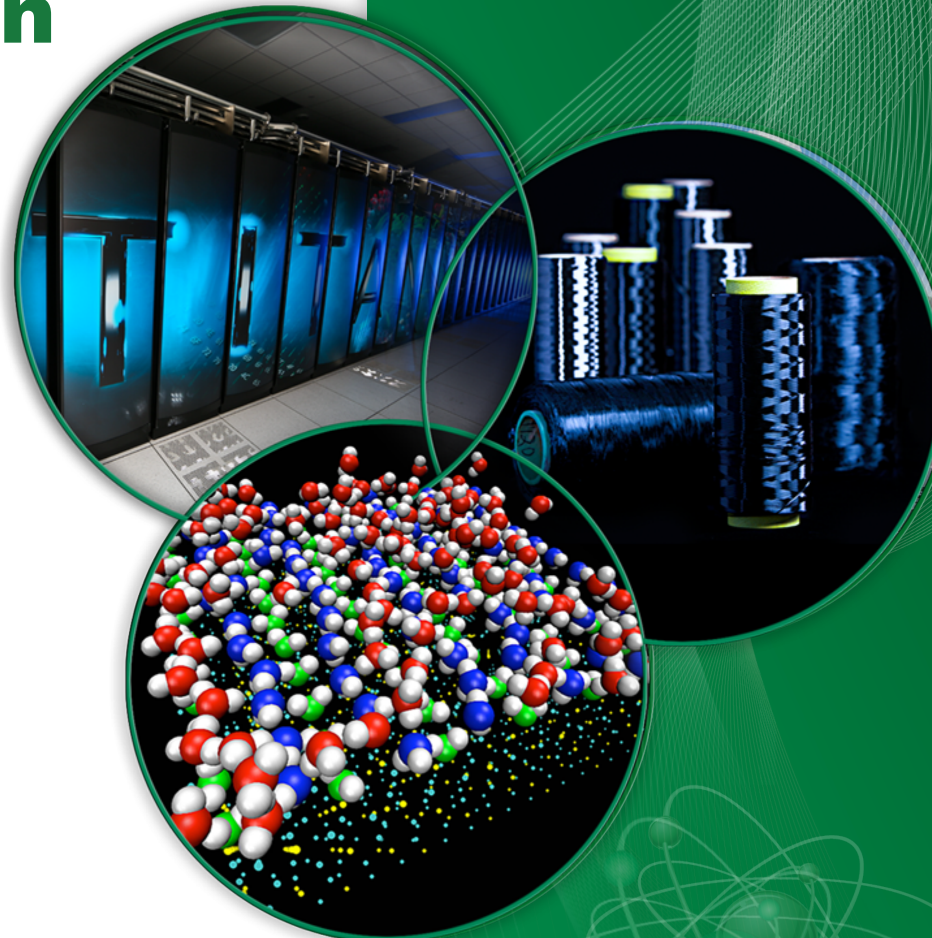
Mantid: Now and in the future



Garrett E. Granroth

Scientific Data Analysis Group Lead

July 23, 2014

ORNL is managed by UT-Battelle
for the US Department of Energy

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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

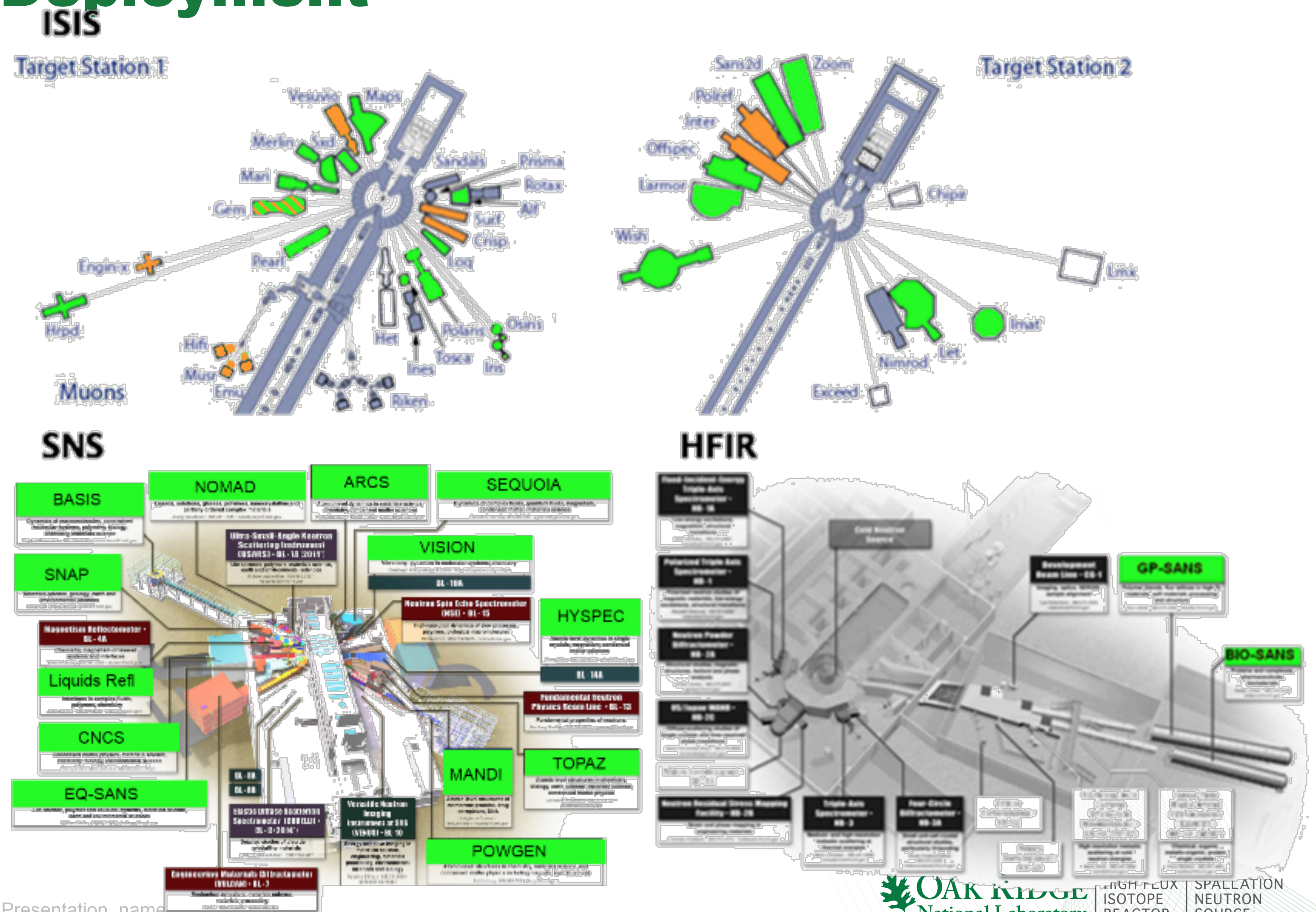
What is Mantid?

- 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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Target Station 1
Vesuvio
Maps
Merlin
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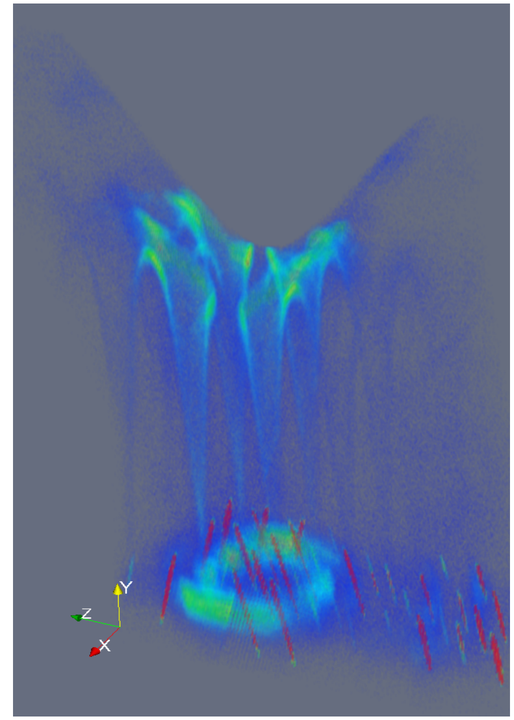
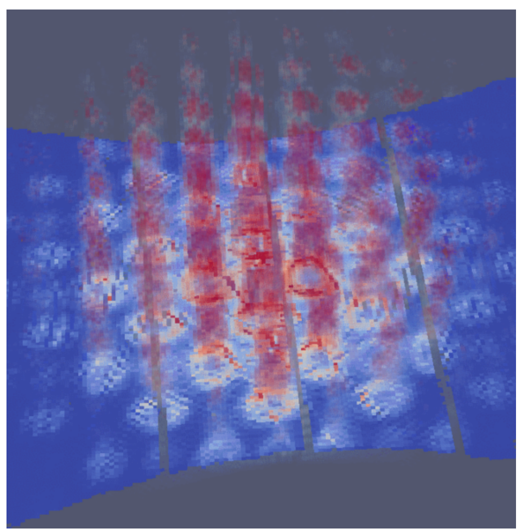
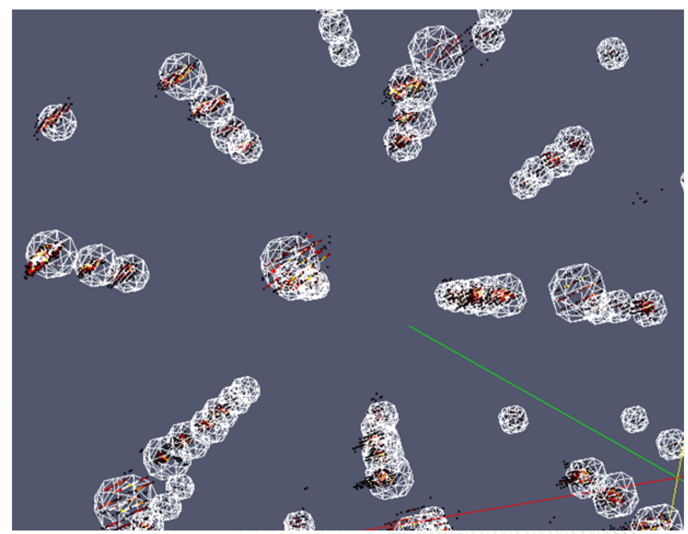
Gem
Sandals
Prisma
Rotax
Alf
Surf
Crisp
Loq
Pearl
Engin-x
Hrpd
Het
Polaris
Osiris
Tosca
Ines
Iris
Hifi
Musr
Emu
Riken
Muons
Target Station 2
Sans2d
Zoom
Polref
Inter
Offspec
Larmor
Chipir
Wish
Lmx
Imat
Let
Nimrod
Exceed
SNS
BASIS
NOMAD
ARCS
SEQUOIA
VISION
SNAP
HYSPEC
Liquids Refl
CNCS
EQ-SANS
MANDI
TOPAZ
POWGEN
HFIR
GP-SANS
BIO-SANS

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/ma…er/Code/Mantid/docs/source/algorithms/SetUB-v1.rst

```
.. 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
enetered, 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::
```

docs.mantidproject.org/nightly/algorithms/SetUB-v1.html

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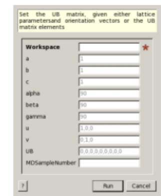
SetUB v1

Table of Contents

- Summary
- Properties
- Description
- Usage



SetUB dialog.

Summary

Set the UB matrix, given either lattice parametersand orientation vectors or the UB matrix elements

Properties

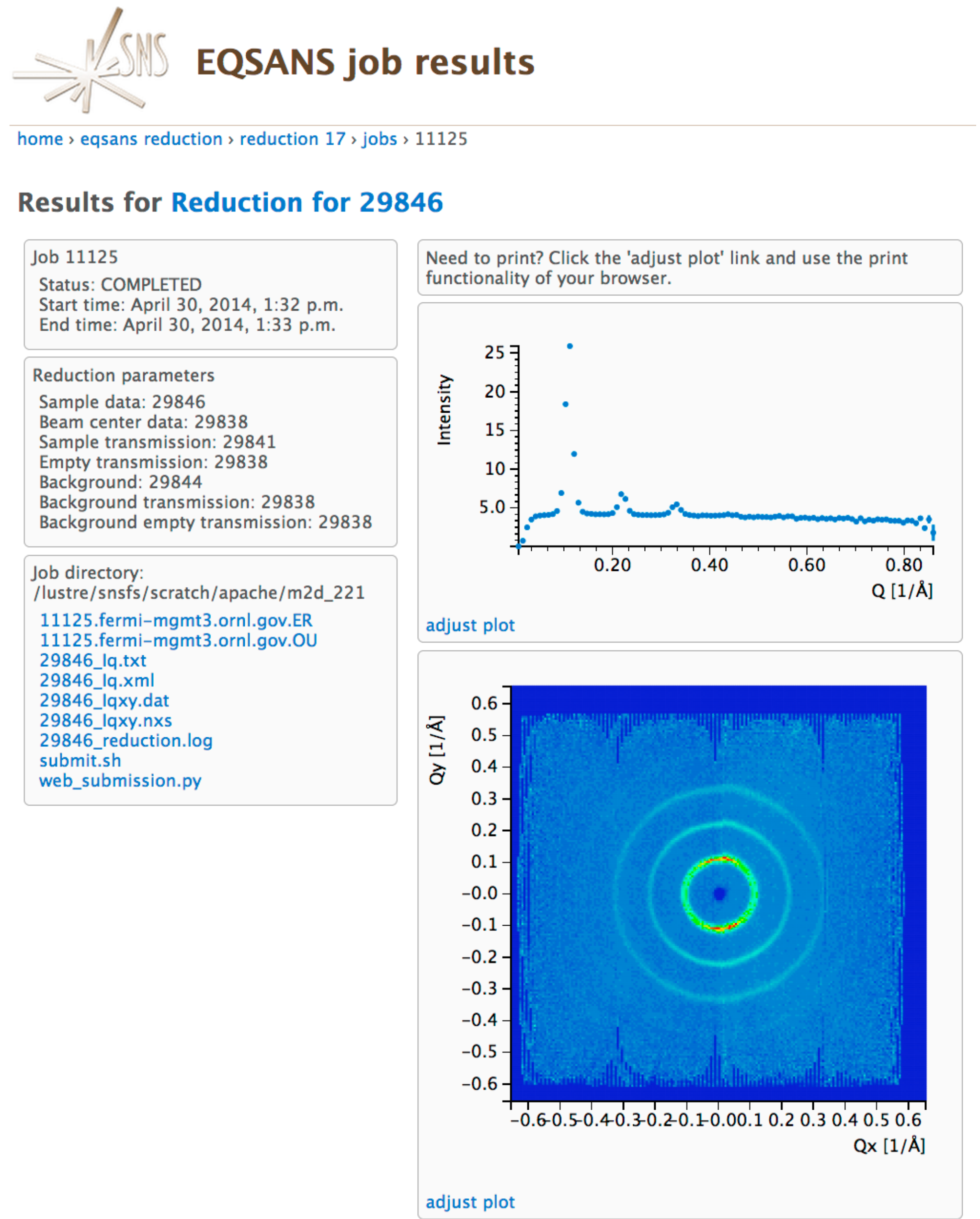
Name	Direction	Type	Default	Description
Workspace	InOut	Workspace	Mandatory	An input workspace.
a	Input	number	1	Lattice parameter a
b	Input	number	1	Lattice parameter b
c	Input	number	1	Lattice parameter c
alpha	Input	number	90	Lattice parameter alpha (degrees)
beta	Input	number	90	Lattice parameter 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	0,0,0,0,0,0,0,0,0	UB Matrix
MDSampleNumber	Input	number	Optional	For an MD workspace, the sample number to wich to attach an oriented lattice (starting from 0). No number, or negative number, means that it will copy to all samples

Description

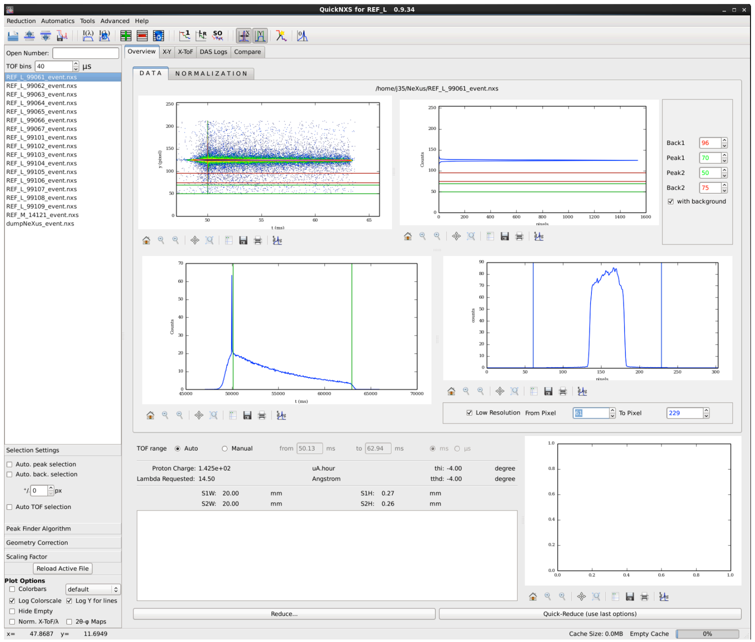
The algorithms will attach an OrientedLattice object to a sample in the workspace. For MD workspaces, you can select to which sample to attach it. If nothing entered, it will attach to all. If bad number is enetered, it will attach to first sample.

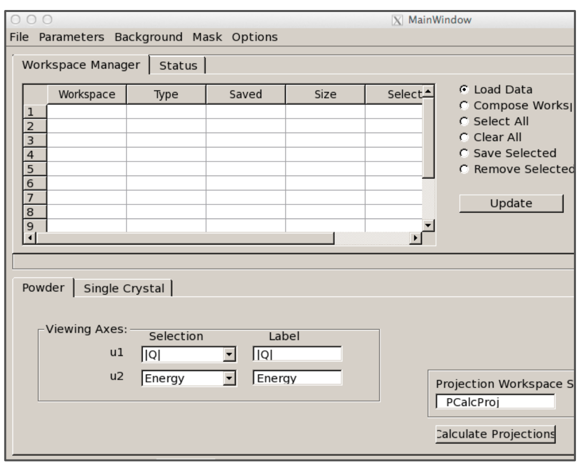
Python- API auto reduction

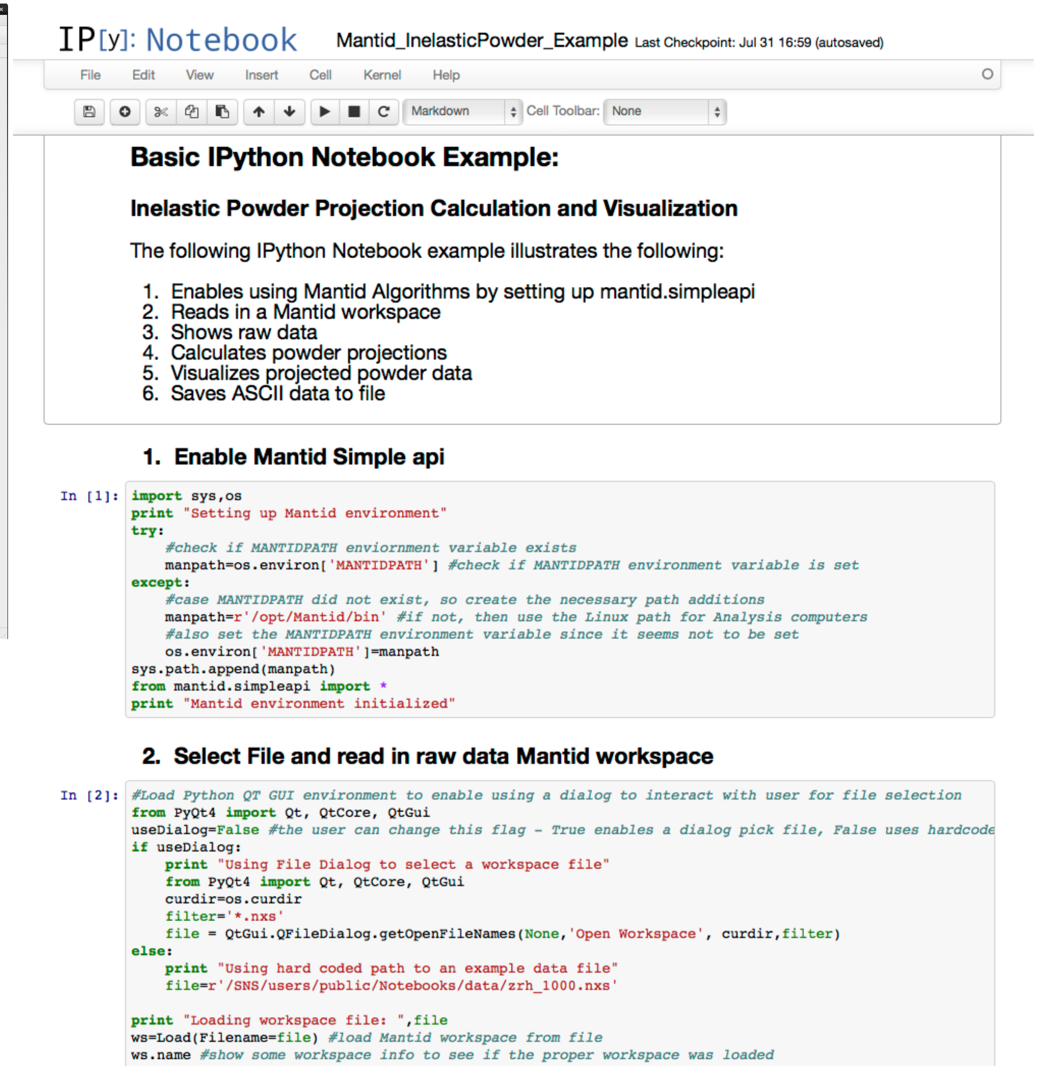
- Simple shell driven script after a run completes
- Prototyping web driven reduction



Python API – use your favorite interface







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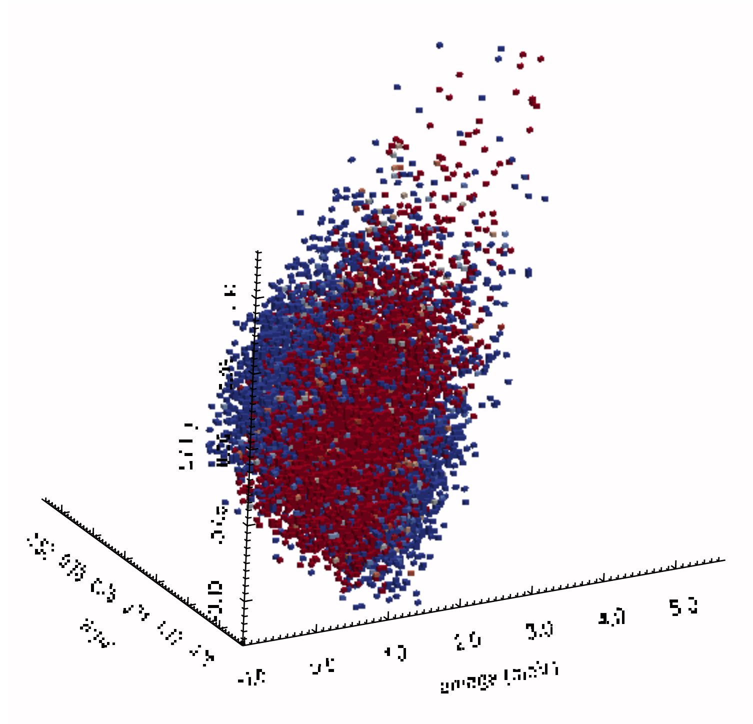
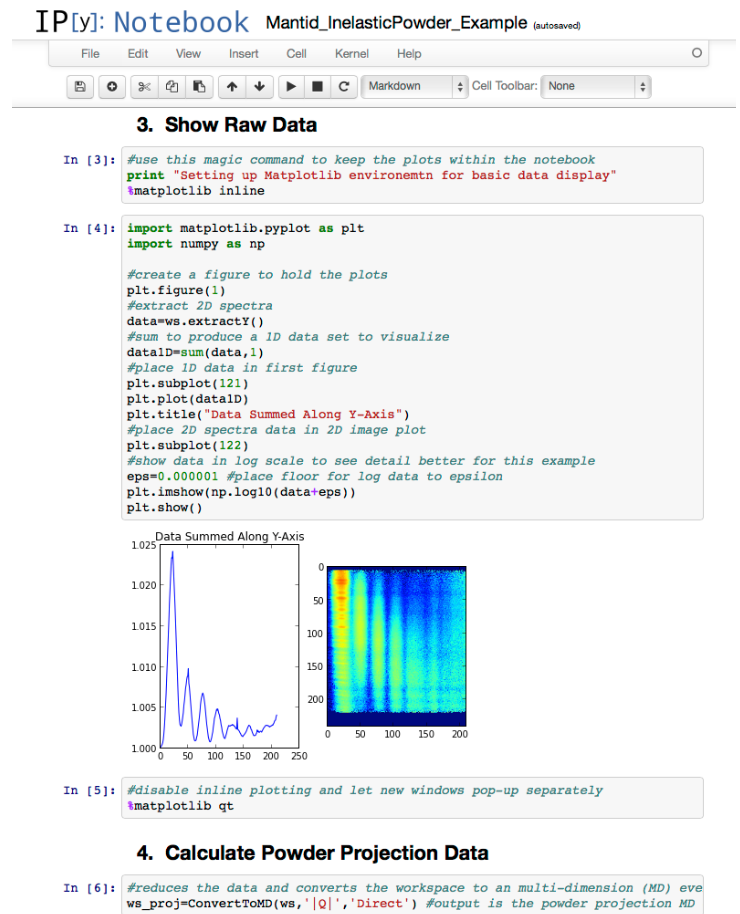
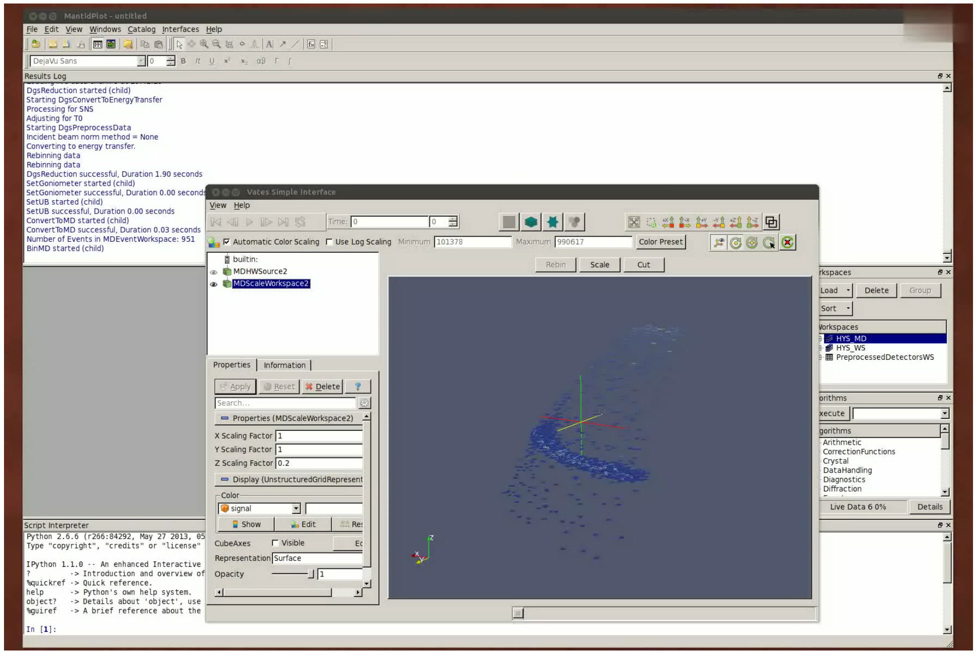
Python API - get data in and out





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



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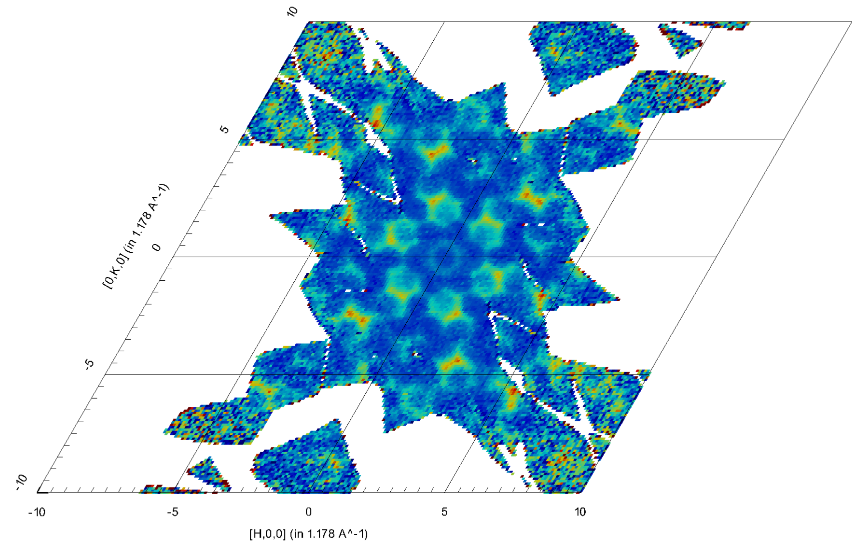
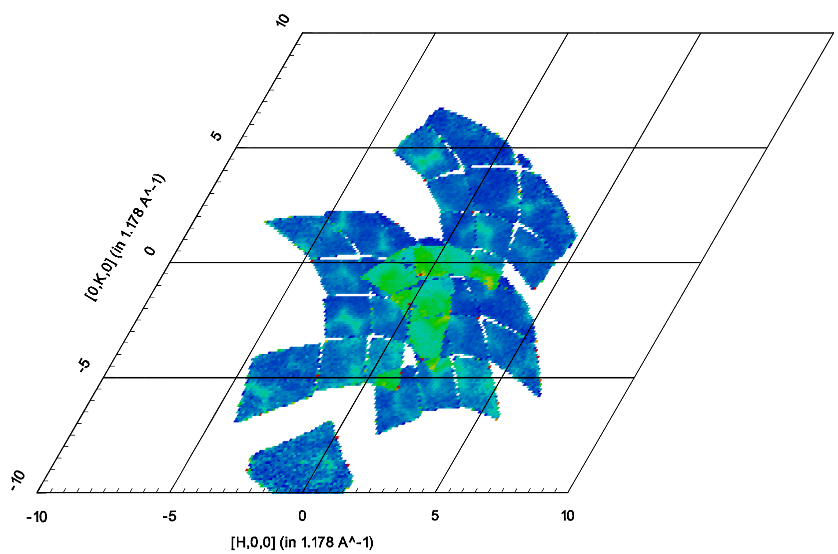
Event Based Data reduction

- 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

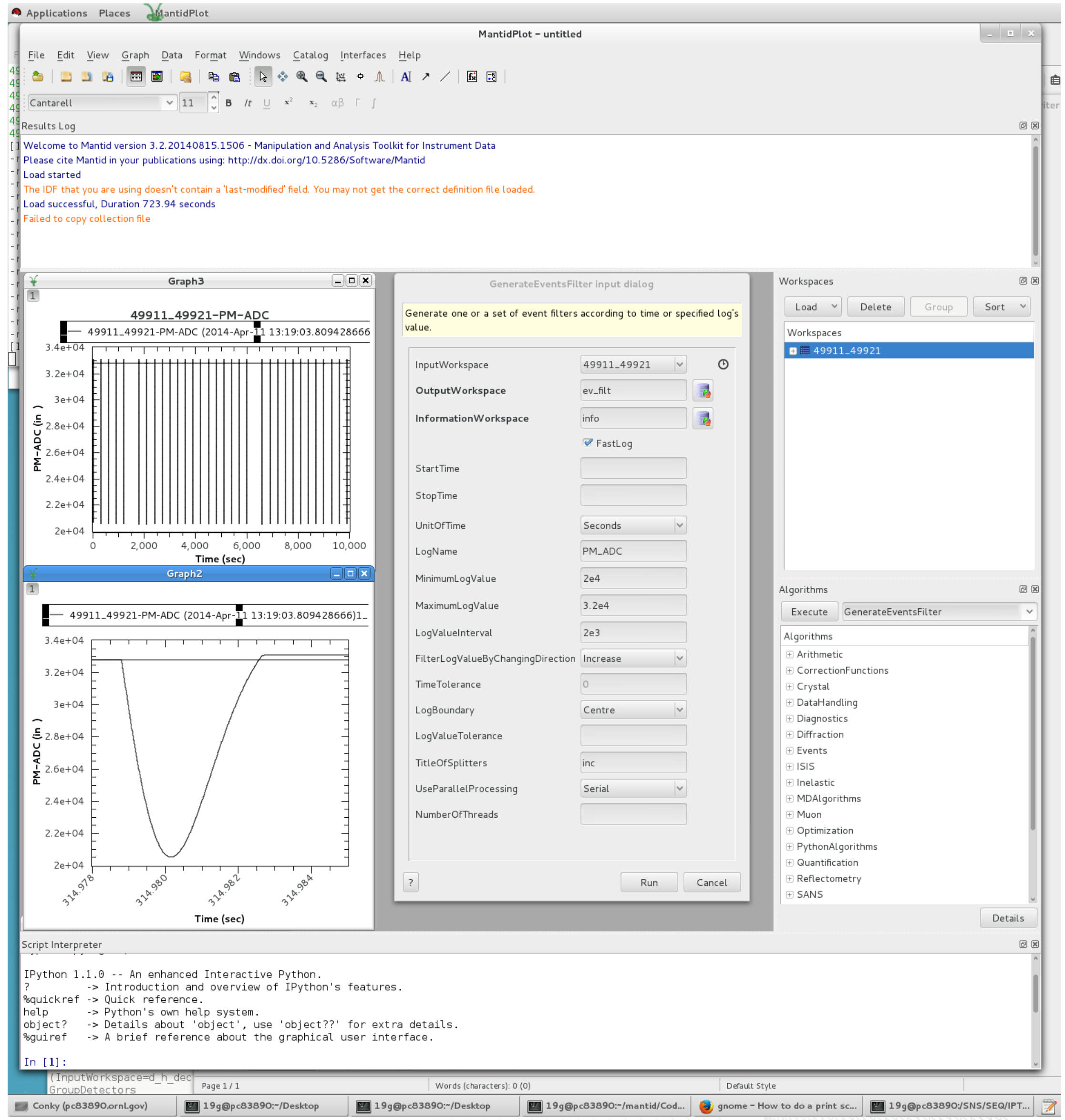
- Most Challenging for diffraction
  - Different Incident flux for every incident wavelength /time bin
- Moving to Inelastic Next





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



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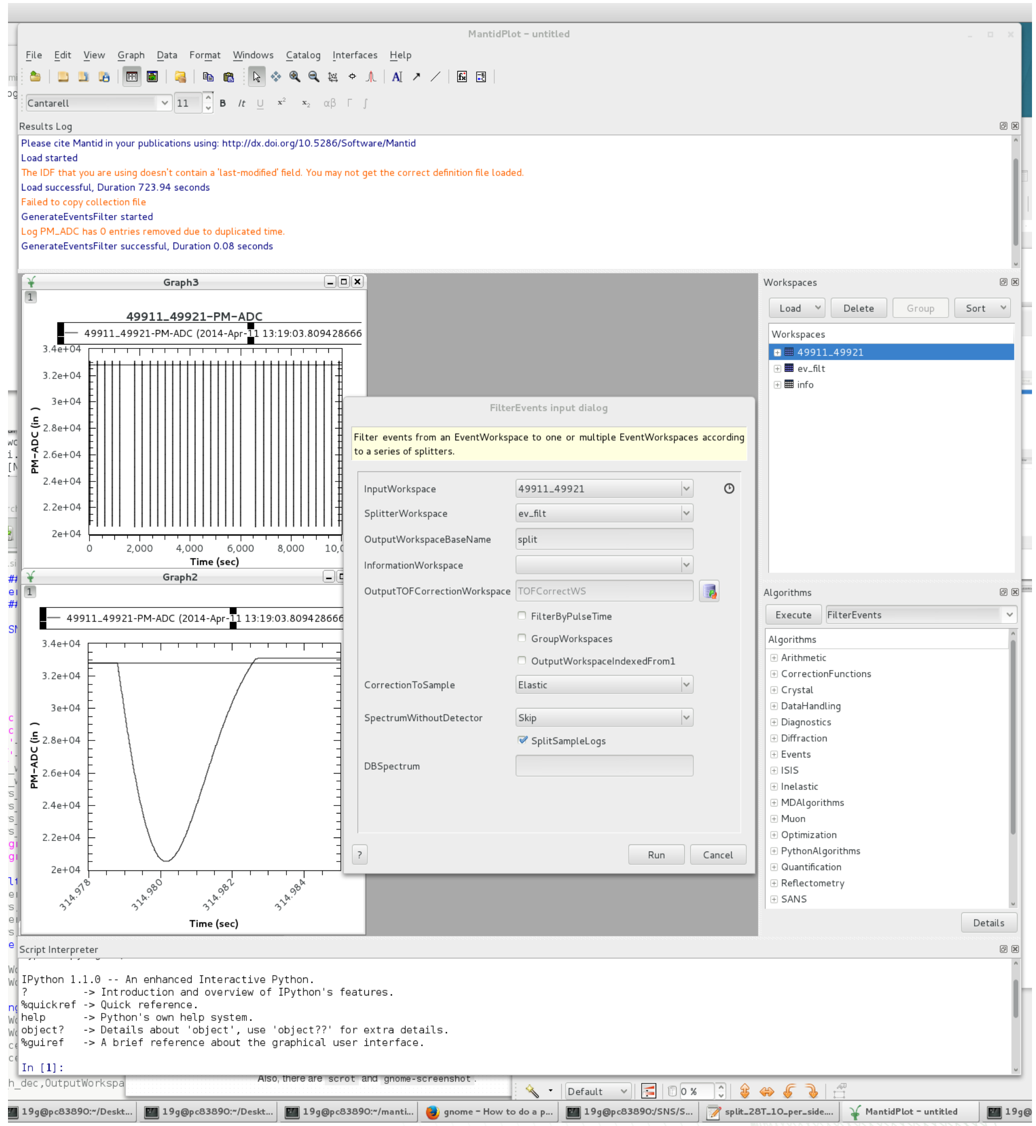
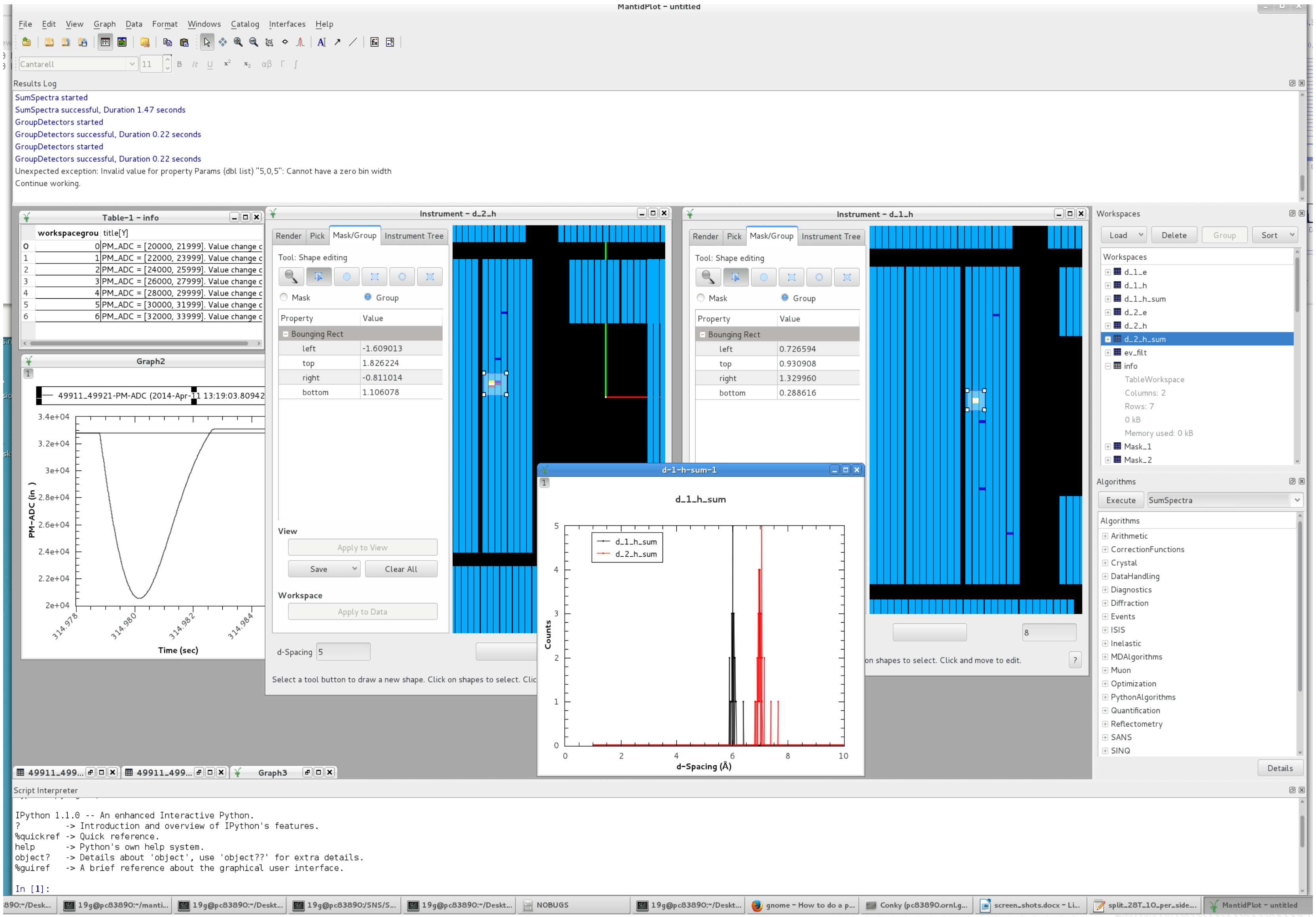
Filter fast logs – a use case

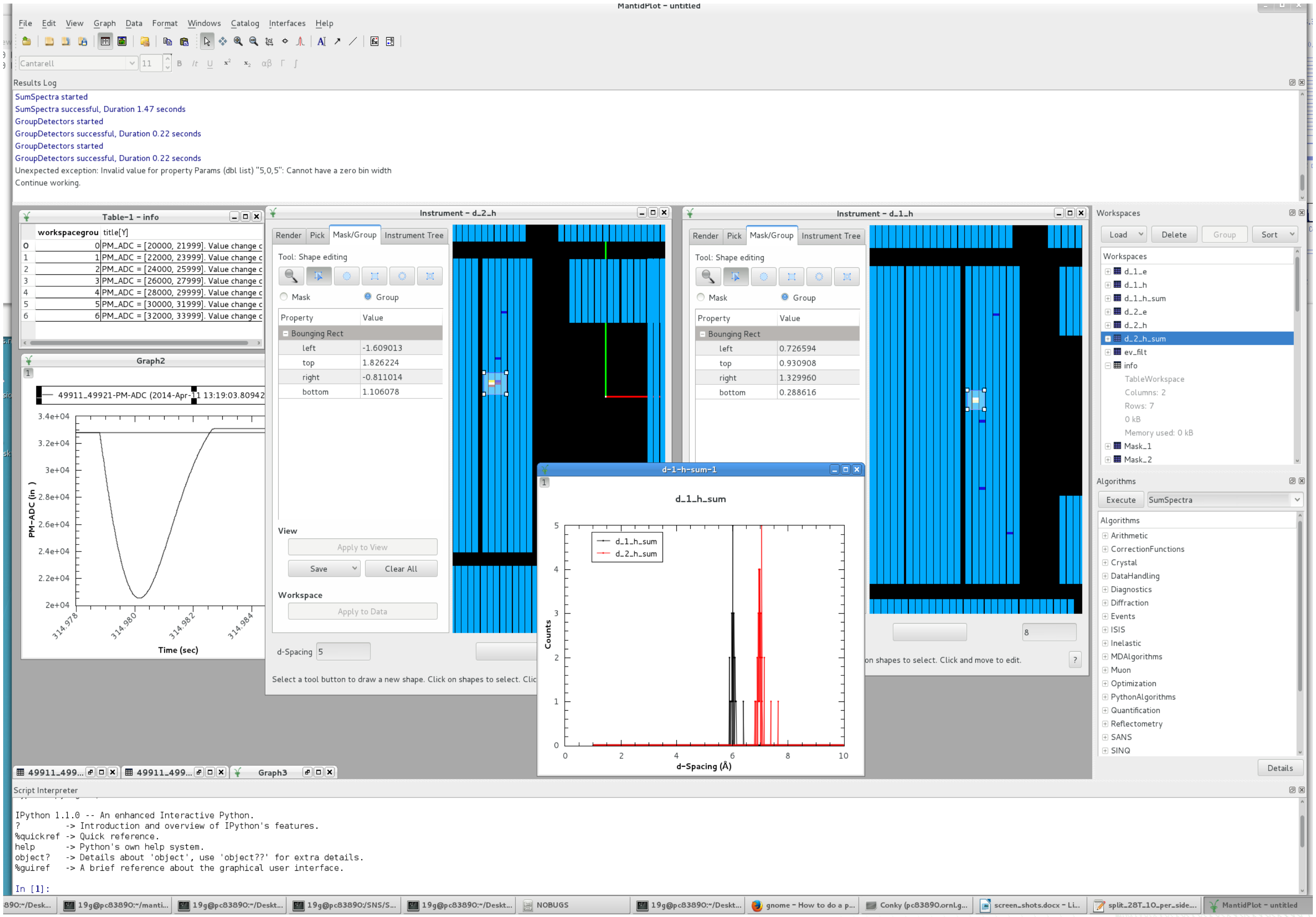
- Interface to perform the filtering



Filter fast logs – a use case



Filter fast logs – a use case



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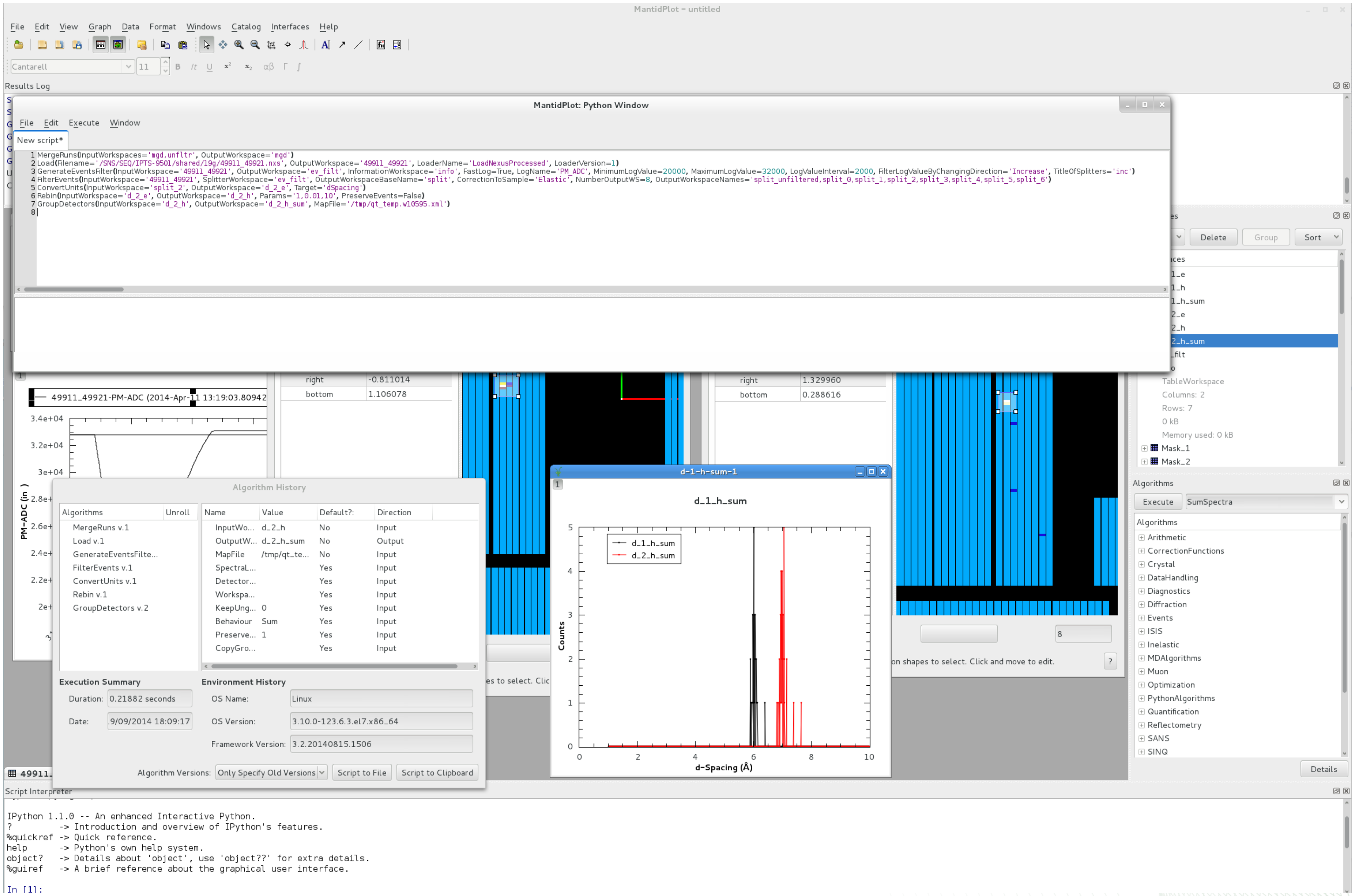
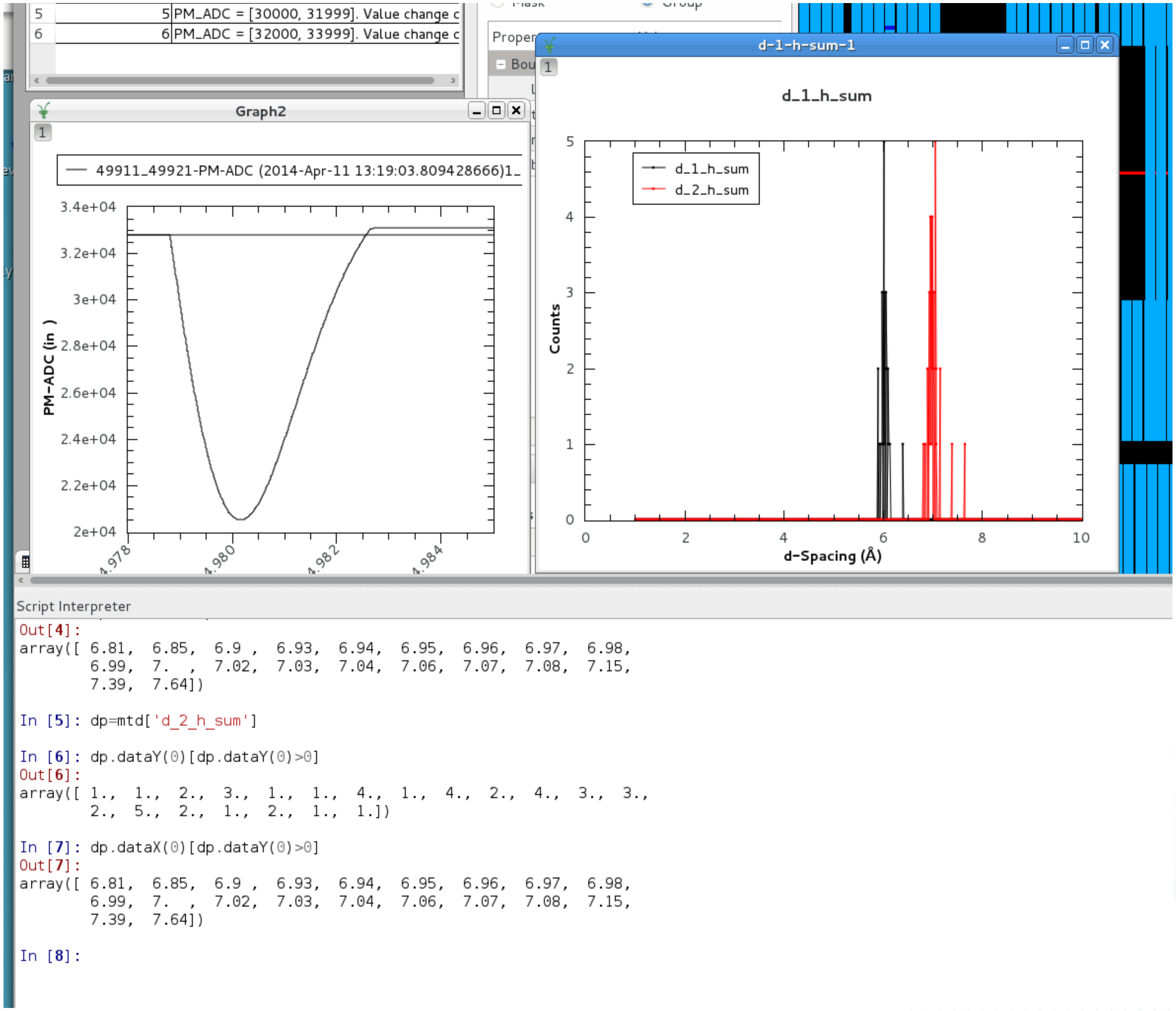
Filter fast logs – a use case



Filter fast logs – a use case



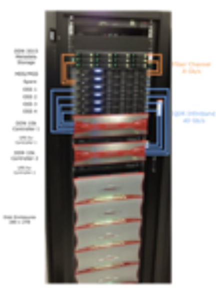
Conclusions

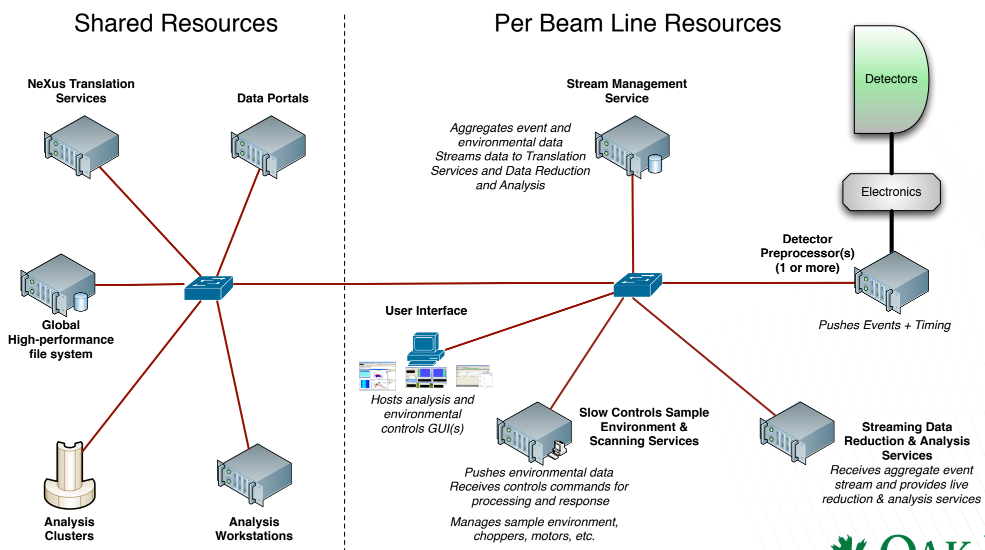
- Mantid is seeing broad use at neutron scattering factilites
- The Python API provides an straightforward and powerful interface to the Mantid Algorithms
- Event based reduction provides added scientific functionality.
- Mantidplot is interface useful for developing scientific workflows in Mantid.

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

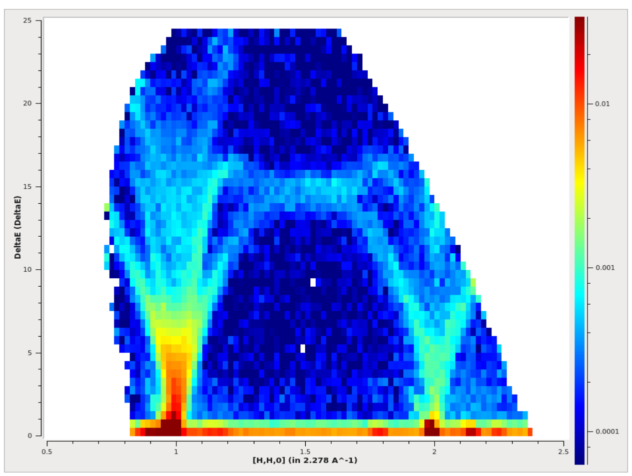


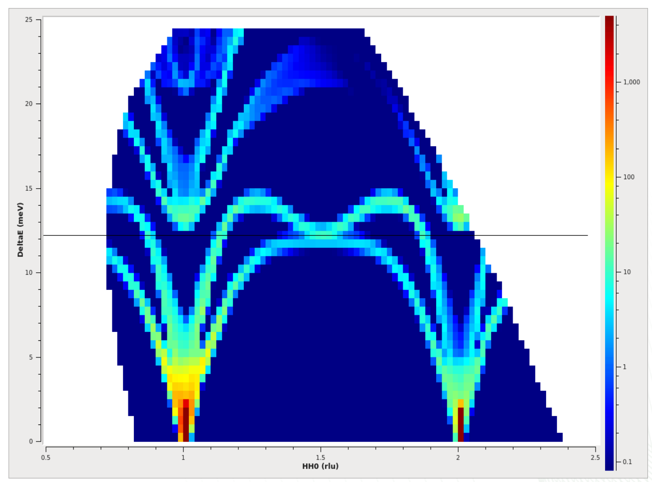


Concurrent Simulations and Experiment

- Ab-initio molecular dynamics (AIMD) simulations on the EOS cluster and experiment on $SrTiO_3$ 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.