

The Mantid Project

The challenges of delivering
flexible HPC for novice end users

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SOS18



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

July 2007
Requirements
& Design

April 2008
V 1.0
First instrument
support

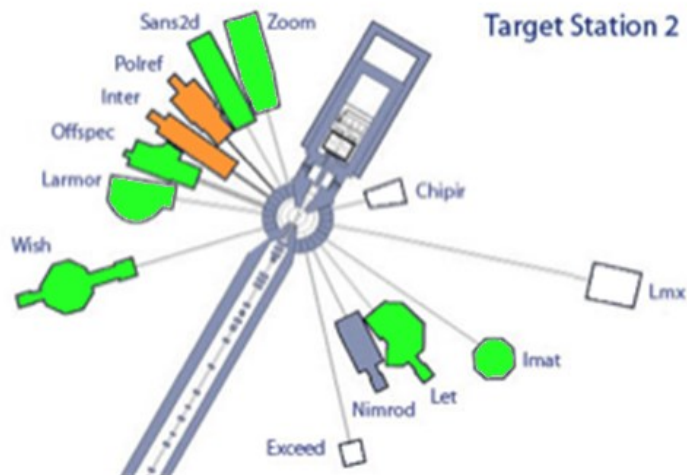
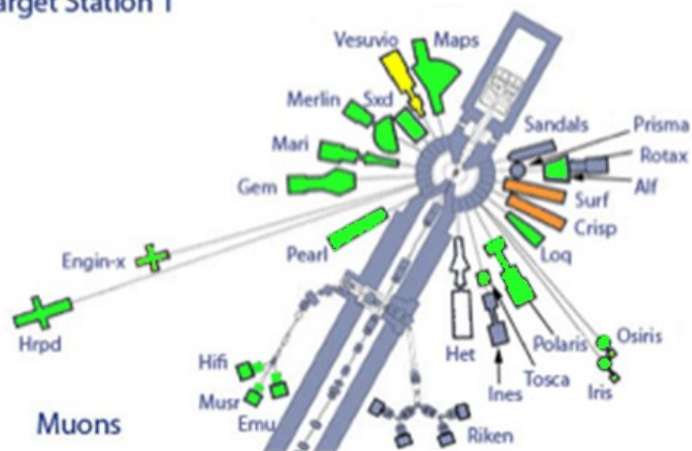
April 2010
Collaboration with
SNS & HFIR

Nov 2012
V2.4
Live Data
Reduction

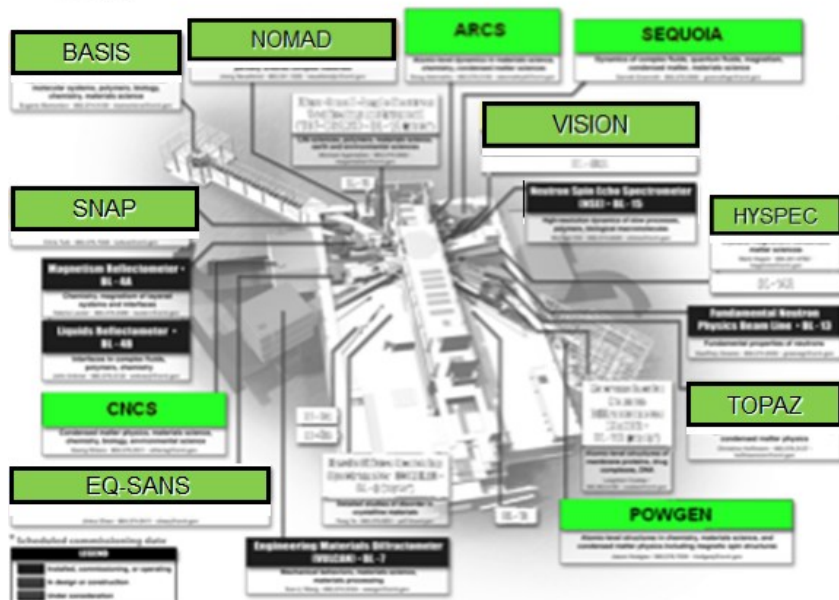
Jan 2014
V3.1
Interest by other
major facilities



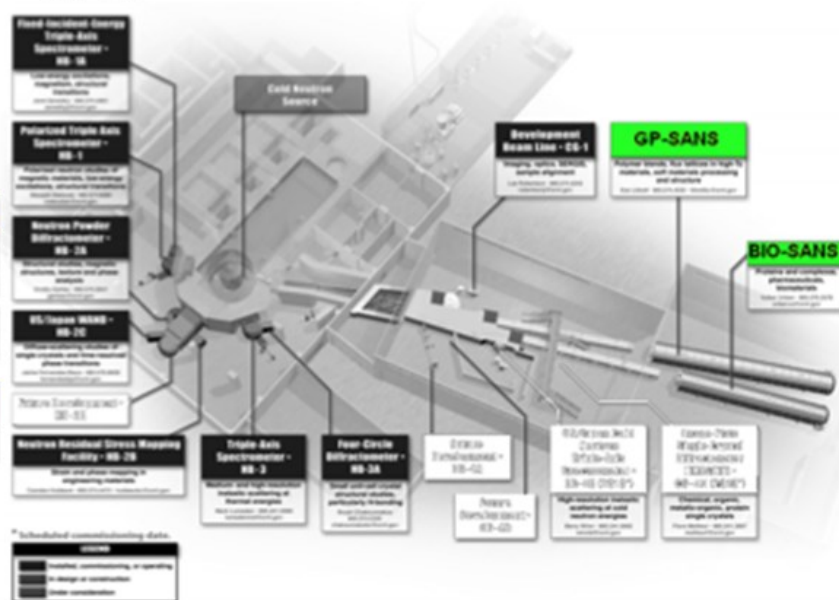
Target Station 1



SNS



HFIR



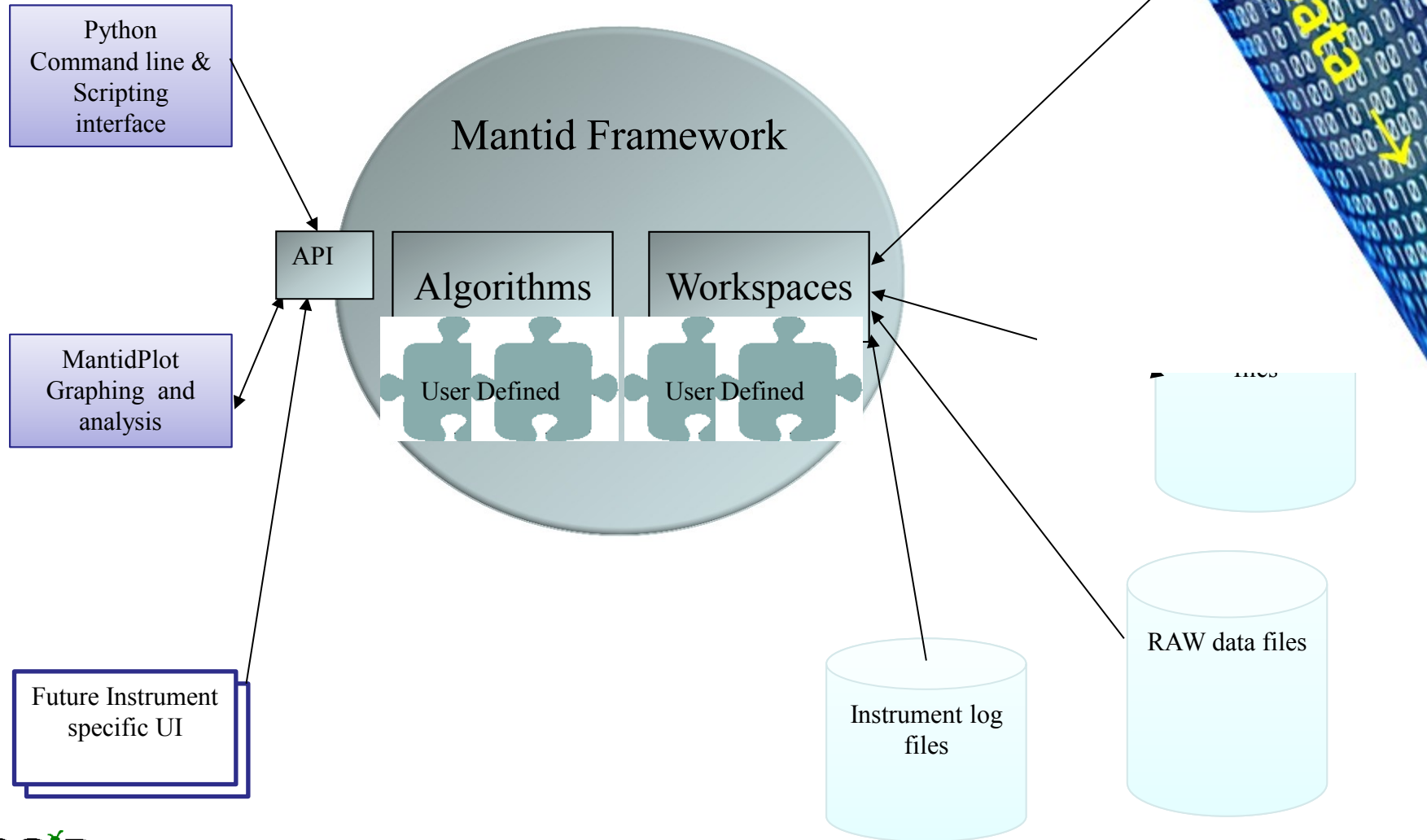


Contributors





Architectural Design Overview





Plug in extensions

GUI

Algorithm Dialogs
Custom Interfaces
Custom Menus

Framework

Python scripts & libraries
Workflow Algorithms
Algorithms

Workspaces

Utility

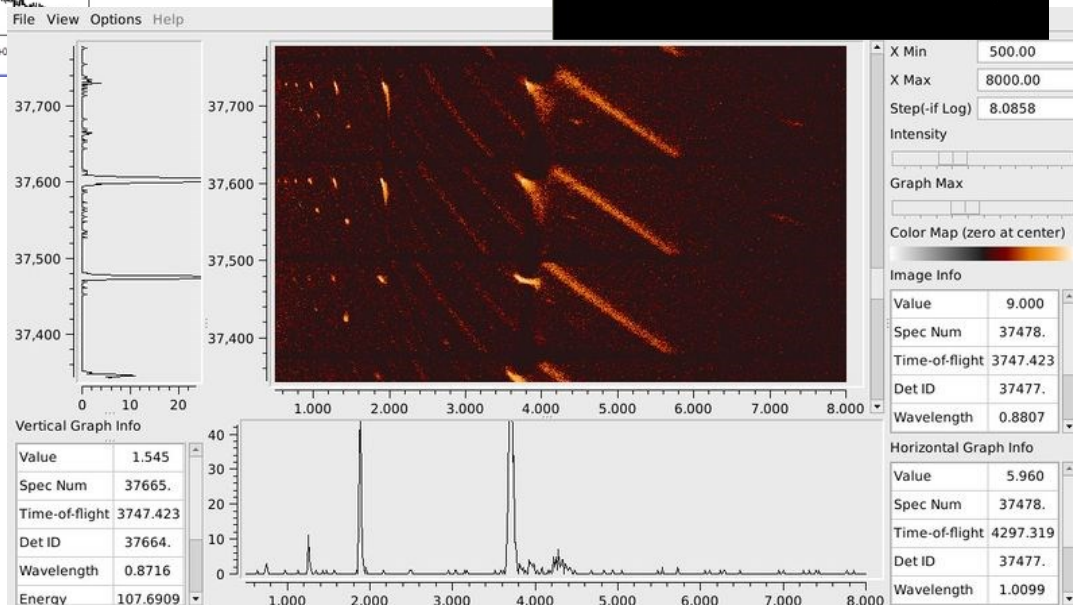
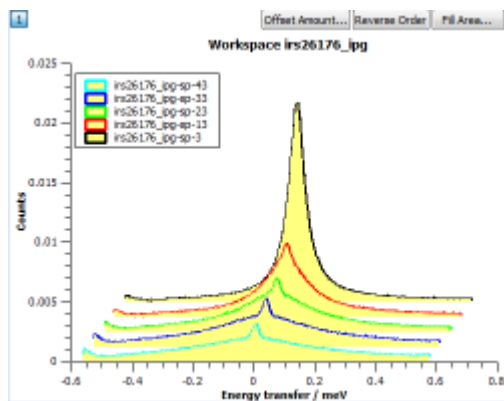
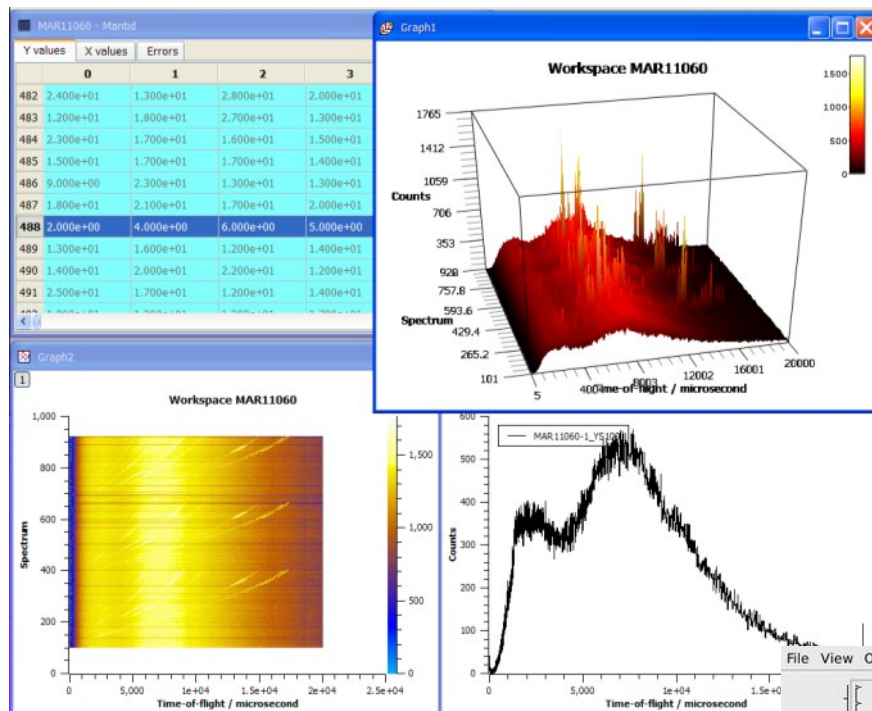
Unit Conversions

Fit Functions
Cost Models
Constraints
Minimizer

Archive Searching
LiveData Listeners
Data Catalogs

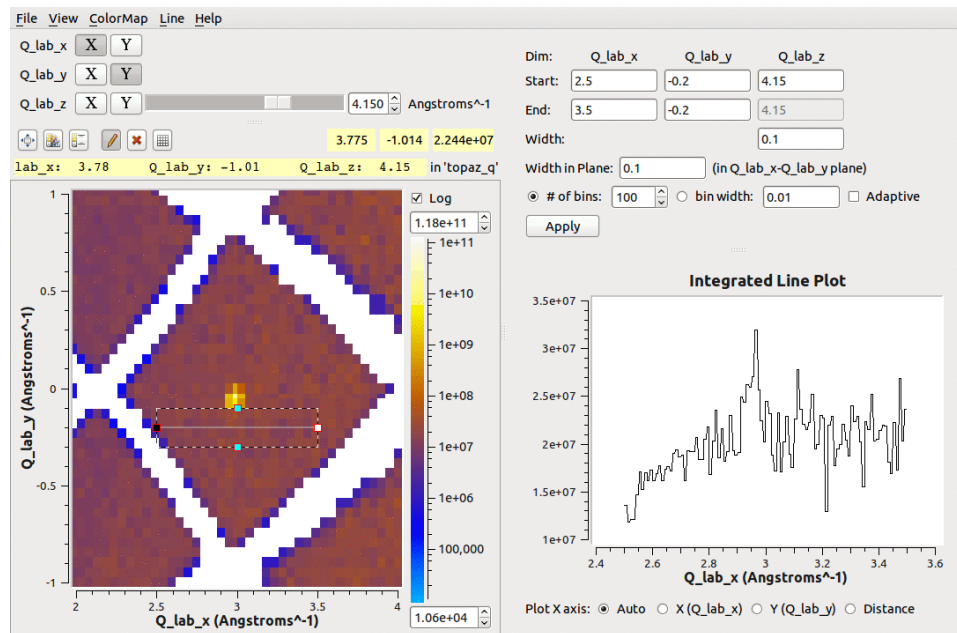
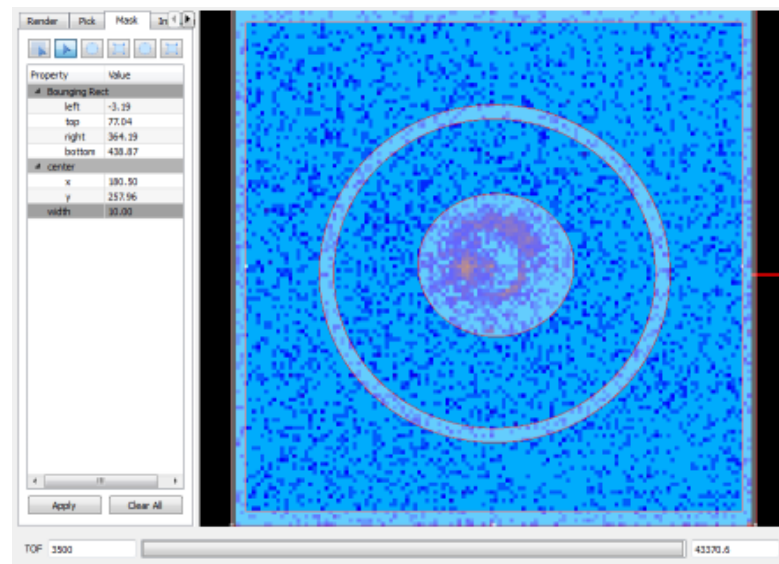
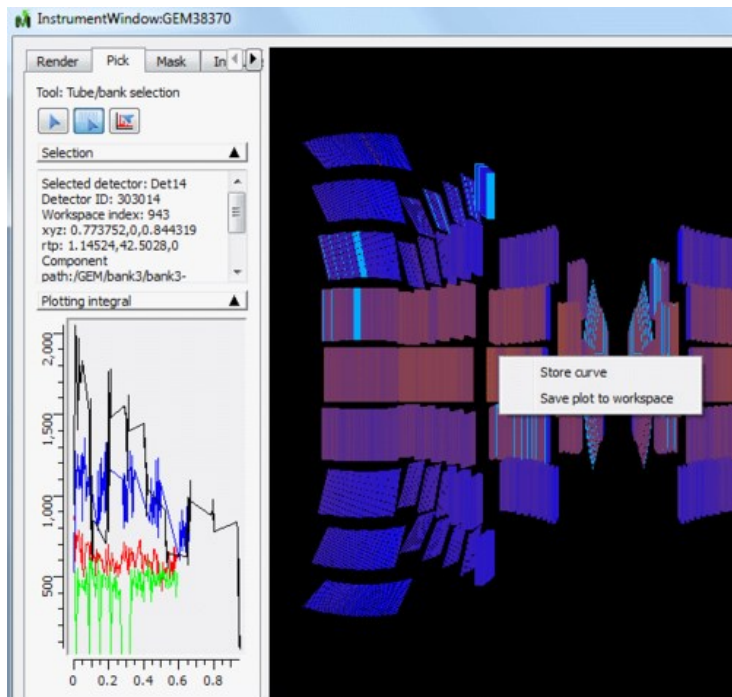


What can we do - Visualization



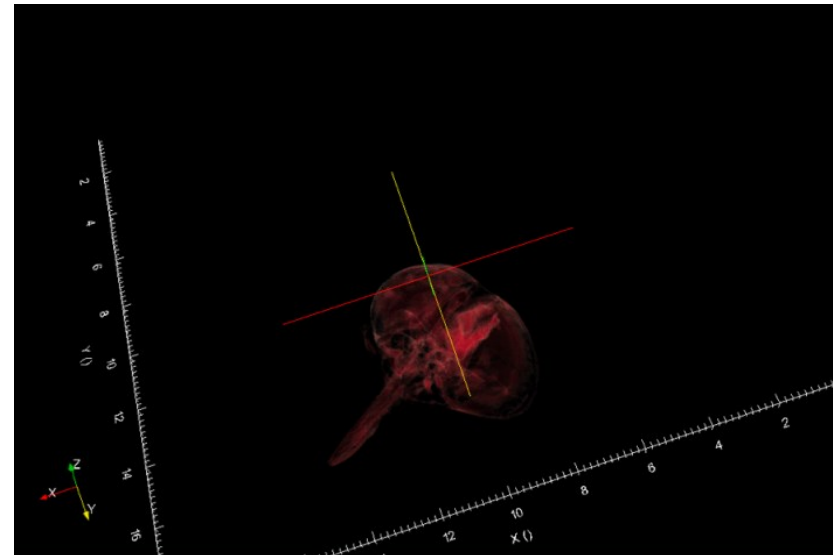
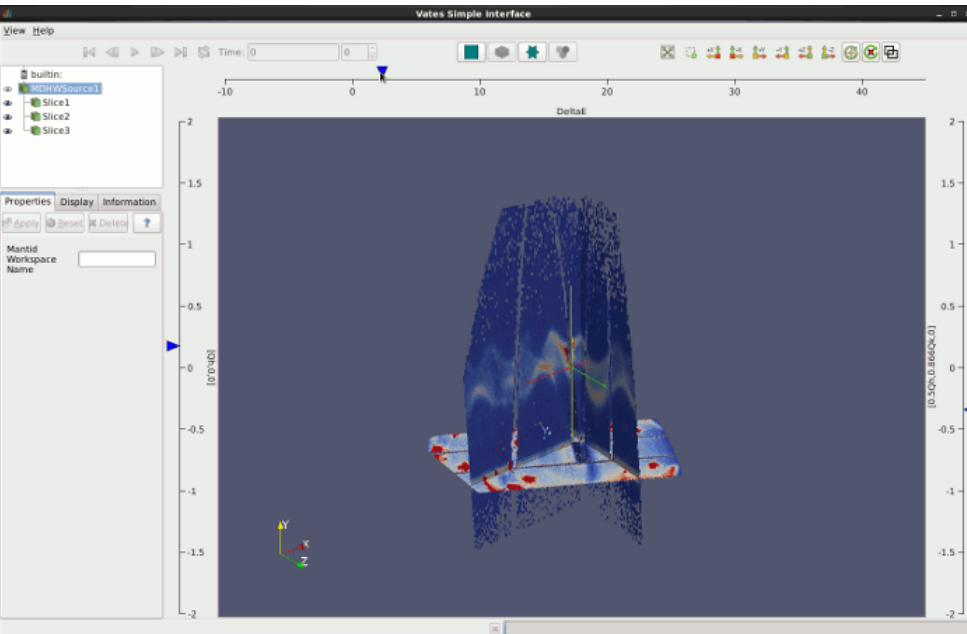
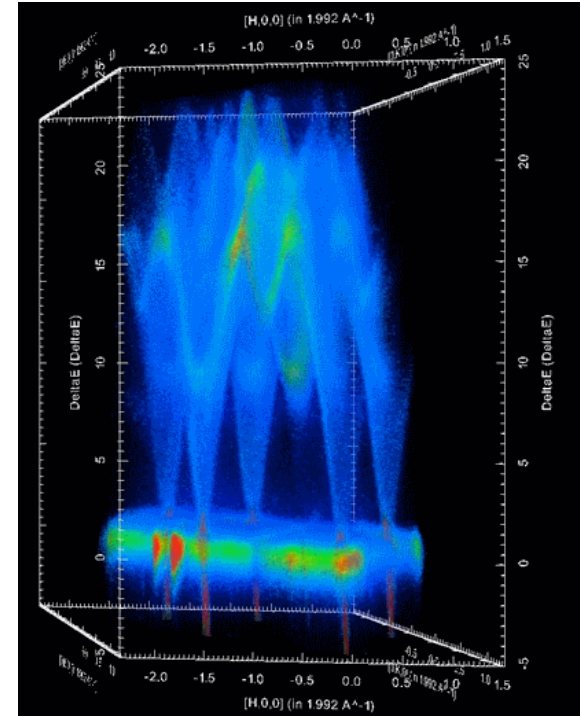
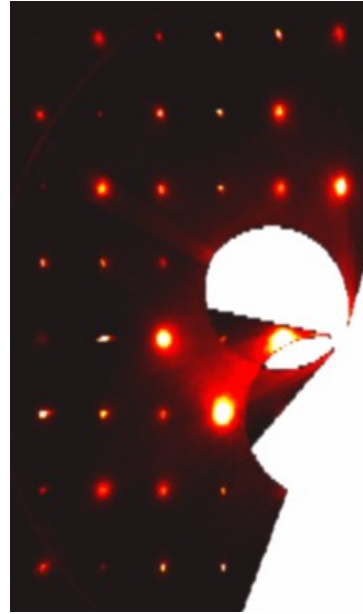
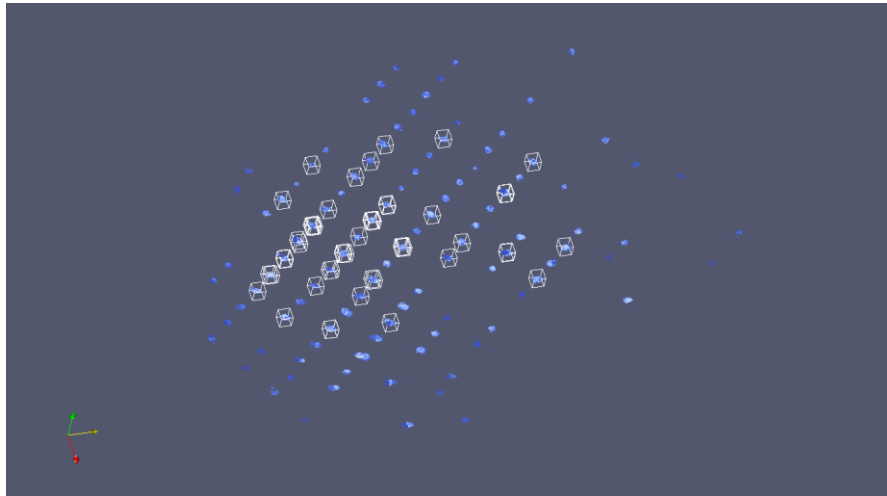


What we can do - Tools





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

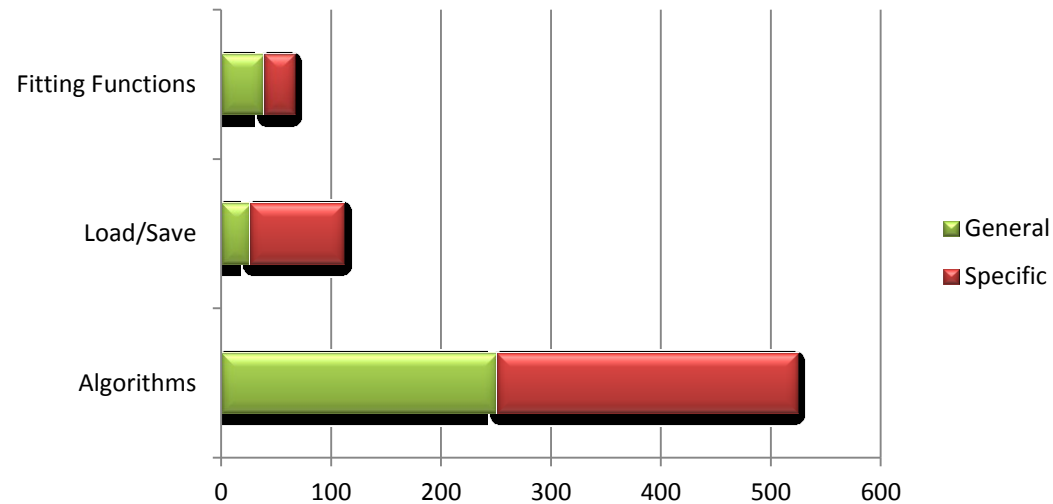
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1 #####
2 #
3 # Mantid-PDF Calculator for POWGEN and NOMAD
4 #
5 # Version 0.1 Prototype.
6 # (i) Hand coded for POWGEN Ni
7 #
8 # Last Edit Location:
9 # * 2011.06.16 bafel
10 # * 2011.06.16 MBP
11 #
12 #
13 #####
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15 _DEBUGOUTPUT = True
16 _DBPATH = "/home/vzz/Projects/Mantid-Project/Tests/PDF-01/"
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22 def prototypemain():
23     """ Main method
24     """
25     # samplers = ["PG3_2581_event.nxs", "PG3_2582_event.nxs"]
26     # vanruns = ["PG3_2548_event.nxs", "PG3_2577_event.nxs"]
27     # canruns = ["PG3_2583_event.nxs", "PG3_2584_event.nxs"]
28     # bkgdruns = ["PG3_2585_event.nxs", "PG3_2586_event.nxs"]
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30     samplers = ["PG3_2581_event.nxs"]
31     vanruns = ["PG3_2548_event.nxs"]
32     canruns = ["PG3_2583_event.nxs"]
33     bkgdruns = ["PG3_2585_event.nxs"]
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What we can do - Algorithms

703

- 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



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



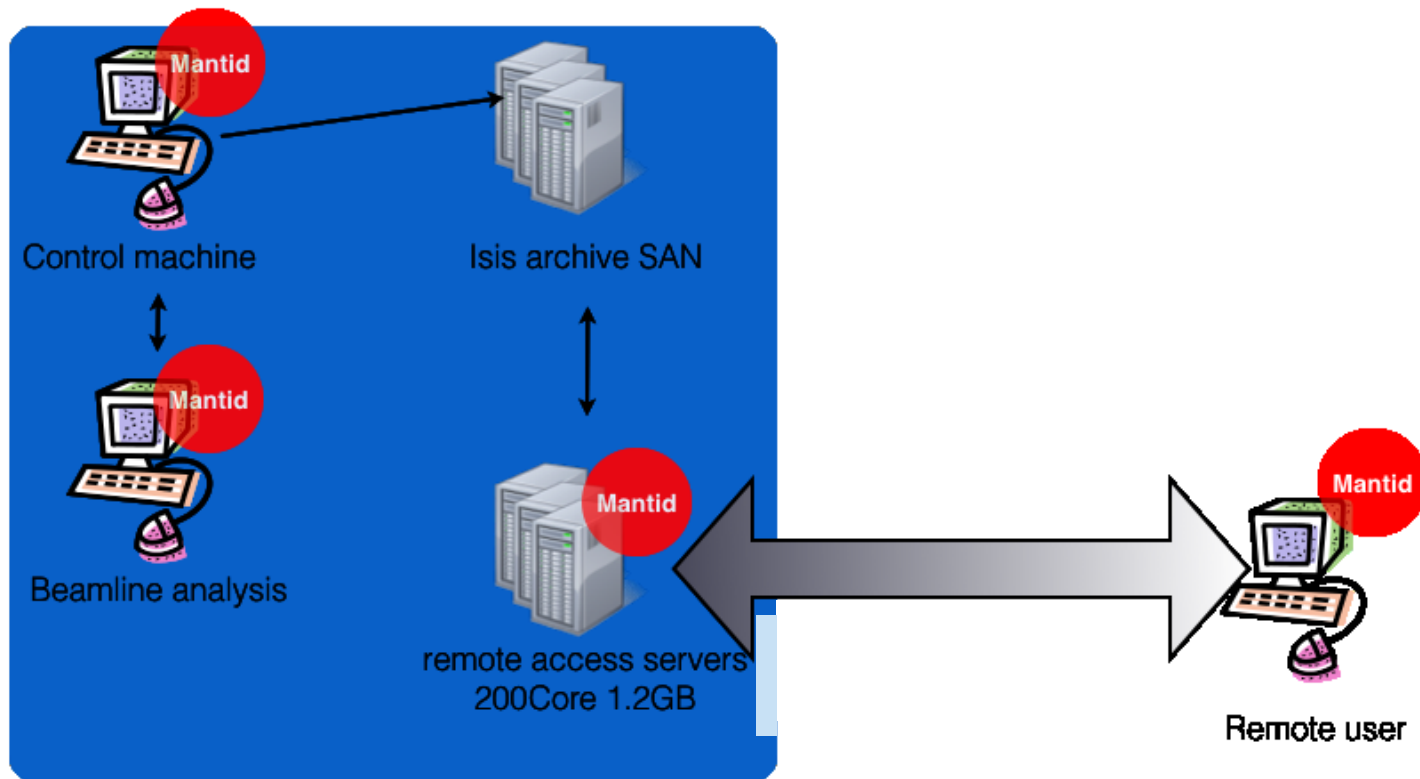
What is a Mantid job?

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



One possible Infrastructure

ISIS user compute infrastructure 1Gbit
cat5





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

The image illustrates the process of configuring a Mantid interface for a specific compute resource, using XML and a dialog box.

XML Configuration (Facilities.xml):

```
300 <facility name="SNS" delimiter="_" FileExtensions=".nxs.h5,_ev
301
302 <archive>
303   <archiveSearch plugin="SNSDataSearch" />
304   <archiveSearch plugin="SNSDataSearchICAT2" />
305 </archive>
306
307 <computeResource name="Fermi">
308   <baseUrl>https://fermi.ornl.gov/MantidRemote</baseUrl>
309 </computeResource>
310
```

Dialog Box (Compute Resource Configuration):

The dialog box shows the configuration for the compute resource:

- Compute resource: Fermi
- Number of nodes: 1
- Number of cores: 16
- Username: MyUserName
- Password: [Redacted]

Main Interface (Sample Setup):

The main interface shows the configuration for the sample setup:

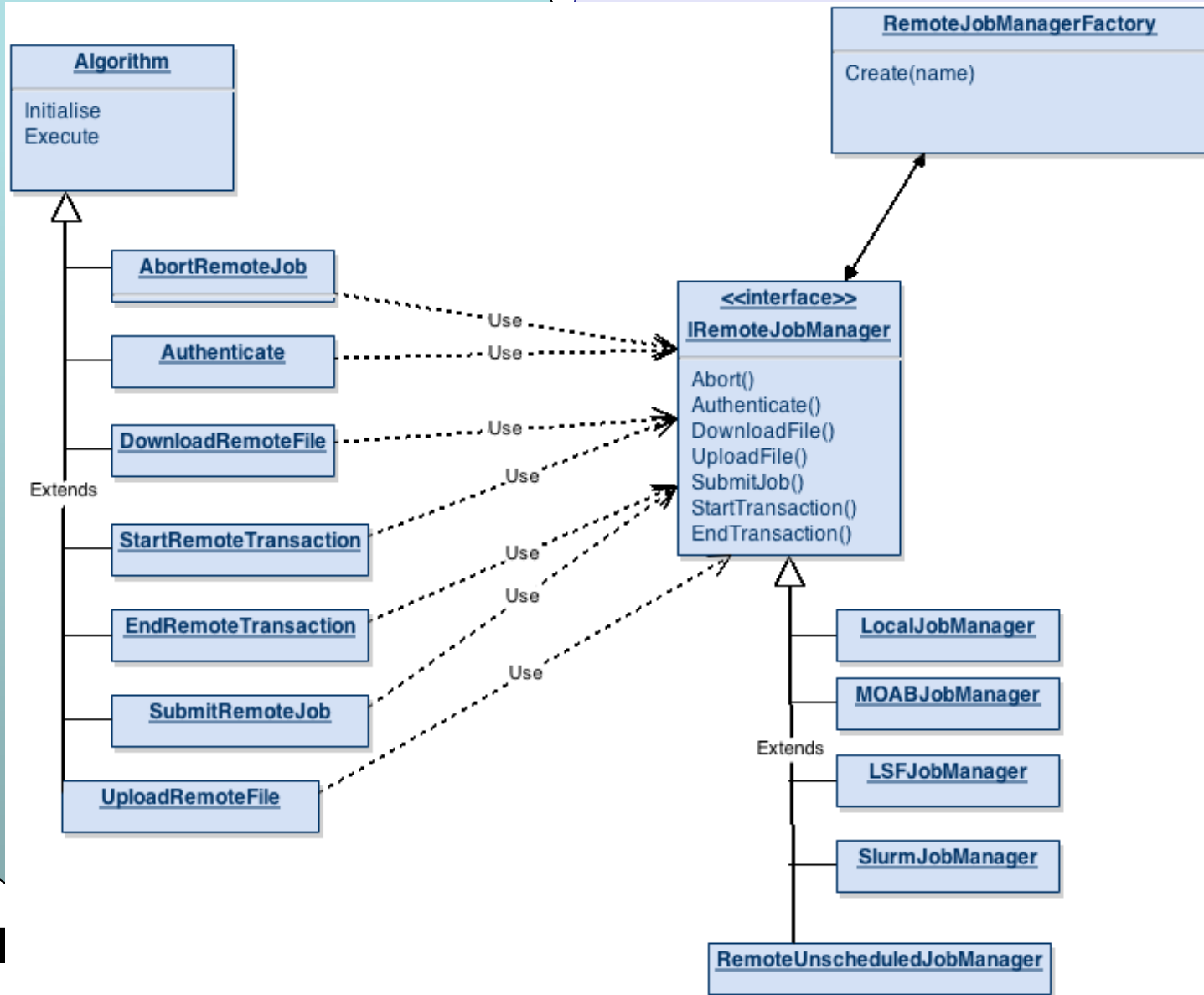
- Sample Data: C:\MantidInstall\data\CNCS_7860_event.nxs
- Output Workspace Name: MyData
- DetCal File: [Redacted]
- Incident Energy Calculation: Incident Energy Guess: 10 meV, TZero Guess: 0.0 microseconds, Monitor Spectrum IDs: 2 and 3
- Energy Transfer Range (meV): Low: 2, Width: 0.1, High: 10
- Hard Mask: [Redacted]
- Grouping: [Redacted]
- Show Intermediate Workspaces: [Redacted]
- Save to folder: c:\MyData\

Buttons:

- Reduce
- Send cluster
- Save
- Export



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



Introduction

A Simple API for Grid and Distributed Applications.

SAGA (*Simple API for Grid Applications*) defines a high-level interface to the most commonly used distributed computing functionality. SAGA provides an access-layer and mechanisms for distributed infrastructure components like job schedulers, file transfer and resource provisioning services. Given the heterogeneity of distributed infrastructure, SAGA provides a much needed interoperability layer that lowers the complexity and improves the simplicity of using distributed infrastructure whilst enhancing the sustainability of distributed applications, services and tools.

SAGA-Python provides a Python module that is compliant with the [OGF GFD.90](#) SAGA specification. Behind the API façade, SAGA-Python implements a flexible *adaptor* architecture. Adaptors are dynamically loadable modules that interface the API with different middleware systems and services. Most application developers use the adaptors that are already part of SAGA-Python, but you can easily implement your own in case your backend system is not supported yet.



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 .. ?



Doesn't this sound a bit like ...

WS_GRAM

The screenshot shows a web browser window with the address bar displaying `toolkit.globus.org/toolkit/docs/3.2/gram/ws/`. The page features a blue header with the Globus logo and navigation links: Home, Globus Online, Globus Toolkit (highlighted), dev.globus, and About Globus. Below the header is a dark blue bar with links: About the Toolkit, Documentation, Downloads, and Support. The main content area is titled "WS GRAM Documentation" and includes a breadcrumb trail: Home -> Toolkit -> Docs -> 3.2 -> Gram -> WS. A Google Custom Search bar is present. The text explains that the Grid Resource Allocation and Management (GRAM) service provides a single interface for requesting and using remote system resources. It mentions two implementations: one based on a proprietary, pre-Web service protocol (Pre-WS GRAM) and another built using Web service interfaces (WS GRAM). The page lists documentation links for WS GRAM, including Overview, Developer's Guide, and System Administrator's Guide.

Home -> Toolkit -> Docs -> 3.2 -> Gram -> WS

Google™ Custom Search

The Grid Resource Allocation and Management (GRAM) service provides a single interface for requesting and using remote system resources for the execution of "jobs". The most common use of GRAM is remote job submission and control. It is designed to provide a uniform, flexible interface to job scheduling systems.

GT3.2 contains two GRAM implementations: one based on a proprietary, pre-Web service protocol ([Pre-WS GRAM](#)) and the second built using Web service interfaces (WS GRAM).

This following documentation links refer to the WS GRAM component.

GRAM Key Concepts

- [Overview](#)

WS GRAM: Developer's Guide

- [Overview](#)
- [GRAM slides](#)
- [API](#)
- [Architecture](#)
- [Fault Tolerance Architecture](#)
- [RSL Schema](#)
- [MJS Fault Types](#)
- [Samples](#)
- [Scheduler interface tutorial](#)
- [Troubleshooting](#)

WS GRAM : System Administrator's Guide

- [Overview](#)

WS GRAM : User's Guide

- [Overview](#)

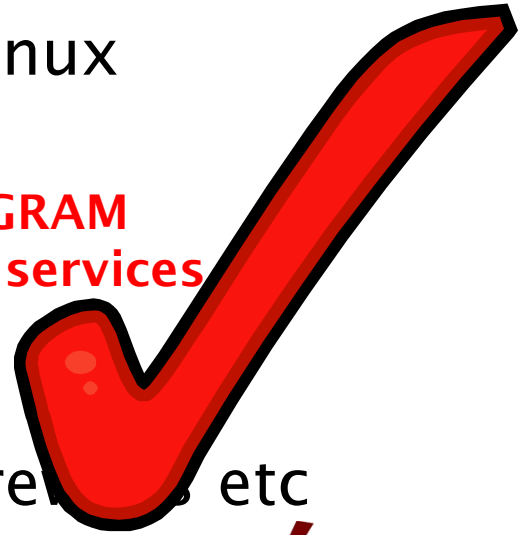


Doesn't this sound a bit like ...

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, firewalls etc
- Does not need Admin or special permissions **X**
- 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

