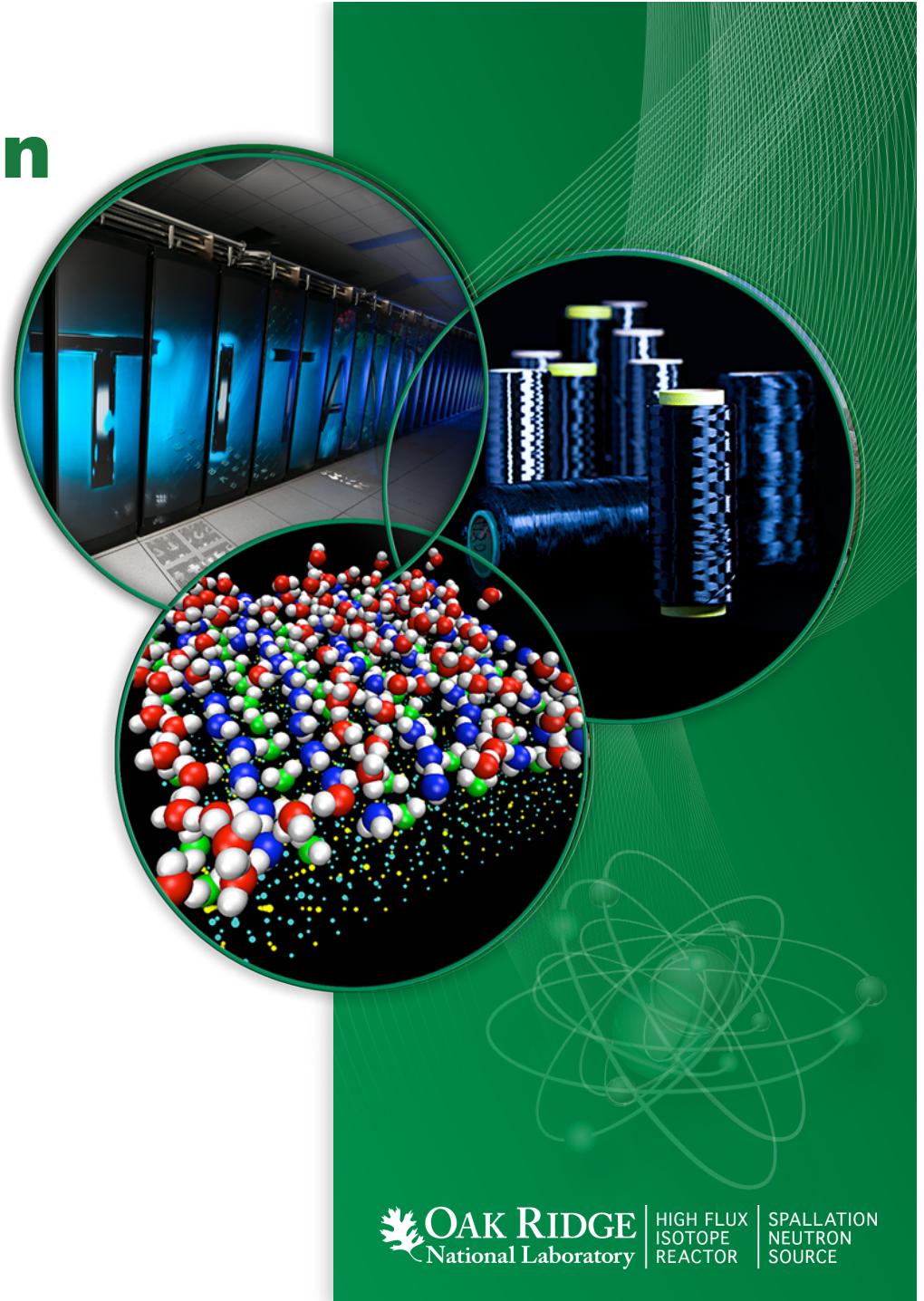


Mantid: Now and in the future

Garrett E. Granroth
Scientific Data Analysis Group
Lead

July 23, 2014

ORNL is managed by UT-Battelle
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Mantid Team



- www.mantidproject.org

NIMA 764, 156 (2014)

Mantid Outline

- Members, Contributors
- Deployment
- Documentation system
- Functionality Highlights and Plans
 - Python API
 - Live
 - Event processing – usage case
- Conclusions

What is Mantid?

- A Framework for Reduction and Analysis of Neutron and Muon Data
 - Can Be accessed by
 - MantidPlot
 - Python Interface
 - C++ API

Partners and Contributors

- Partners



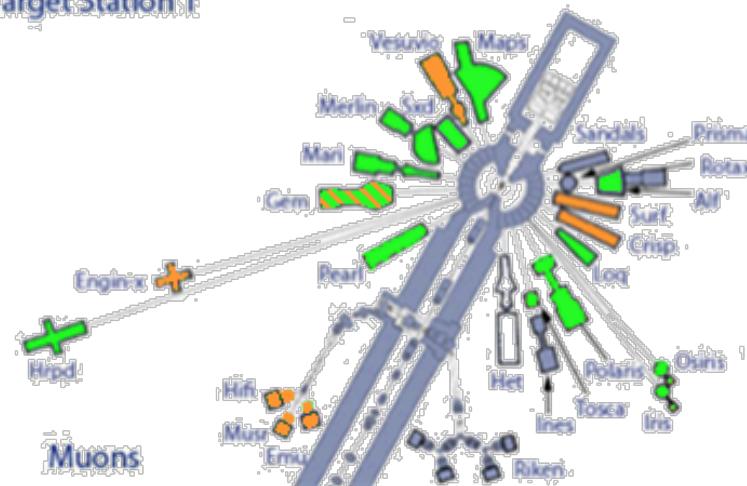
- Contributors



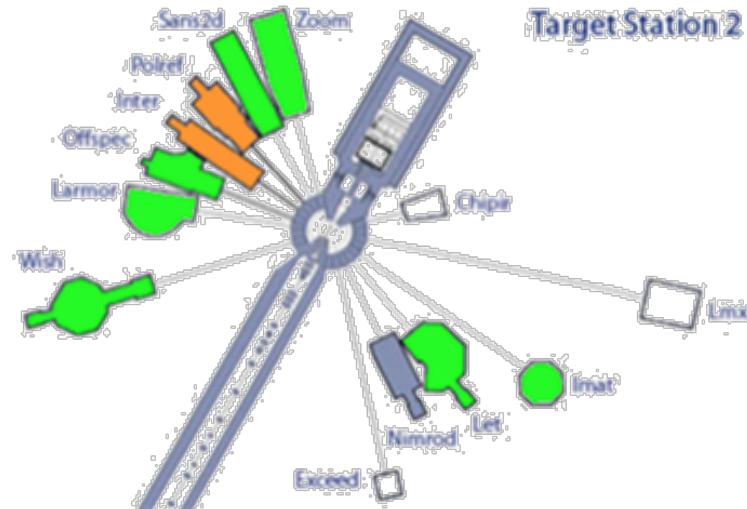
Deployment

ISIS

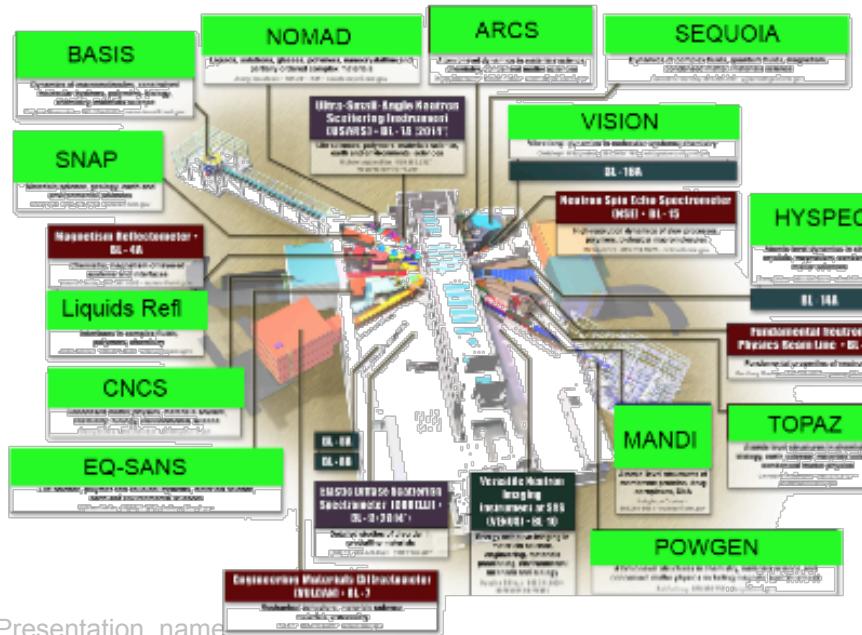
Target Station 1



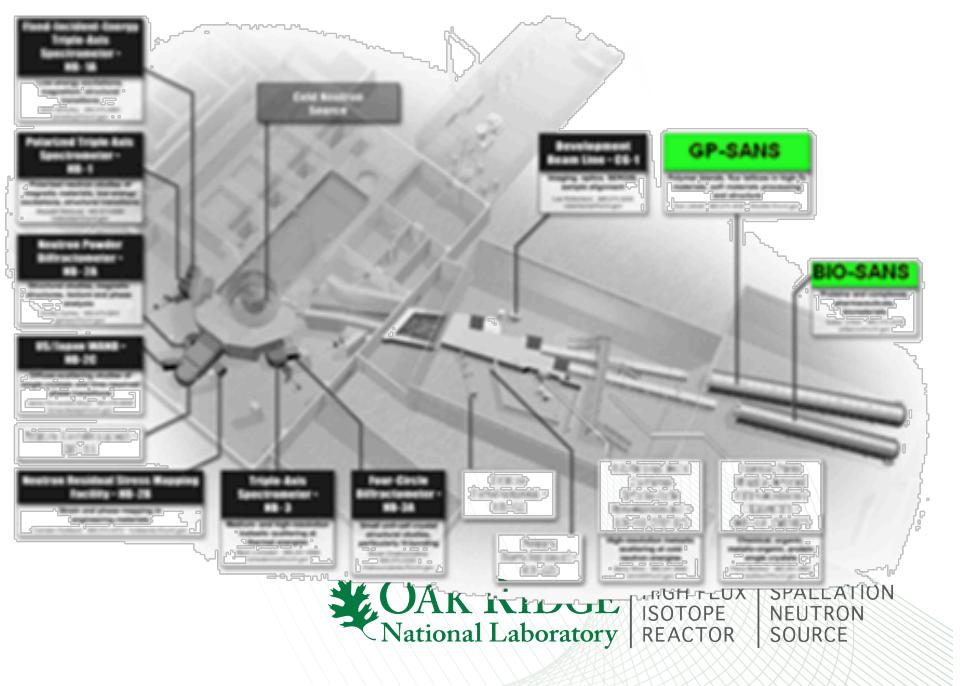
Target Station 2



SNS



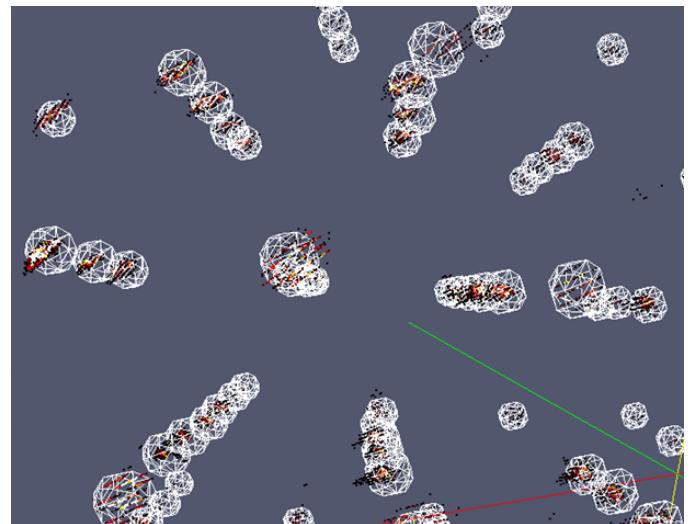
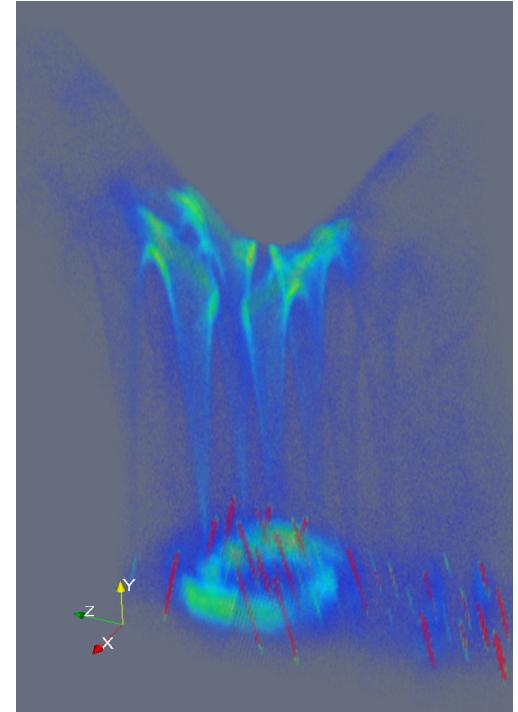
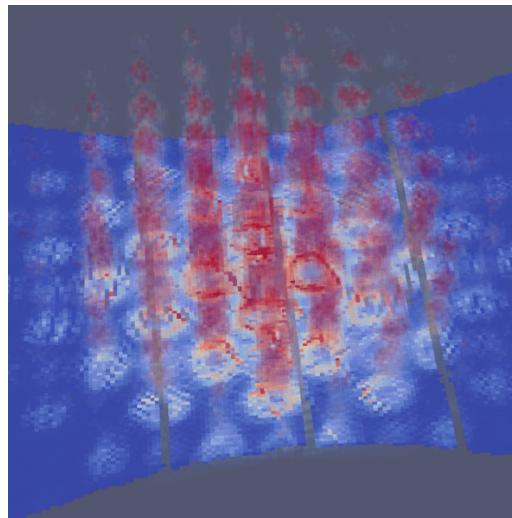
HFIR



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Advanced Visualization

- Vates /integrated Paraview
- Future
 - Moving to Paraview 4.2
 - Production interface in Mantid workflow
 - Improved GUI



Improved Sphinx based documentation

```
○ ○ ○ https://raw.githubusercontent.com/mantidproject/mantid/docs/source/algorithms/SetUB-v1.rst
○ ○ ○ https://raw.githubusercontent.com/mantidproject/mantid/master/Code/Mantid/docs/source/algorithms/SetUB-v1.rst
Apple iCloud Facebook Twitter Wikipedia Yahoo News Popular Reader

.. algorithm::

.. summary::

.. alias::

.. properties::

Description
-----
The algorithms will attach an OrientedLattice object to a sample in the workspace. For MD workspaces, you can select to which sample to attach it. If nothing entered, it will attach to all. If bad number is entered, it will attach to first sample.

If UB matrix elements are entered, lattice parameters and orientation vectors are ignored. The algorithm will throw an exception if the determinant is 0. If the UB matrix is all zeros (default), it will calculate it from lattice parameters and orientation vectors (MSlice and Horace style). The algorithm will throw an exception if u and v are collinear, or one of them is very small in magnitude.

Usage
-----
.. testcode:: SetUB

# create a workspace (or you can load one)
ws=CreateSingleValuedWorkspace(5)

#set a UB matrix using the vector along k_i as 1,1,0, and the 0,0,1 vector in the horizontal plane
SetUB(ws,a=5,b=6,c=7,alpha=90, beta=90, gamma=90, u="1,1,0", v="0,0,1")

#check that it works
from numpy import *
mat=array(ws.sample().getOrientedLattice().getUB())
print "UB matrix"
print array_str(mat,precision=3, suppress_small=True)

.. testcleanup:: SetUB

DeleteWorkspace(ws)

Output:
.. testoutput:: SetUB

UB matrix
[[ -0.        0.       0.143]
 [ 0.128   -0.128    0.      ]
 [ 0.154    0.107   -0.      ]]

.. categories::
```



SetUB v1

Table of Contents

- Summary
- Properties
- Description
- Usage

Summary

Set the UB matrix, given either lattice parameters and orientation vectors or the UB matrix elements.

Properties

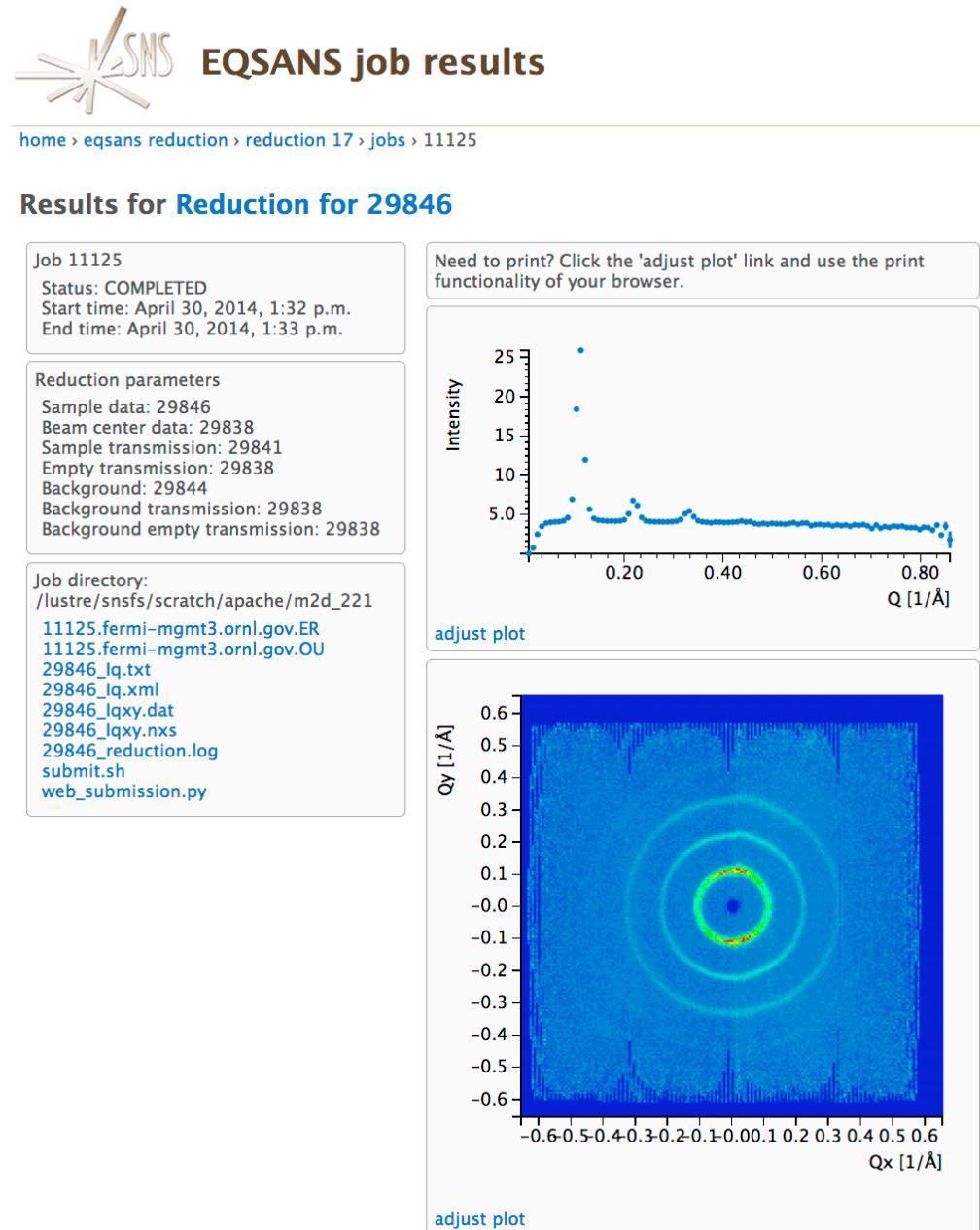
Name	Direction	Type	Default	Description
Workspace	InOut	Workspace	Mandatory	An input workspace.
a	Input	number	1	Lattice parameter a
b	Input	number	1	Lattice parameter b
c	Input	number	1	Lattice parameter c
alpha	Input	number	90	Lattice parameter alpha (degrees)
beta	Input	number	90	Lattice parameter beta (degrees)
gamma	Input	number	90	Lattice parameter gamma(degrees)
u	Input	dbl list	1,0,0	Vector along k_i, when goniometer is at 0
v	Input	dbl list	0,1,0	In plane vector perpendicular to k_i, when goniometer is at 0
UB	Input	dbl list	0,0,0,0,0,0,0	UB Matrix
MDSampleNumber	Input	number	Optional	For an MD workspace, the sample number to which to attach an oriented lattice (starting from 0). No number, or negative number, means that it will copy to all samples

Description

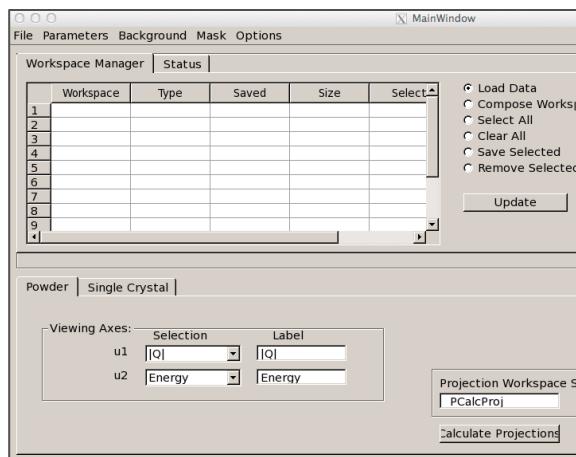
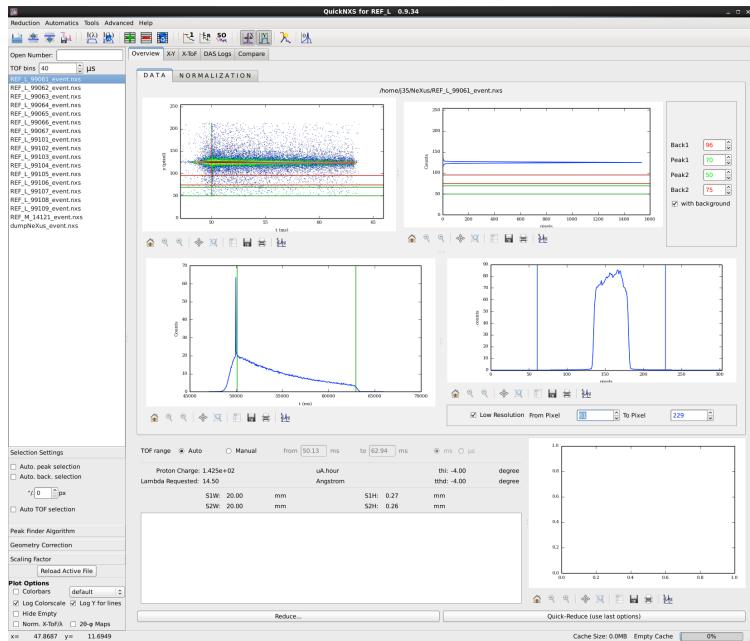
The algorithms will attach an OrientedLattice object to a sample in the workspace. For MD workspaces, you can select to which sample to attach it. If nothing entered, it will attach to all. If bad number is entered, it will attach to first sample.

Python- API auto reduction

- Simple shell driven script after a run completes
- Prototyping web driven reduction



Python API – use your favorite interface



IP[y]: Notebook Mantid_InelasticPowder_Example Last Checkpoint: Jul 31 16:59 (autosaved)

Basic IPython Notebook Example:

Inelastic Powder Projection Calculation and Visualization

The following IPython Notebook example illustrates the following:

1. Enables using Mantid Algorithms by setting up `mantid.simpleapi`
2. Reads in a Mantid workspace
3. Shows raw data
4. Calculates powder projections
5. Visualizes projected powder data
6. Saves ASCII data to file

1. Enable Mantid Simple api

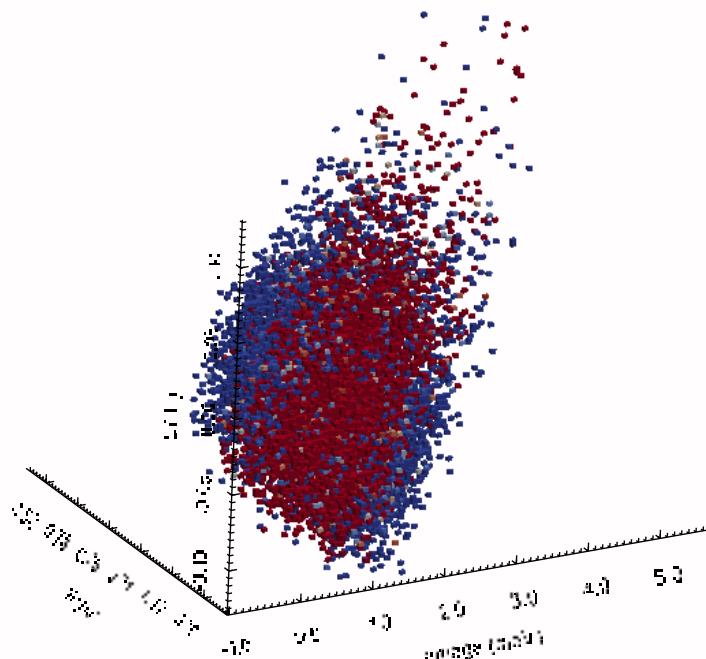
```
In [1]: import sys,os
print "Setting up Mantid environment"
try:
    #check if MANTIDPATH enviornment variable exists
    manpath=os.environ['MANTIDPATH'] #check if MANTIDPATH environment variable is set
except:
    #case MANTIDPATH did not exist, so create the necessary path additions
    manpath=r'/opt/Mantid/bin' #if not, then use the Linux path for Analysis computers
    #also set the MANTIDPATH environment variable since it seems not to be set
    os.environ['MANTIDPATH']=manpath
sys.path.append(manpath)
from mantid.simpleapi import *
print "Mantid environment initialized"
```

2. Select File and read in raw data Mantid workspace

```
In [2]: #Load Python QT GUI environment to enable using a dialog to interact with user for file selection
from PyQt4 import Qt, QtCore, QtGui
useDialog=False #the user can change this flag - True enables a dialog pick file, False uses hardcoded
if useDialog:
    print "Using File Dialog to select a workspace file"
    from PyQt4 import Qt, QtCore, QtGui
    curdir=os.curdir
    filter='*.nxs'
    file = QtGui.QFileDialog.getOpenFileNames(None,'Open Workspace', curdir,filter)
else:
    print "Using hard coded path to an example data file"
    file=r'/SNS/users/public/Notebooks/data/zrh_1000.nxs'

print "Loading workspace file: ",file
ws=Load(filename=file) #load Mantid workspace from file
ws.name #show some workspace info to see if the proper workspace was loaded
```

Python API - get data in and out



IP[y]: Notebook Mantid_InelasticPowder_Example (autosaved)

File Edit View Insert Cell Kernel Help

3. Show Raw Data

```
In [3]: #use this magic command to keep the plots within the notebook
print "Setting up Matplotlib environment for basic data display"
%matplotlib inline
```

```
In [4]: import matplotlib.pyplot as plt
import numpy as np

#create a figure to hold the plots
plt.figure(1)
#extract 2D spectra
data=ws.extractY()
#sum to produce a 1D data set to visualize
data1D=np.sum(data,1)
#place 1D data in first figure
plt.subplot(121)
plt.plot(data1D)
plt.title("Data Summed Along Y-Axis")
#place 2D spectra data in 2D image plot
plt.subplot(122)
#show data in log scale to see detail better for this example
eps=0.00001 #place floor for log data to epsilon
plt.imshow(np.log10(data+eps))
plt.show()
```

Data Summed Along Y-Axis

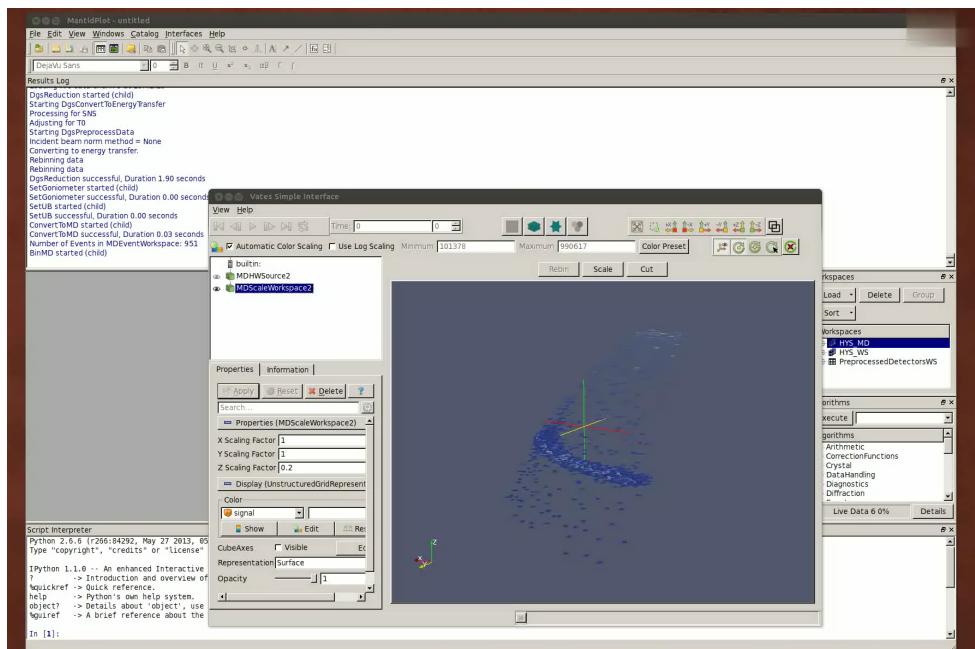
```
In [5]: #disable inline plotting and let new windows pop-up separately
%matplotlib qt
```

4. Calculate Powder Projection Data

```
In [6]: #reduces the data and converts the workspace to an multi-dimension (MD) eve
ws_proj=ConvertToMD(ws,'|Q|','Direct') #output is the powder projection MD
```

Live Data

- Converting to instrument units (Q and ω) as things come in.
- On Hyspec, SEQUOIA, Vision, Correlli, and USANS at SNS
- ENGIN-X, MERLIN, LET, OFFSPEC, SANS2D at ISIS

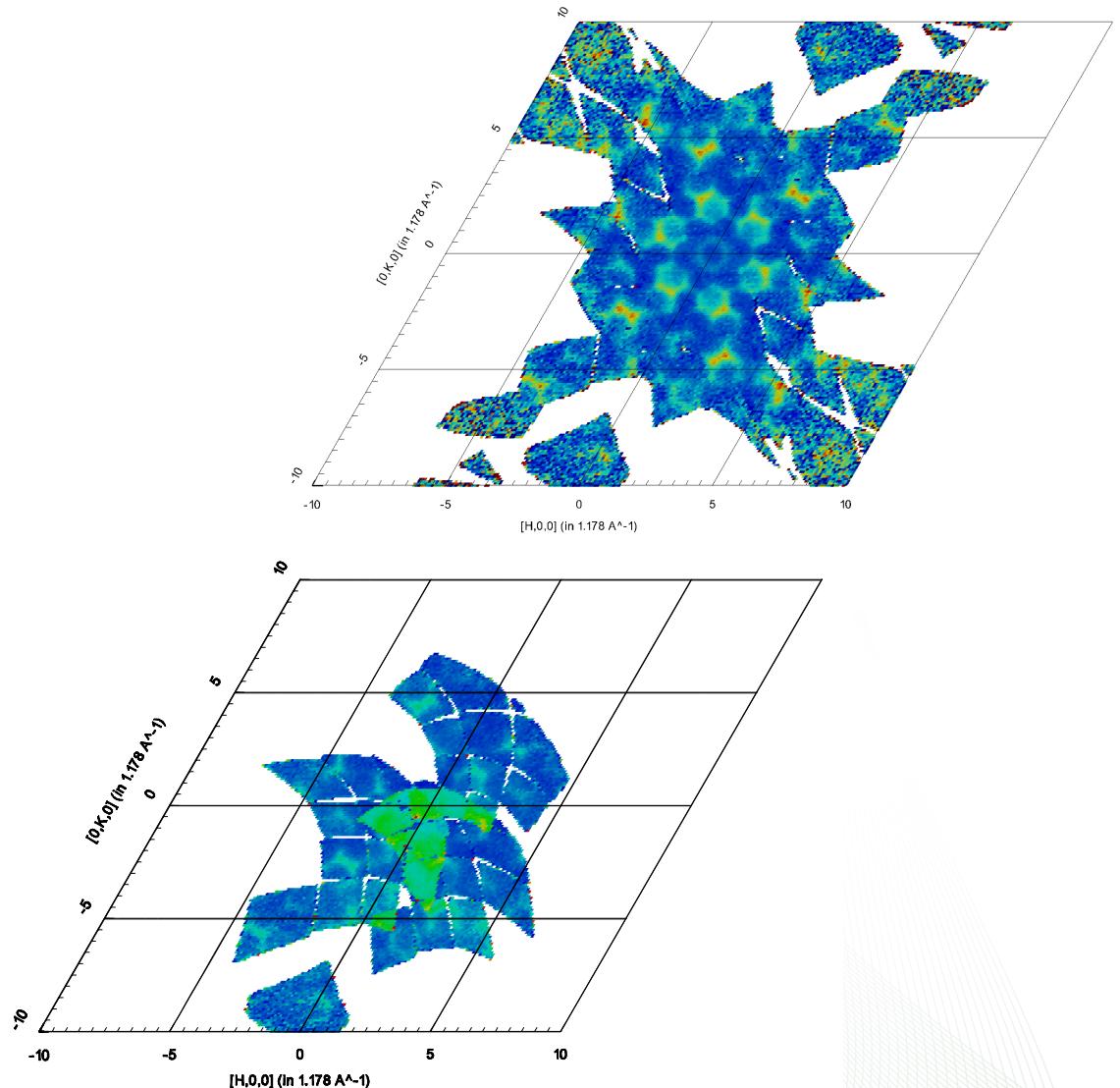


Event Based Data reduction

- Allows for faster processing in most cases
- Not all Mathematics is straightforward
- Currently Working through Normalization of different statistic runs
- Allows for pump probe filter experiments

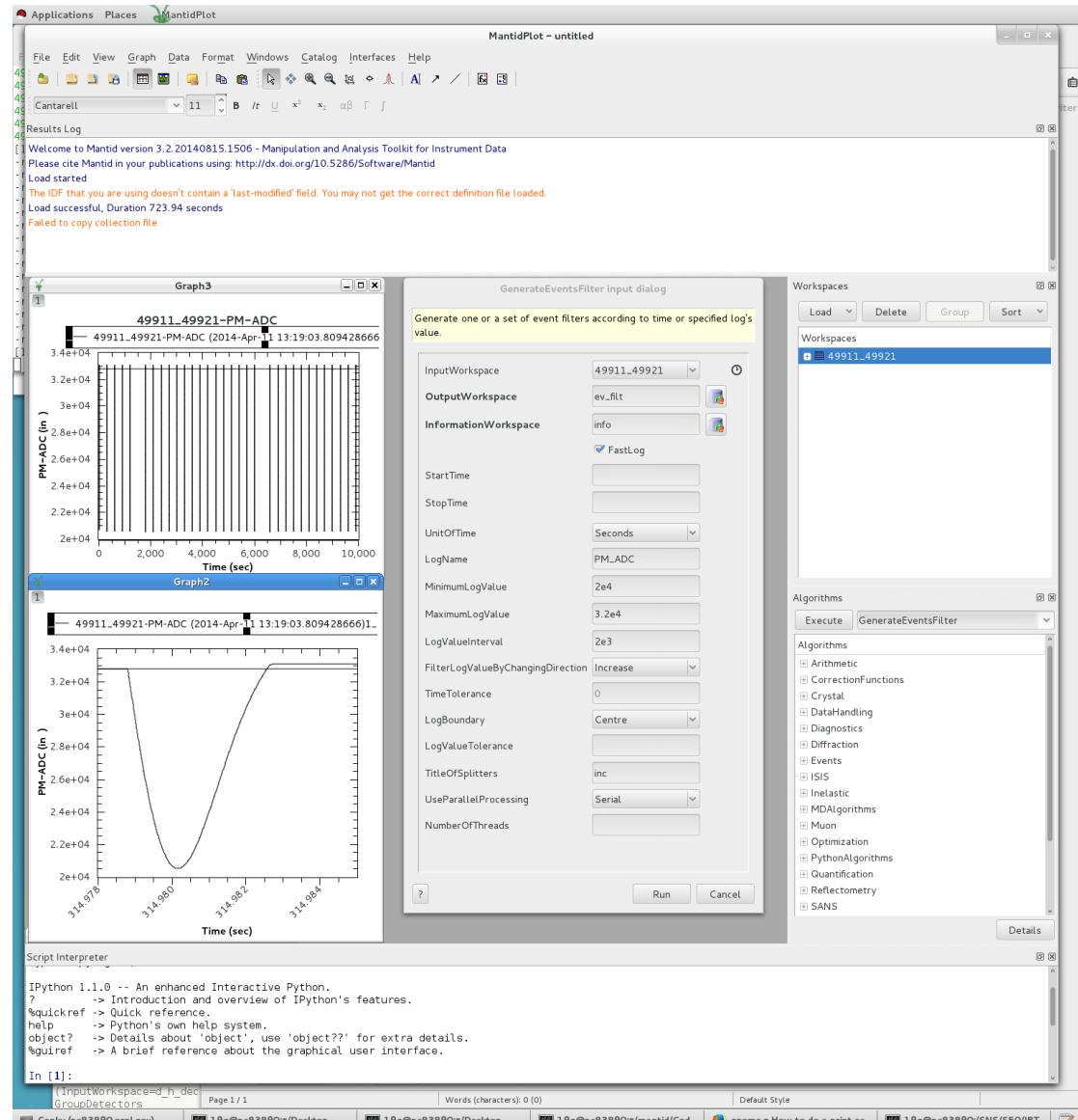
Event Diffraction Data Normalization

- Most Challenging for diffraction
 - Different Incident flux for every incident wavelength /time bin
- Moving to Inelastic Next



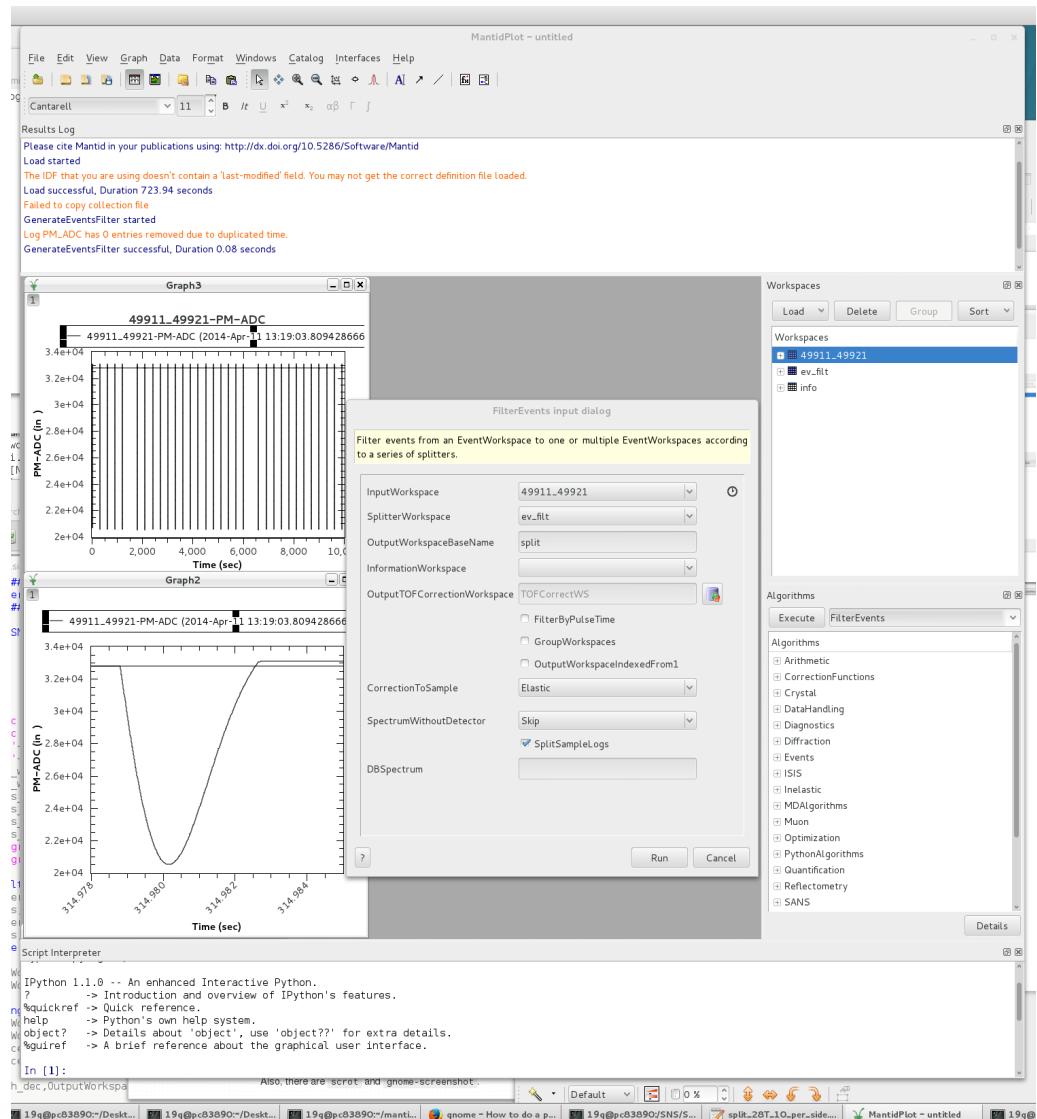
Filter fast logs – a use case

- Generate Filter on Pulsed Magnet log
- Prepare to put events in 5 workspaces corresponding to rising edge on magnet signal

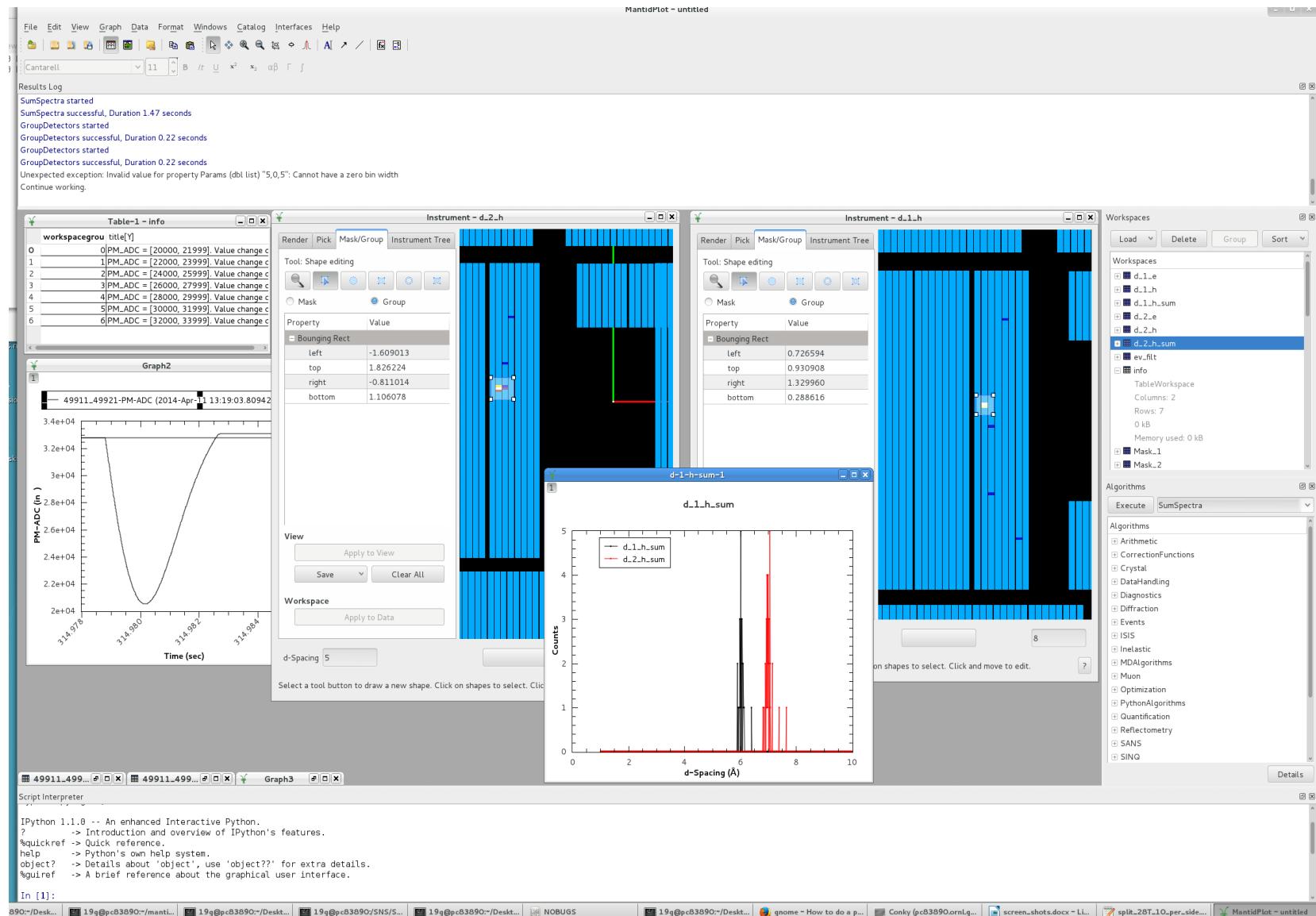


Filter fast logs – a use case

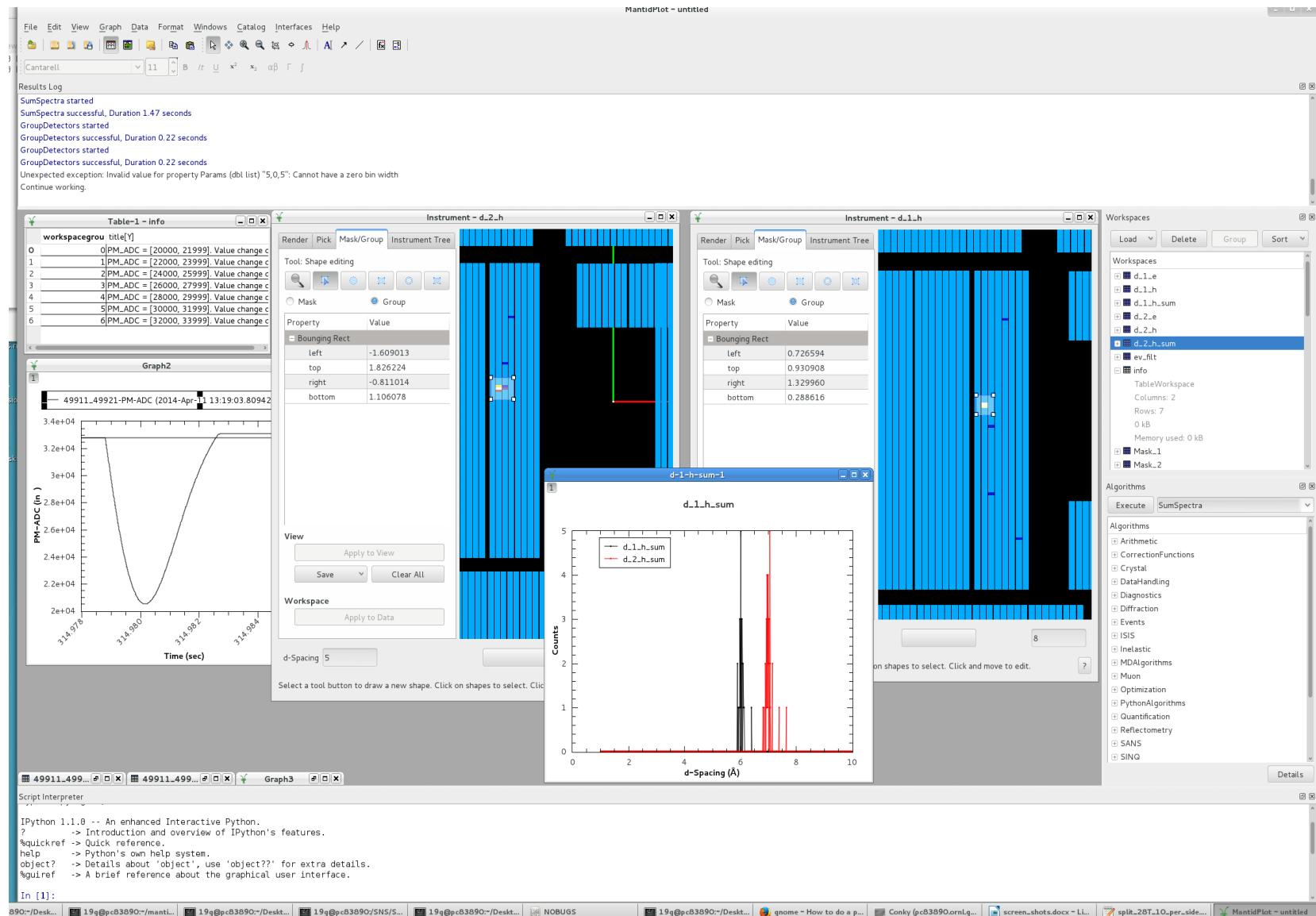
- Interface to perform the filtering



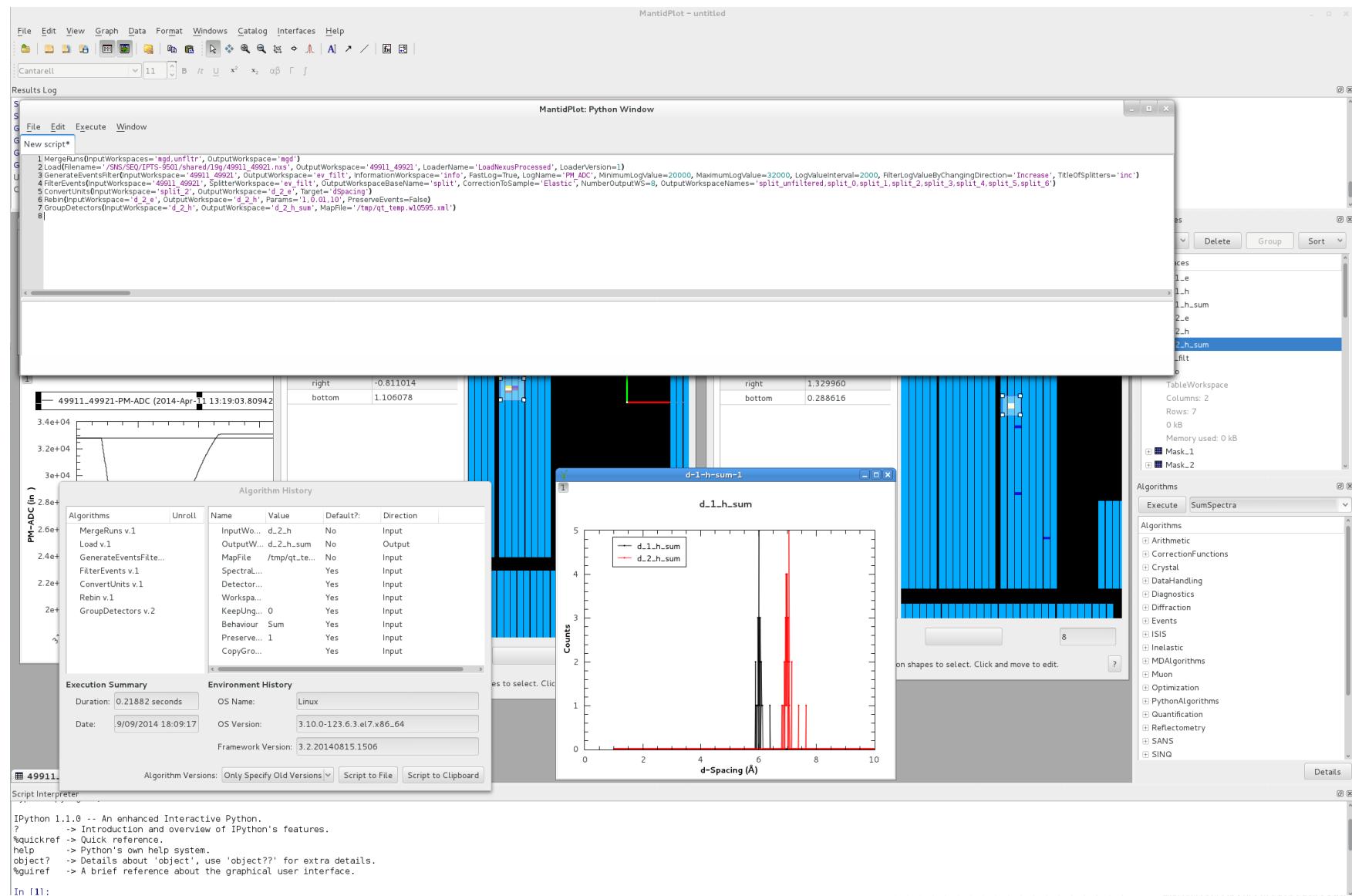
Filter fast logs - a use case



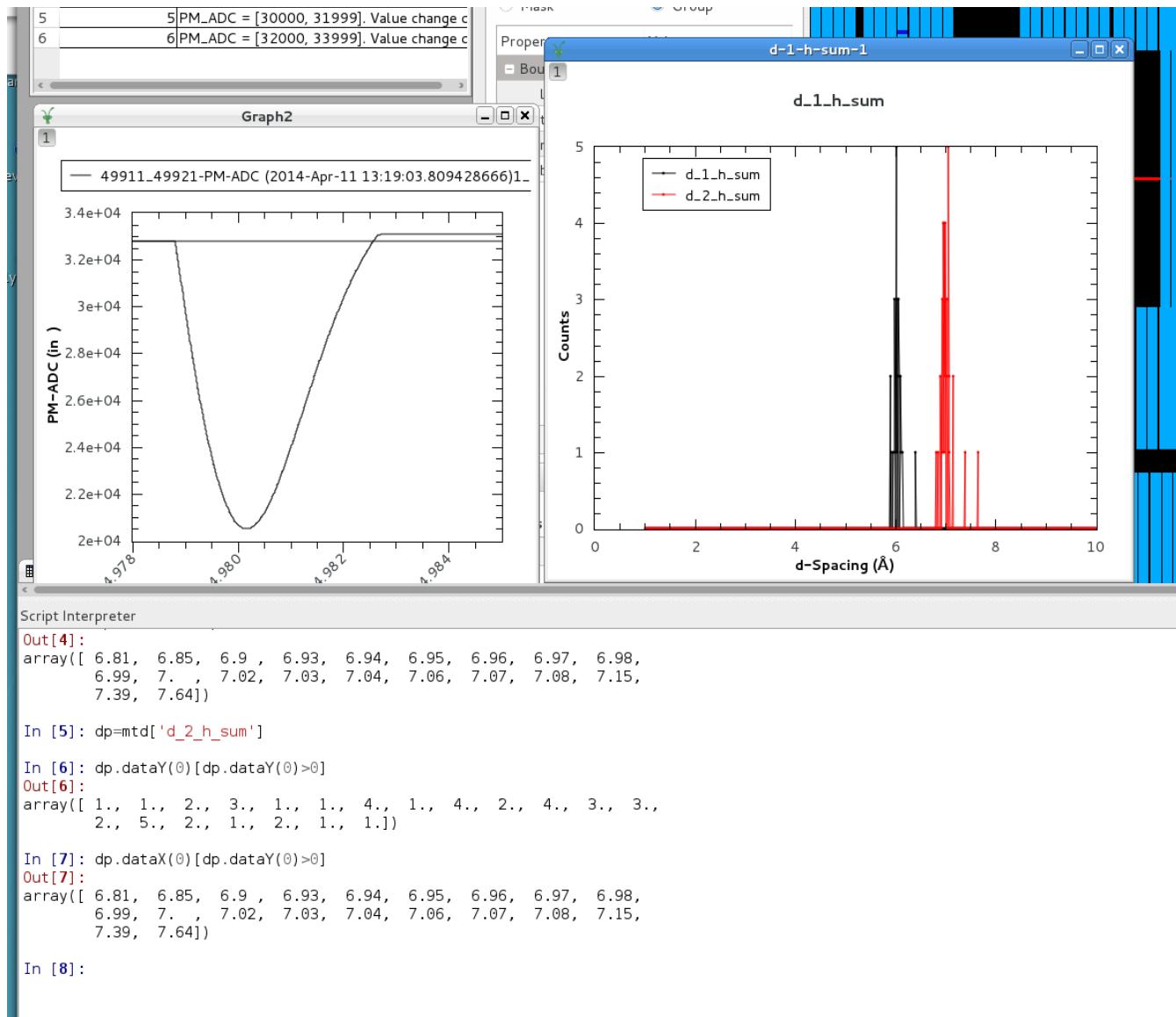
Filter fast logs - a use case



Filter fast logs - a use case



Filter fast logs - a use case



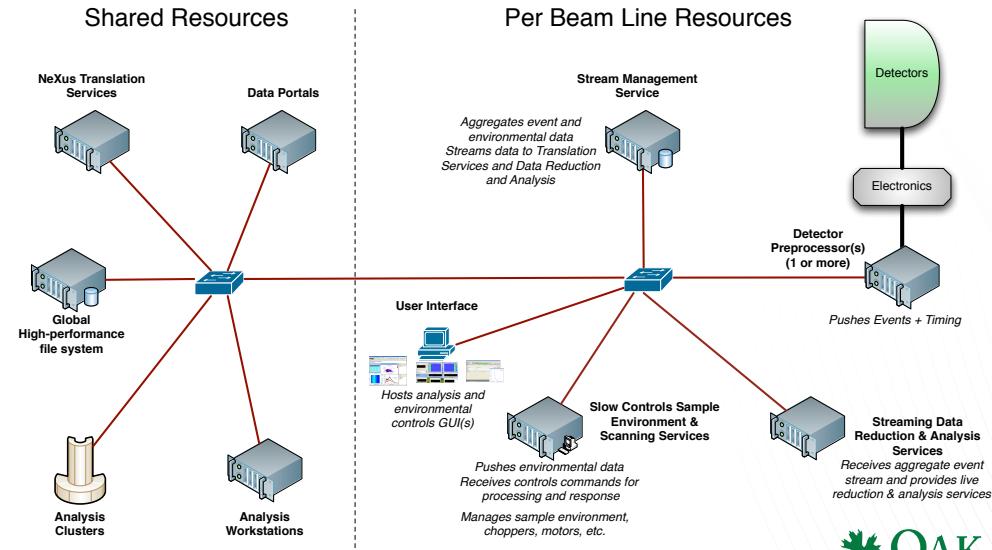
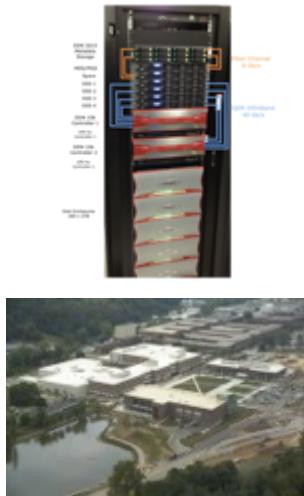
Conclusions

- Mantid is seeing broad use at neutron scattering facilities
- The Python API provides an straightforward and powerful interface to the Mantid Algorithms
- Event based reduction provides added scientific functionality.
- Mantidplot is interface useful for developing scientific workflows in Mantid.

Improving Acquisition



- Accelerating Data Acquisition, Reduction, and Analysis at SNS
- We stream data (neutron and SE) from the DAS to a publish subscribe system
 - **Stream Management Service (SMS)**
- We re-configure the data translation (file creation) to read the data stream from SMS and create the files while the run is taking place... end of run = close file [file appears “instantly”]
 - **Streaming Translation Service (STS)**
- We modify MANTID (data reduction) to read from the data stream live from SMS
 - **Streaming Reduction Service (SRS)**
- Files are created on an HPC infrastructure for subsequent parallel analysis and data reduction



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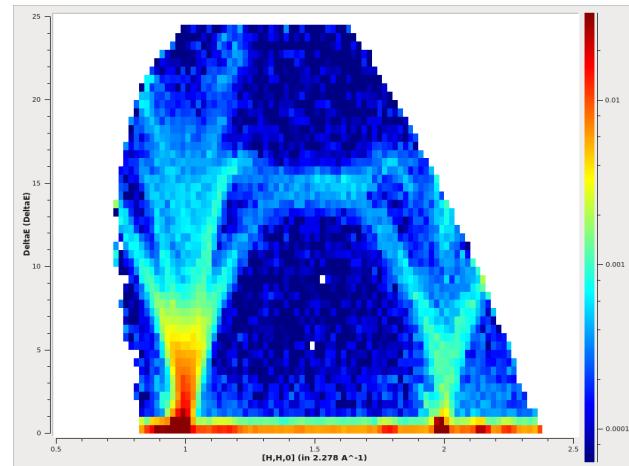
HIGH FLUX
ISOTOPE
REACTOR

SPALLATION
NEUTRON
SOURCE

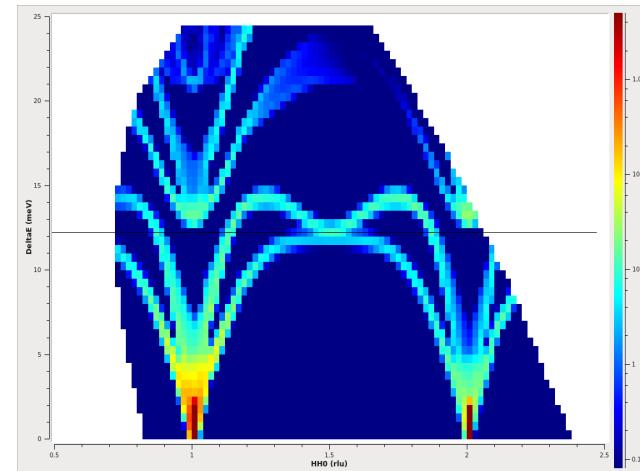
Concurrent Simulations and Experiment

- Ab-initio molecular dynamics (AIMD) simulations on the EOS cluster and experiment on SrTiO₃ on the HYSPEC instrument at the SNS.
- Used dedicated 23,000 computing cores on EOS (a Cray XC30 cluster).
- Large AIMD calculations capture the anharmonic renormalization (stabilization) of phonon dispersions and achieve good agreement with the experiments.
- Parameters in the simulations were adjusted based on observed scattering intensity.
- The simulations also helped refine the range of crystal orientations collected.
- Volume datasets from HYSPEC measurements and SimPhonies simulations were visualized side-by-side with MANTID SliceView

HYSPEC



EOS



S(Q,E) from experiment (left) and simulation (right) along [HH1] direction.