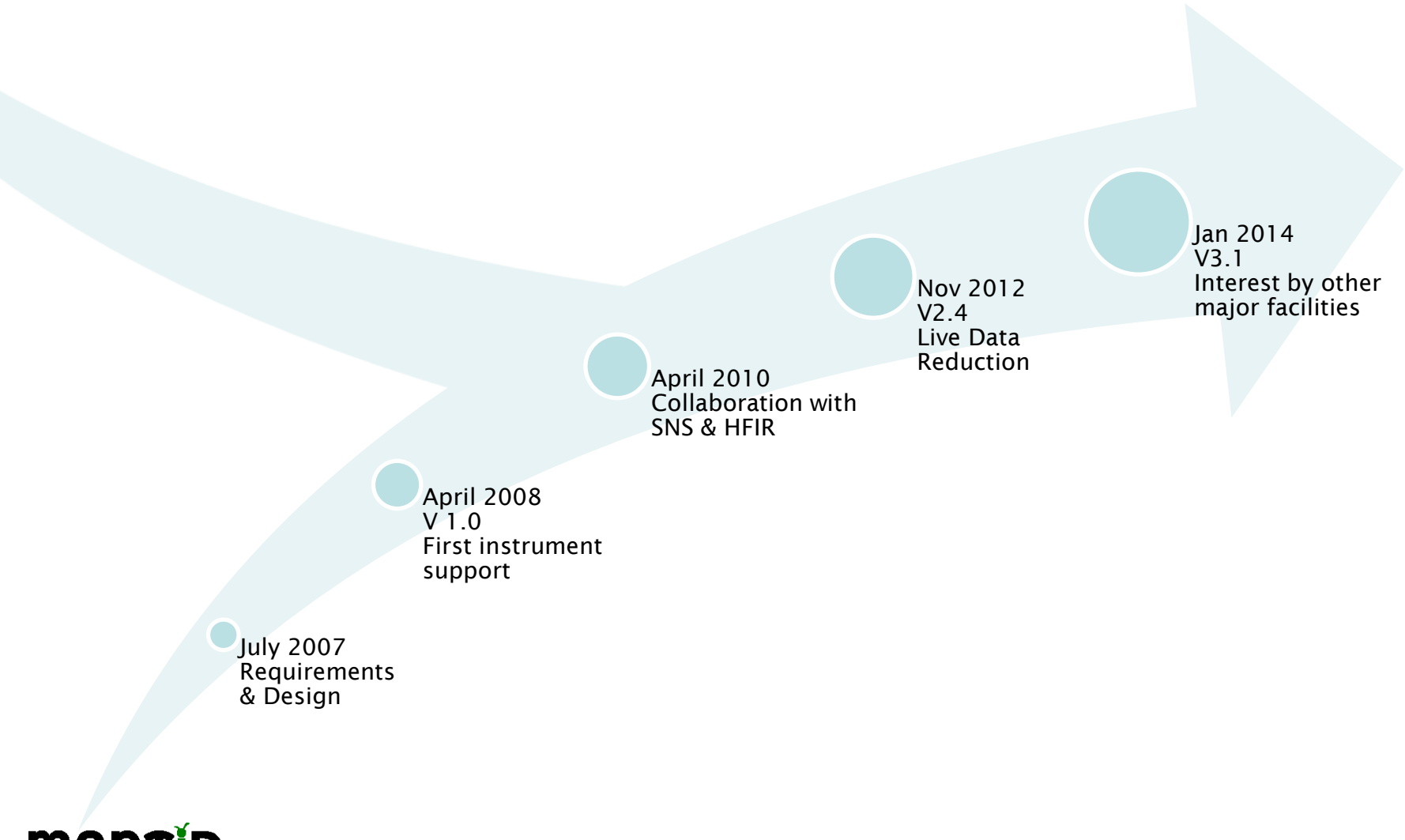
Tessella
Technology & Consulting

SNS
SPALLATION NEUTRON SOURCE

What Is Mantid

- A framework that supports high-performance computing and visualisation of scientific data.
- Manipulate and analyse Neutron and Muon data.
  - Neutron Scattering
    - Diffraction, spectroscopy, small angle, reflectometry
  - Muon Spectroscopy
  - Could be applied to other techniques
- Open Source
- Multiple Platforms
  - Windows, Linux, Mac

Project History



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Members

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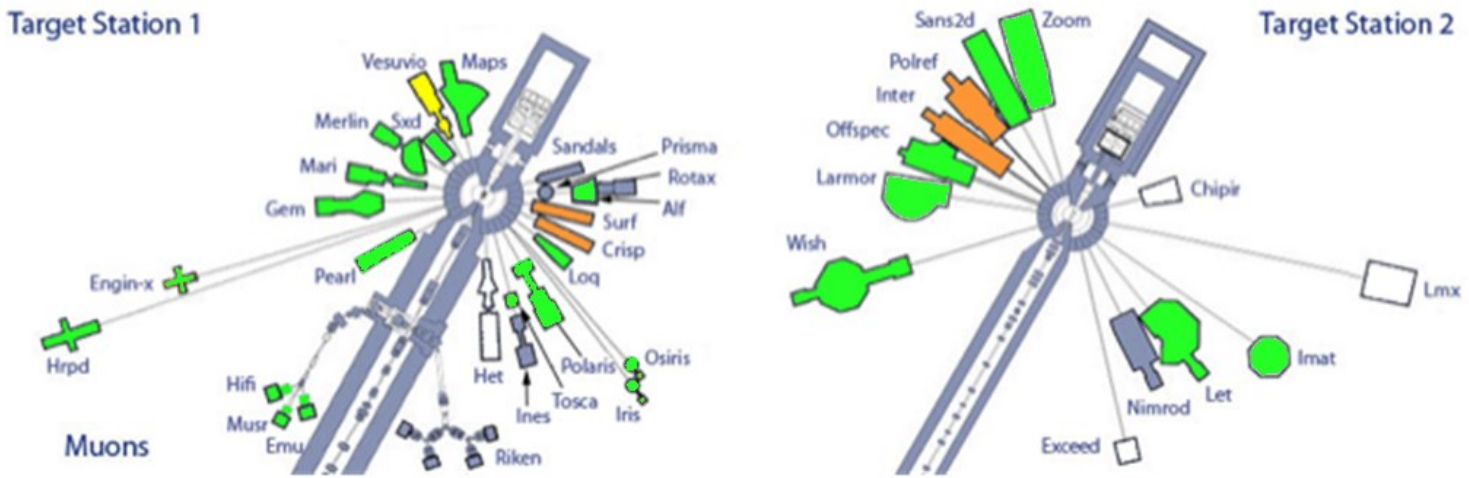

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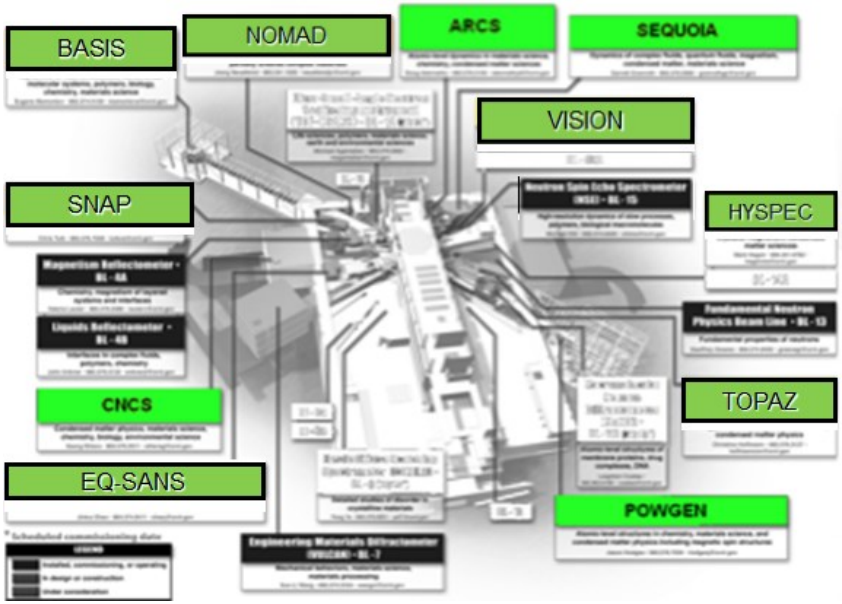
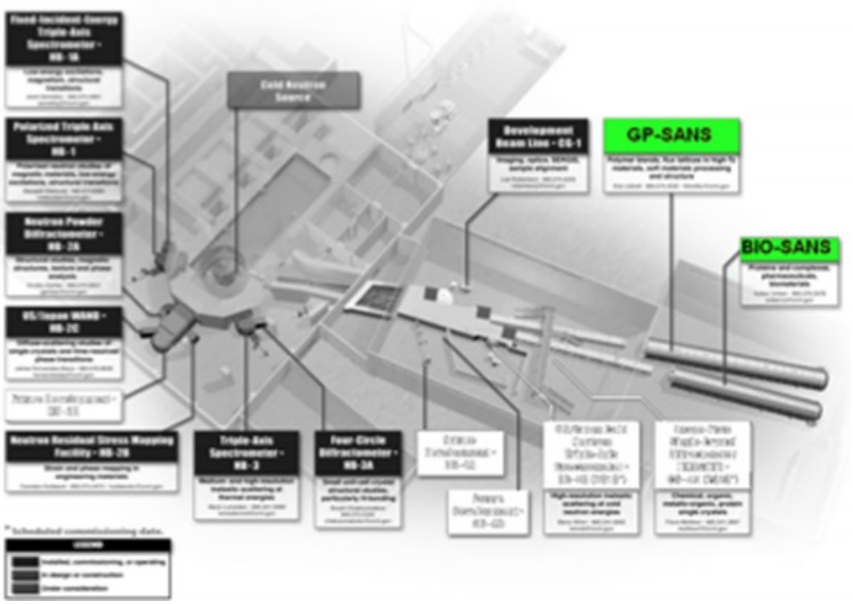


HFIR



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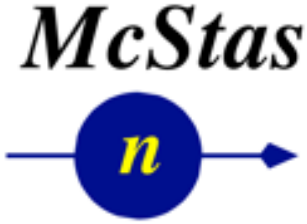
Contributors



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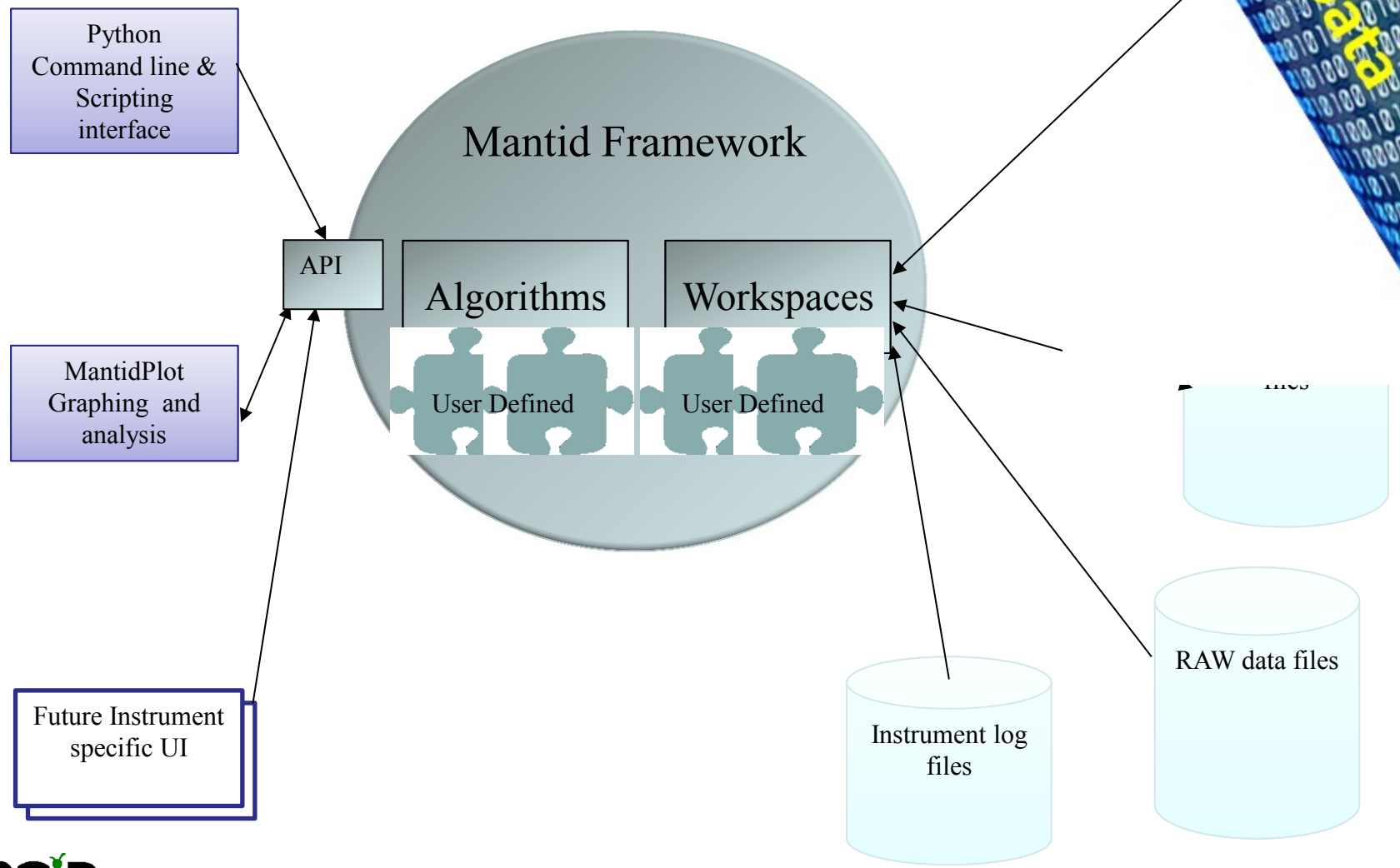
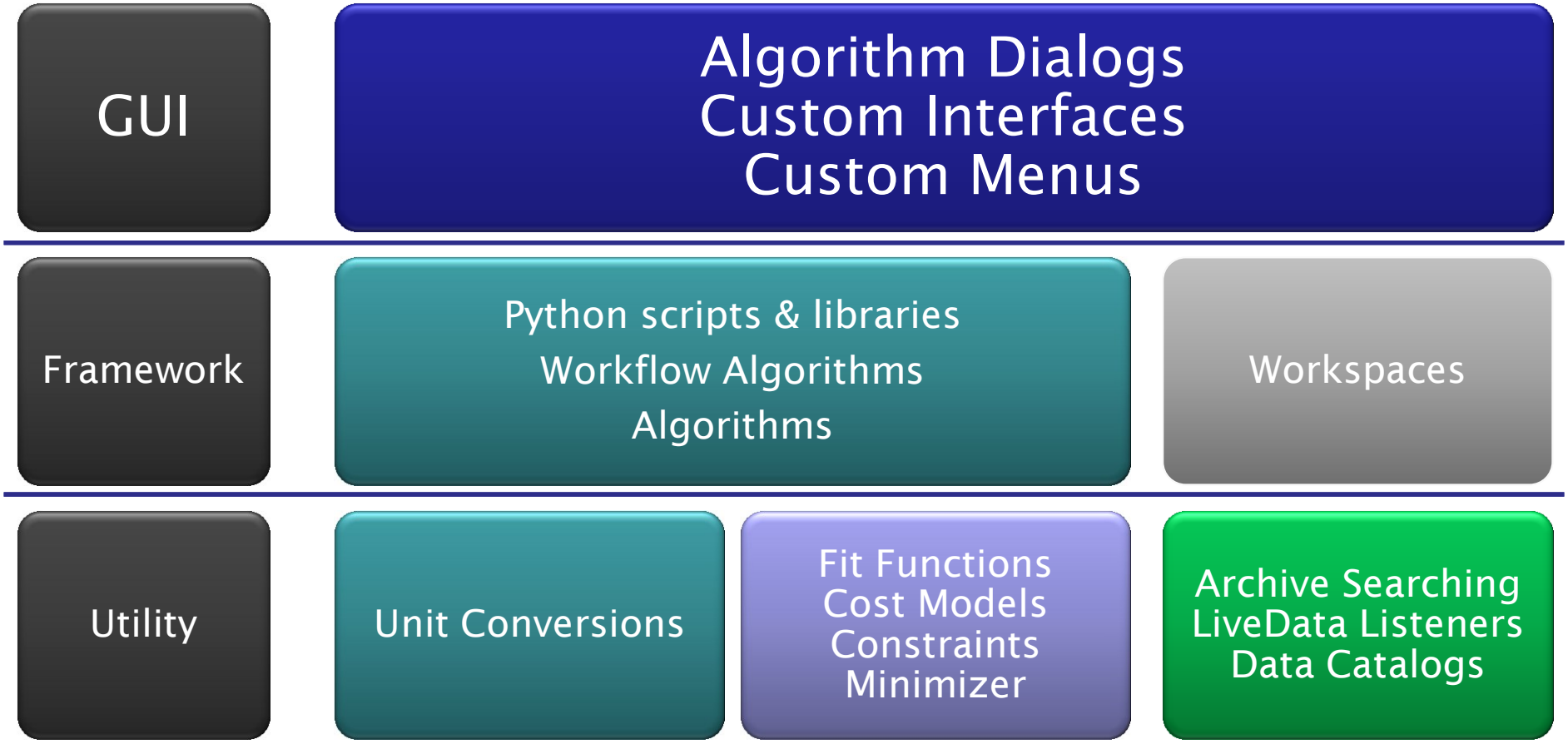
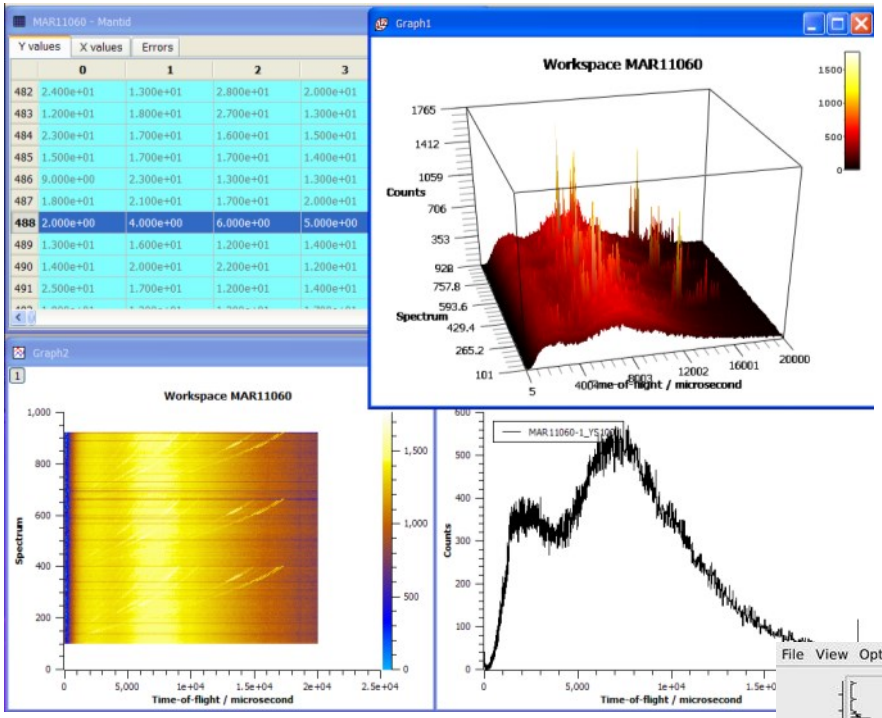
Architectural Design Overview

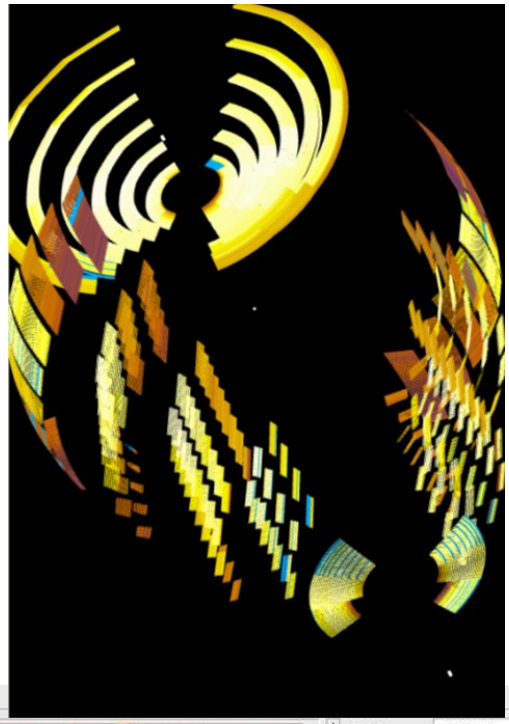


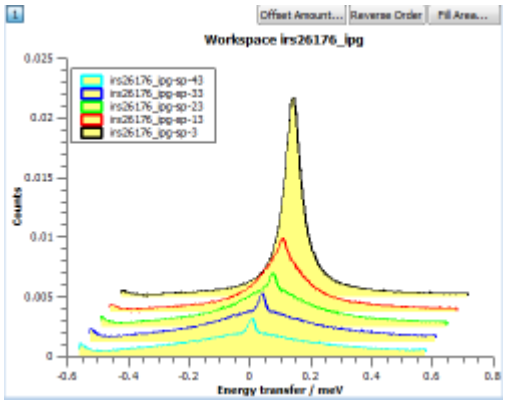
Plug in extensions

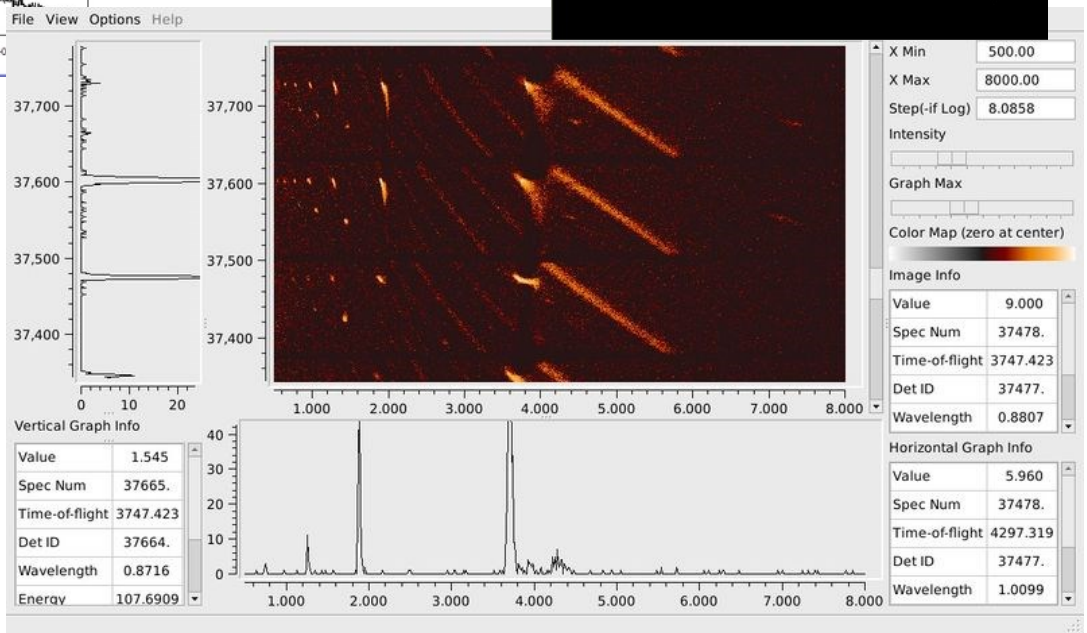


What can we do - Visualization









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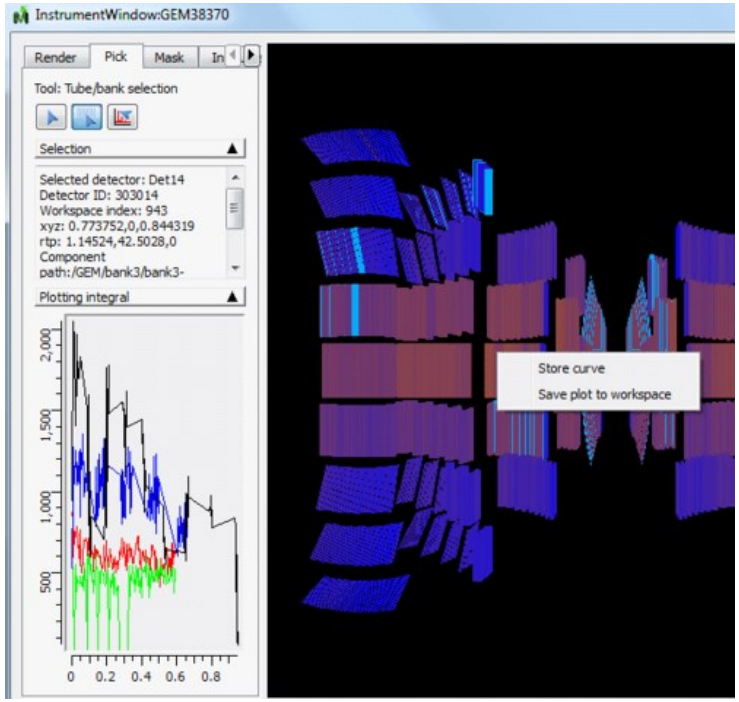
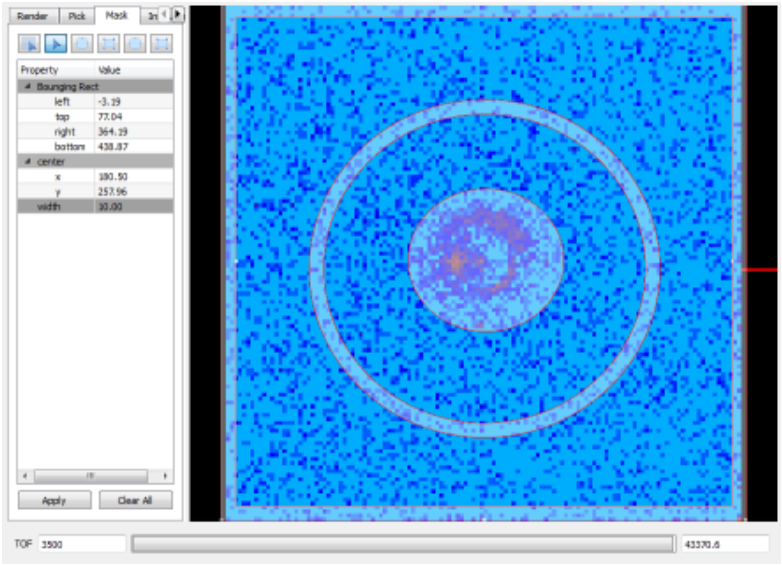
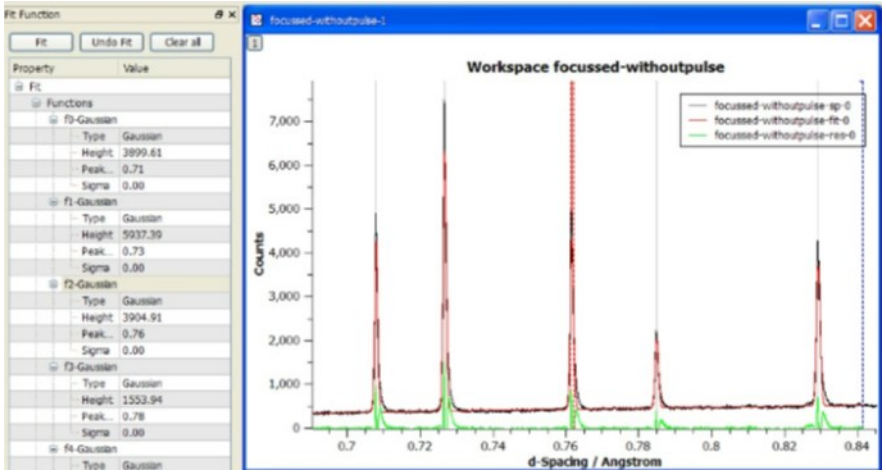
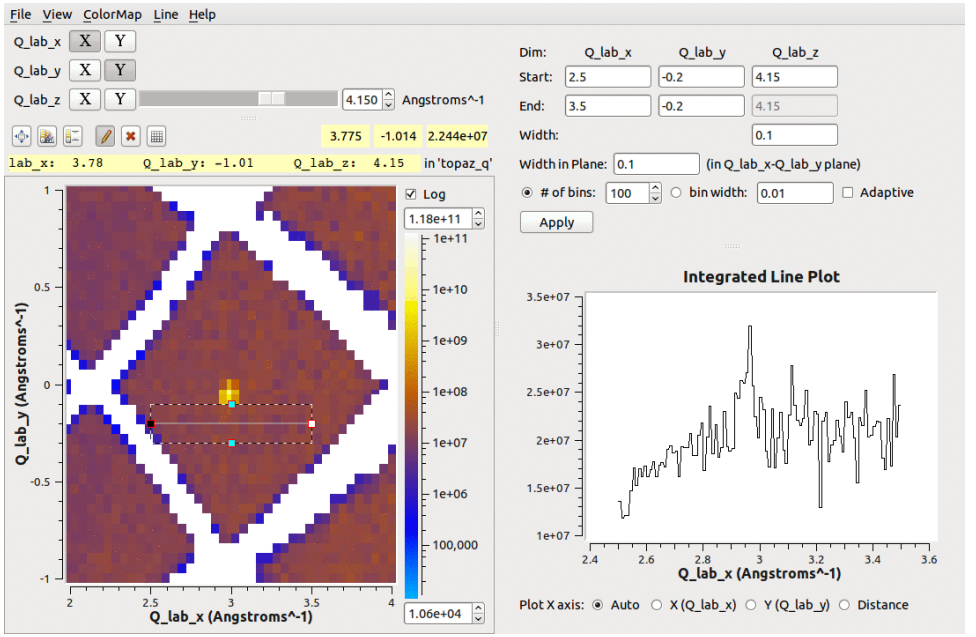
What we can do - Tools









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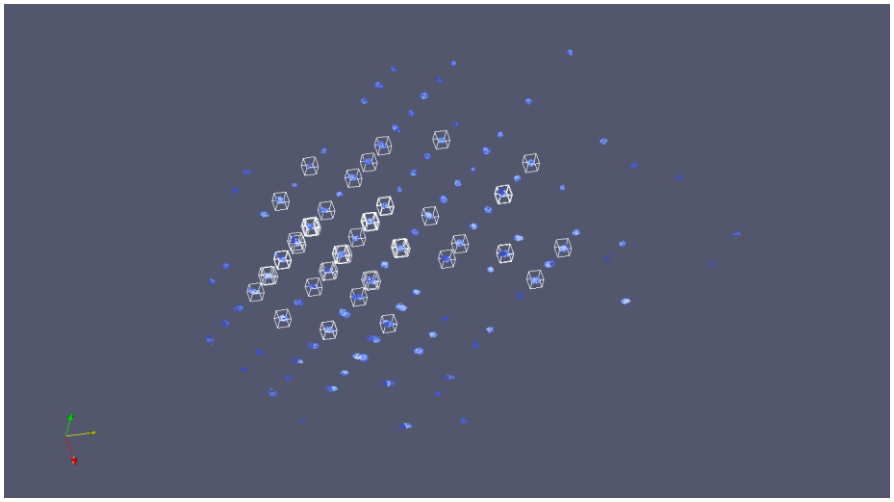
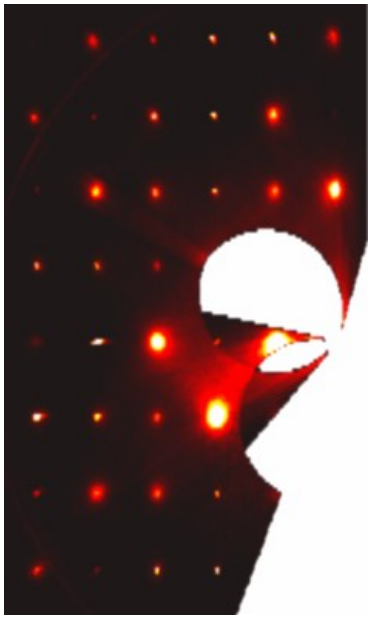
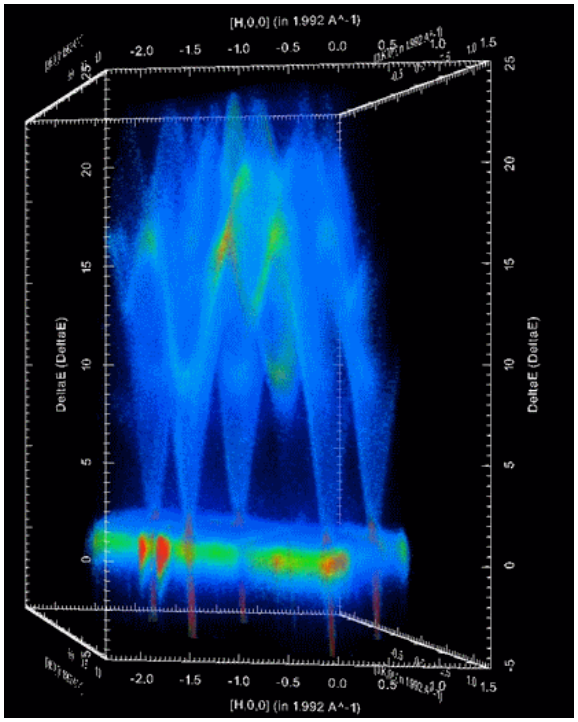
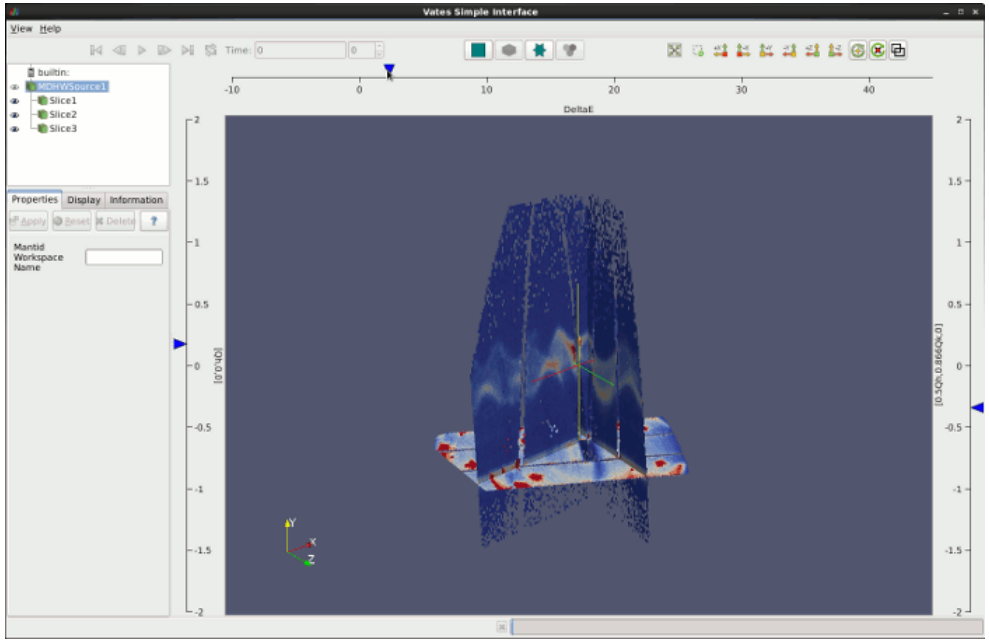
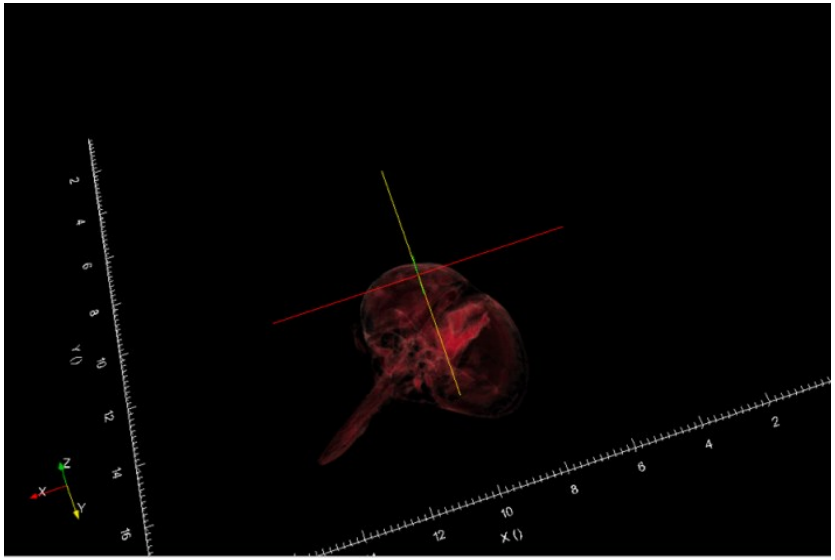
What can we do - Visualization





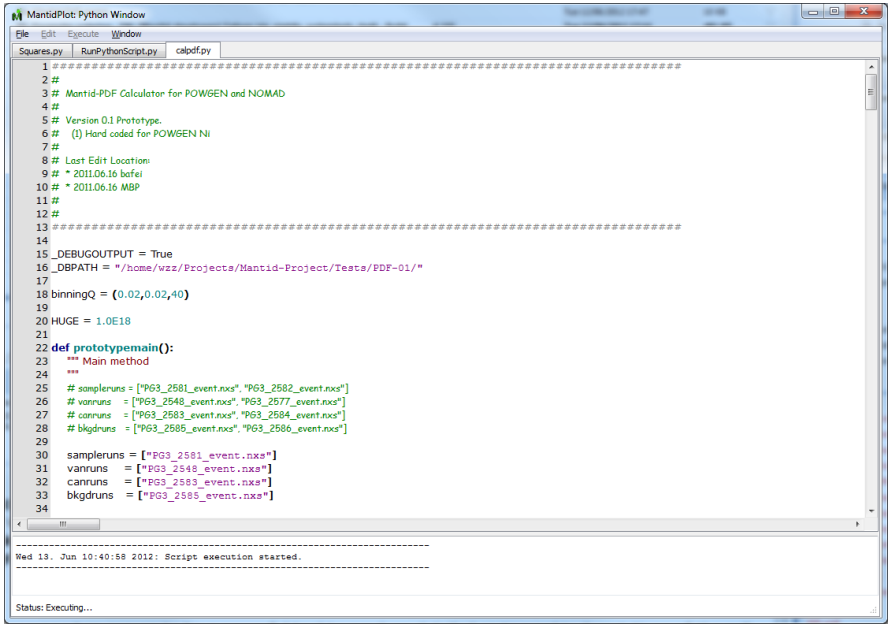


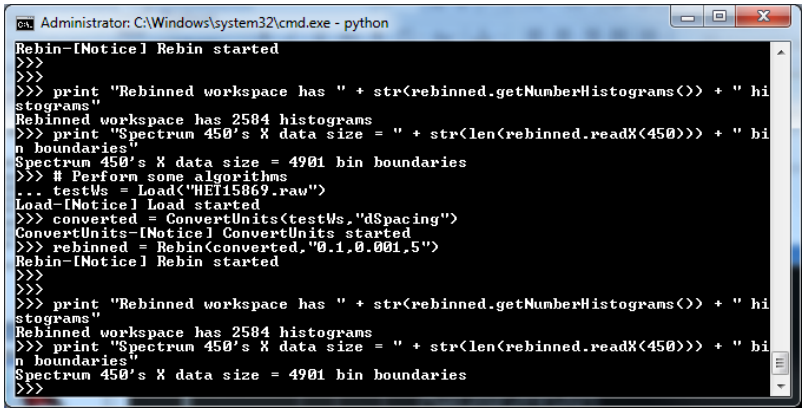


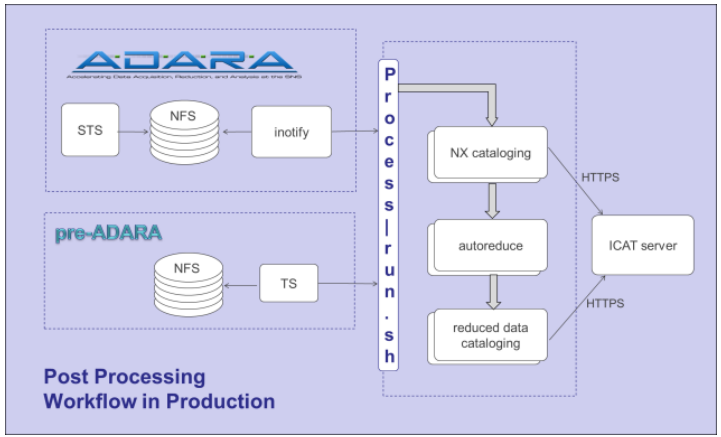


What we can do - Scripting

- Python Control
  - Within MantidPlot or command line
  - iPython Shell
  - Integrated numPy
  - Python Plugins
    - Algorithms
    - Fitting functions
    - User interfaces
  - Automated reduction







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What we can do - Algorithms

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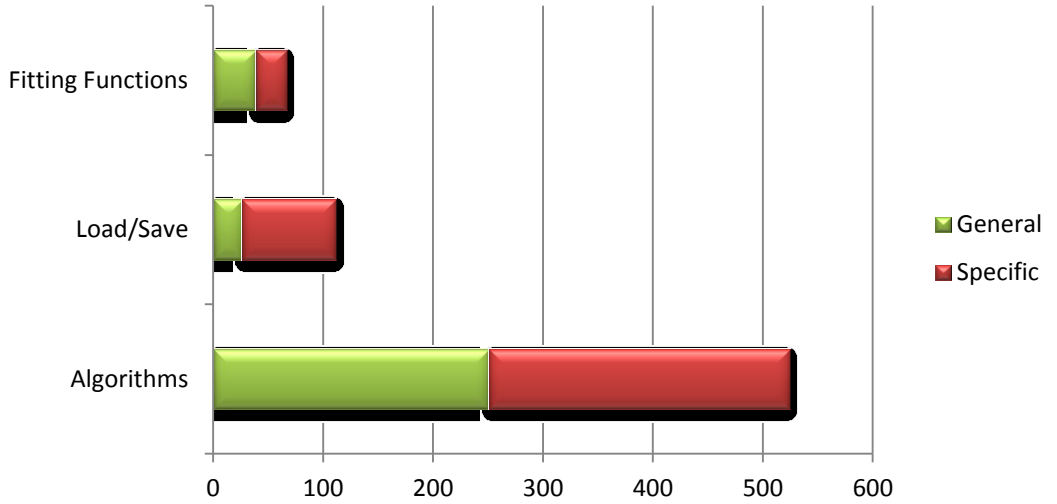
- Arithmetic
- Correction Functions
  - Absorption
  - Background
  - Efficiency
- Technique
  - Single Crystal
  - Inelastic
  - SANS
  - Powder diffraction
- Data handling



- Diagnostics
- Event Filtering
- Optimization
- Transforms
  - Masking
  - Grouping
  - Smoothing
  - Unit conversions

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The Mantid Environment

- Users
  - From scientific experts, who will understand HPC to some extent, but have limited time.
  - To visiting scientists, who just want results, and have little time to understand systems or learn new processes.

- Compute environments
  - Local computer only
  - Powerful workstations
  - Facility HPC facilities
  - University facilities
  - Commercial Cloud resources
  - National HPC facility

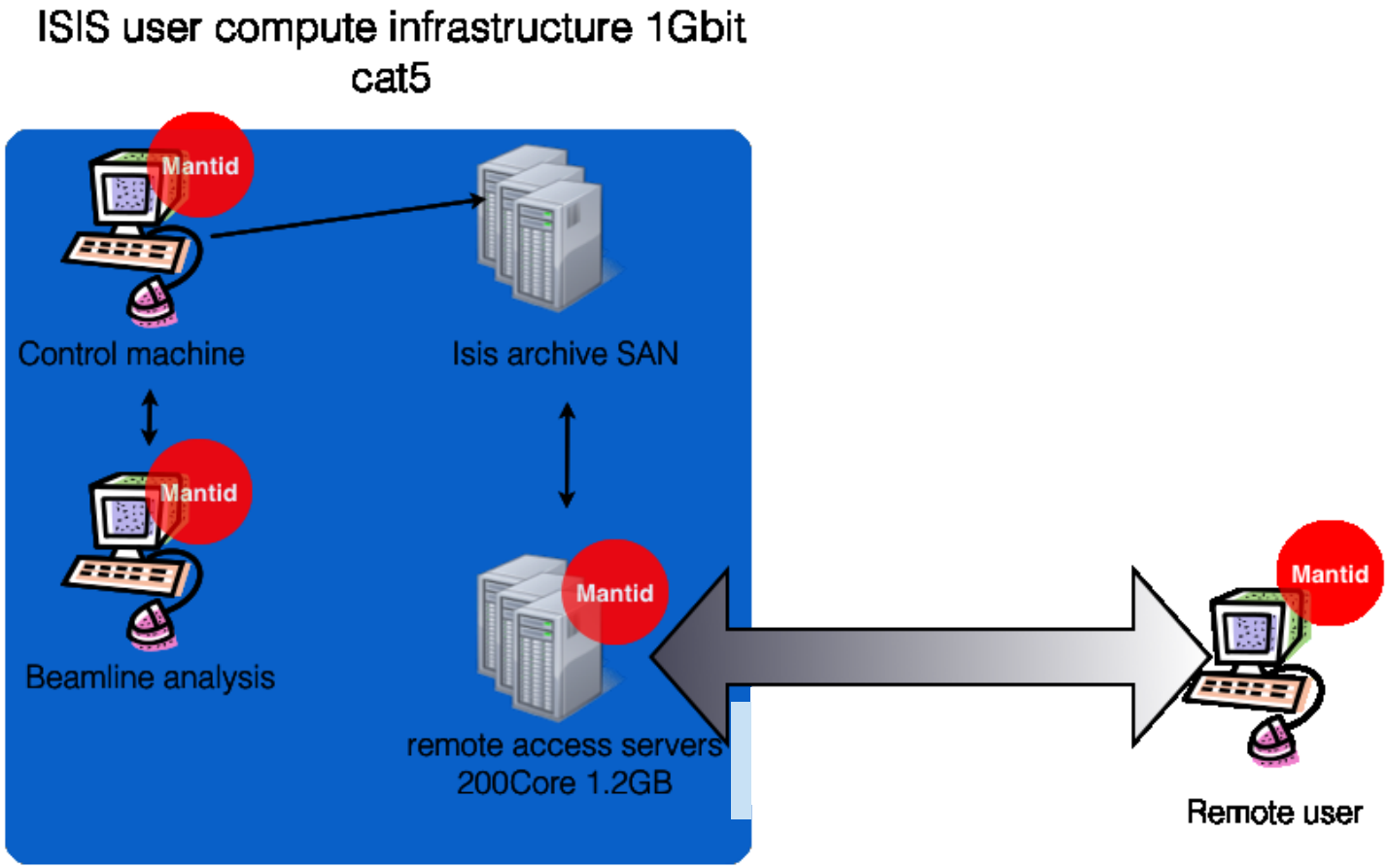
Mantid and Distributed Computing

- Not all operations in Mantid would benefit from distributed or HPC computing
  - Small data volume
  - Large data volume, local to client, simple operations
- For some operations the need is clear
  - Large Data Volume, fast access by cluster
  - Complex scalable operations
    - Monte Carlo instrument simulations
    - Absorption corrections
  - Use of third party codes
    - Molecular dynamics simulations
  - Computationally expensive optimisations of models to experimental data

What is a Mantid job?

- Input data
  - Shared File Location
  - Uploaded File
- Python Script
- Output data
  - Shared File Location
  - Downloaded File

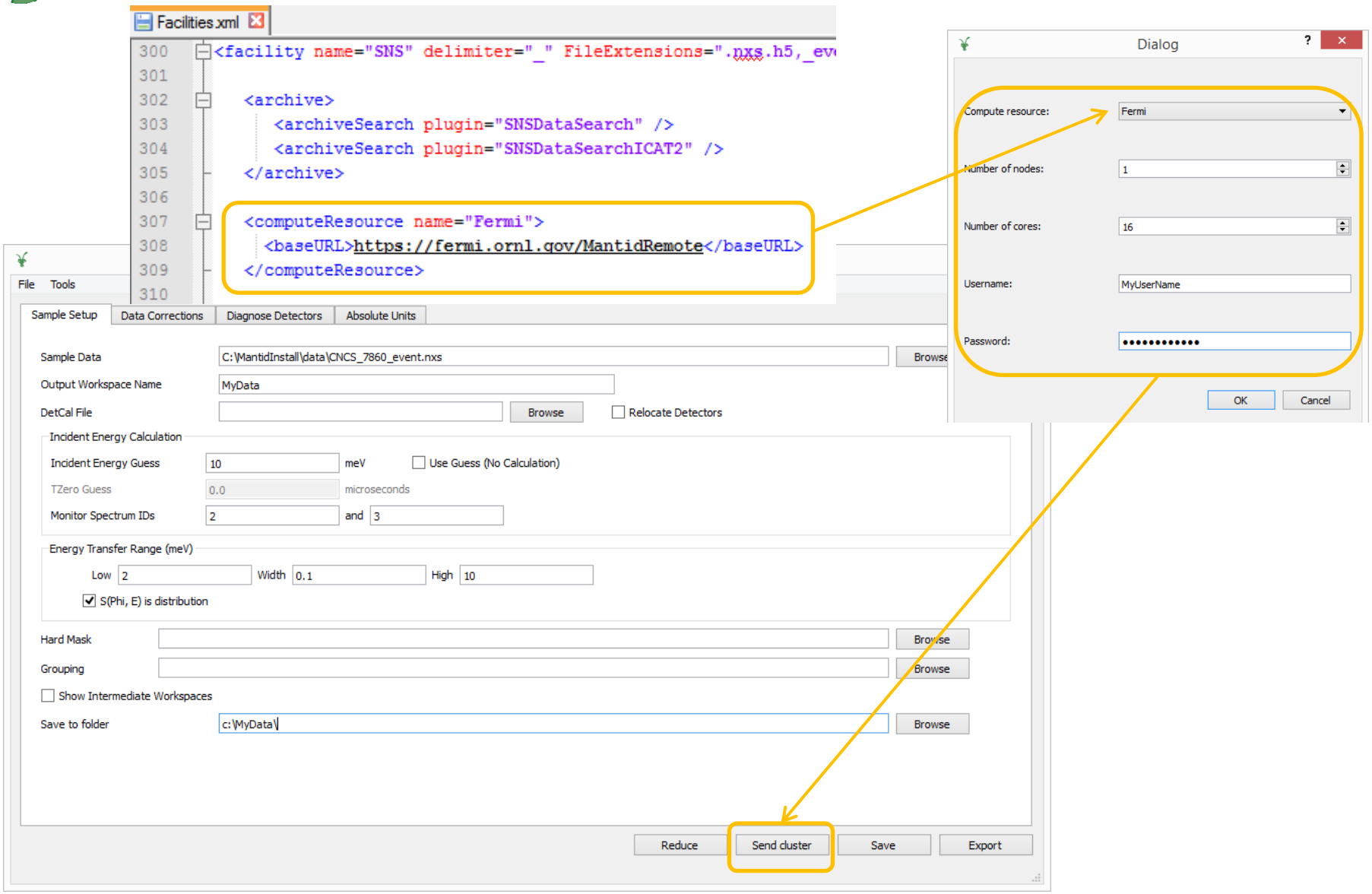
One possible Infrastructure



Challenges

- Different facility infrastructures
  - Authentication
    - Username/password, certificates, need to physically turn up with ID.
  - Job Schedulers
    - Few accessible via web services
    - Of those that do not few work well with C++ cross platform
  - Locating resources

Interfaces - Keep it simple



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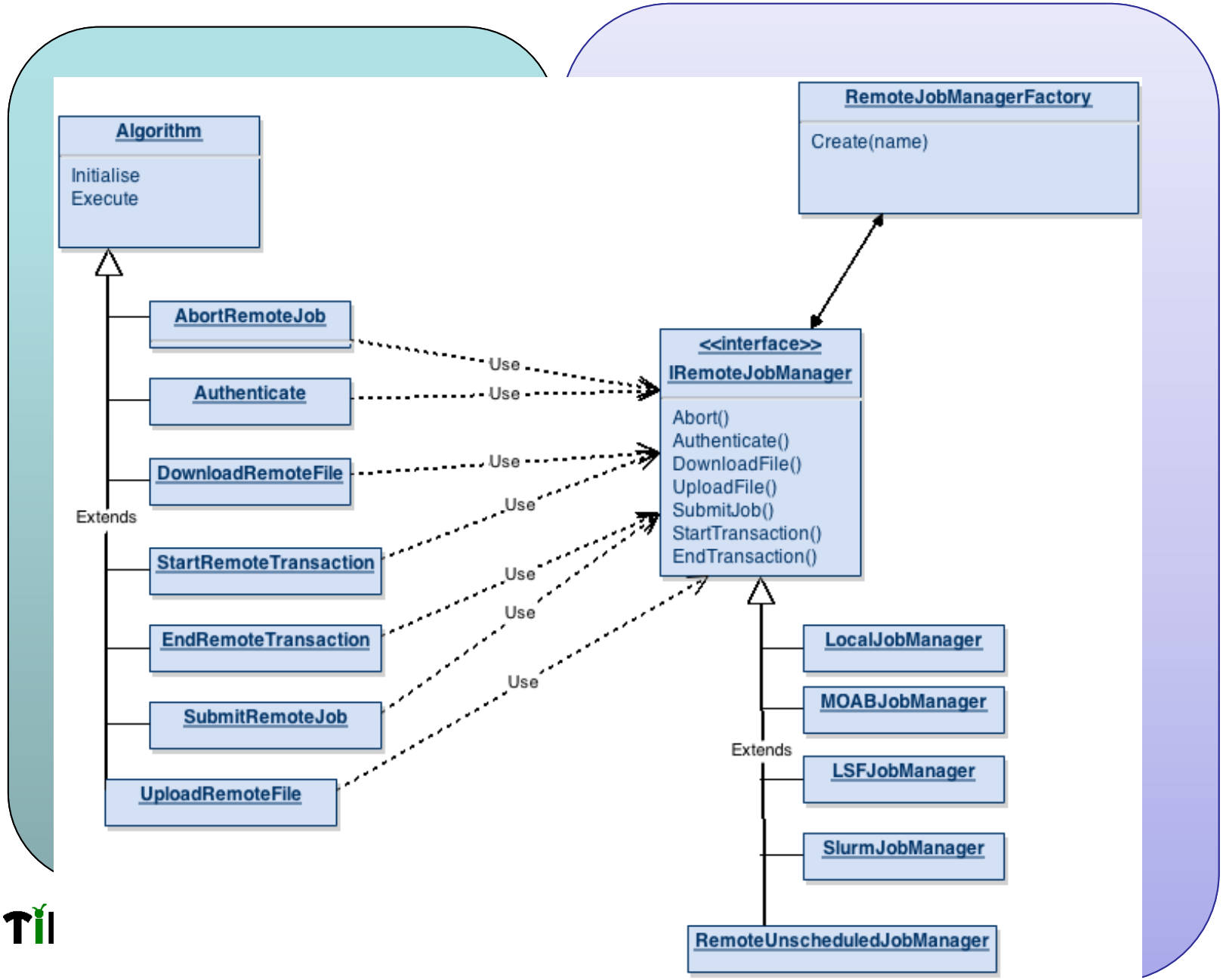
Under the bonnet

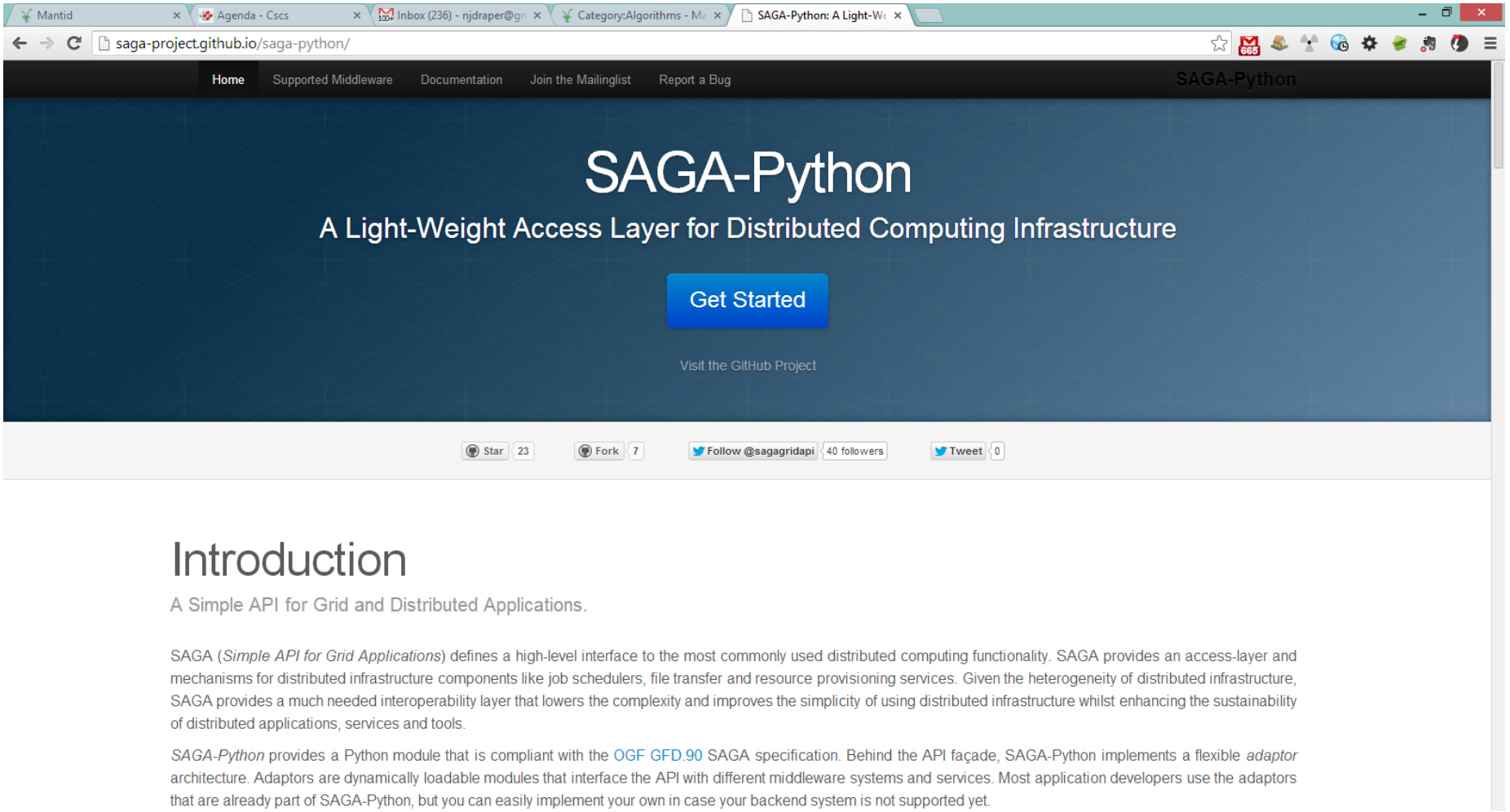


The Ideal Middleware

- Removes the need to care what job scheduler is in use.
- Compiles easily on Windows, Mac, Linux
- Packages easily for deployment
- APIs
  - C++, Python
  - others
- Needs to handle network proxies, firewalls etc
- Does not need Admin or special permissions
- Easy to add additional Job Managers
- Just works …

Doesn't this sound a bit like …

SAGA



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Doesn't this sound a bit like …
SAGA

- Removes the need to care what job scheduler is in use.
- Compiles easily on Windows, Mac, Linux
- Packages easily for deployment
- APIs — Development stopped 2 yrs ago
  - C++, Python
  - others — Java
- Needs to handle network proxies, firewalls etc — SSH only
- Does not need Admin or special permissions
- Easy to add additional Job Managers
- Just works ..

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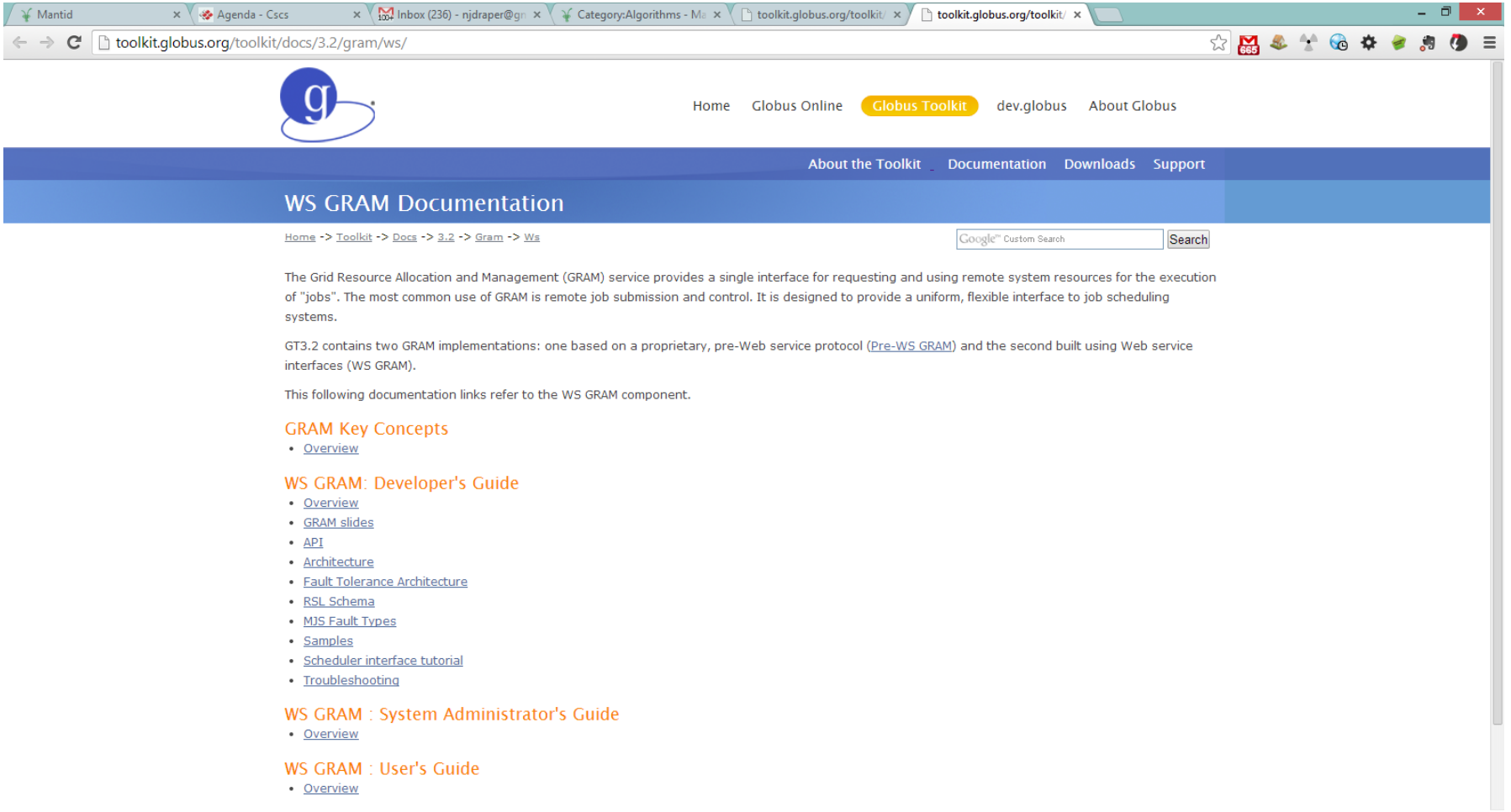
Doesn't this sound a bit like …

WS_GRAM



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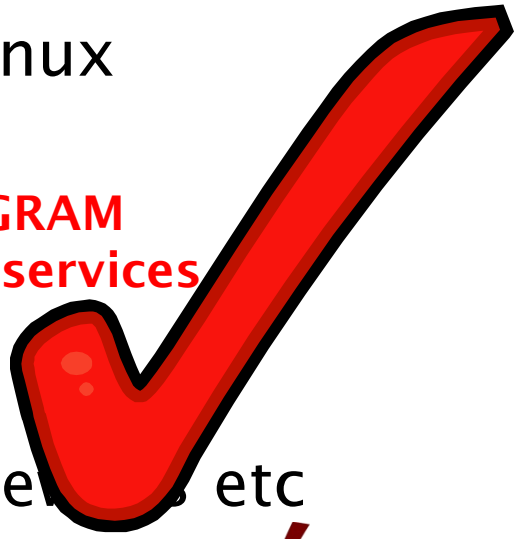
Doesn't this sound a bit like …
WS_GRAM

- Removes the need to care what job scheduler is in use. ? Not local or remote workstation
- Compiles easily on Windows, Mac, Linux
- Packages easily for deployment
- APIs
  - C++, Python
  - others
- Needs to handle network proxies, fire[illegible] etc
- Does not need Admin or special permissions
- Easy to add additional Job Managers ?
- Just works .. ?



WS_GRAM
Web services

File Transfer
needs GridFTP

Further information

- Project web page - www.mantidproject.org

- Many Thanks to the Project Sponsors
- And the development team

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