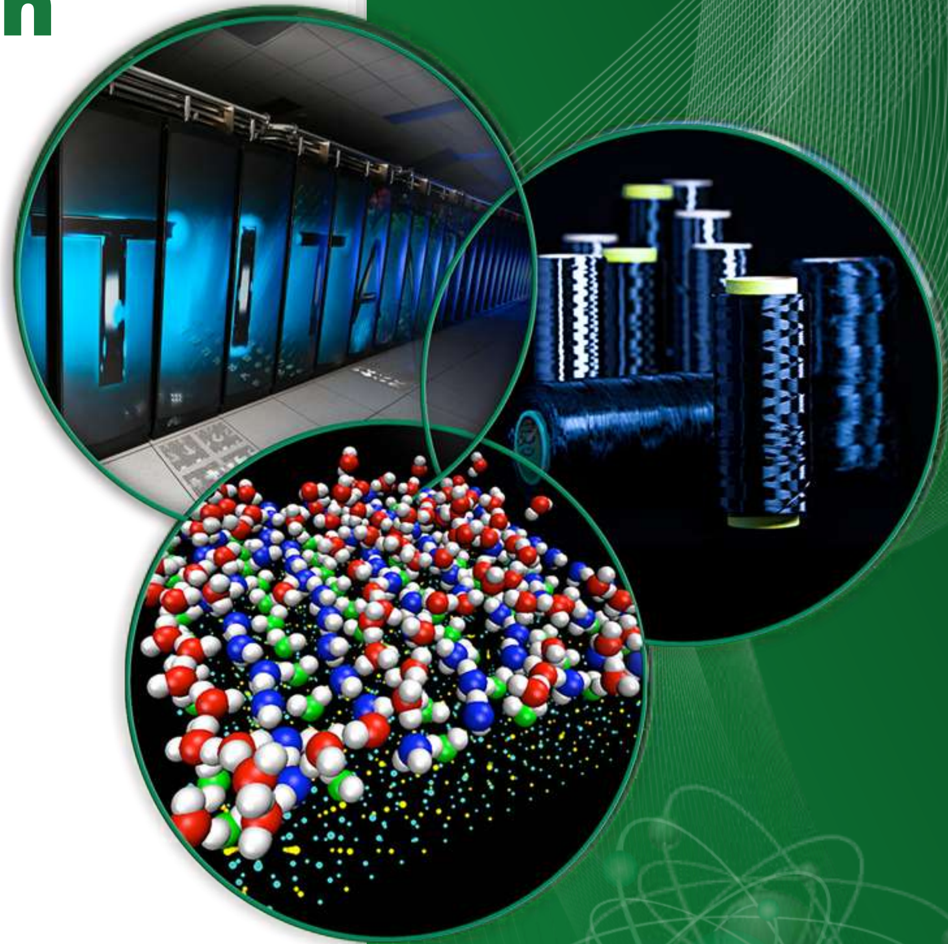
Mantid: Now and in the future



Garrett E. Granroth

Scientific Data Analysis Group Lead

Sept 26, 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

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What is Mantid?

- A Framework for Reduction and Analysis of Neutron and Muon Data
  - Can Be accessed by
    - MantidPlot
    - Python Interface
    - C++ API
  - Has a set of data objects, methods and Algorithms well suited towards scattering science

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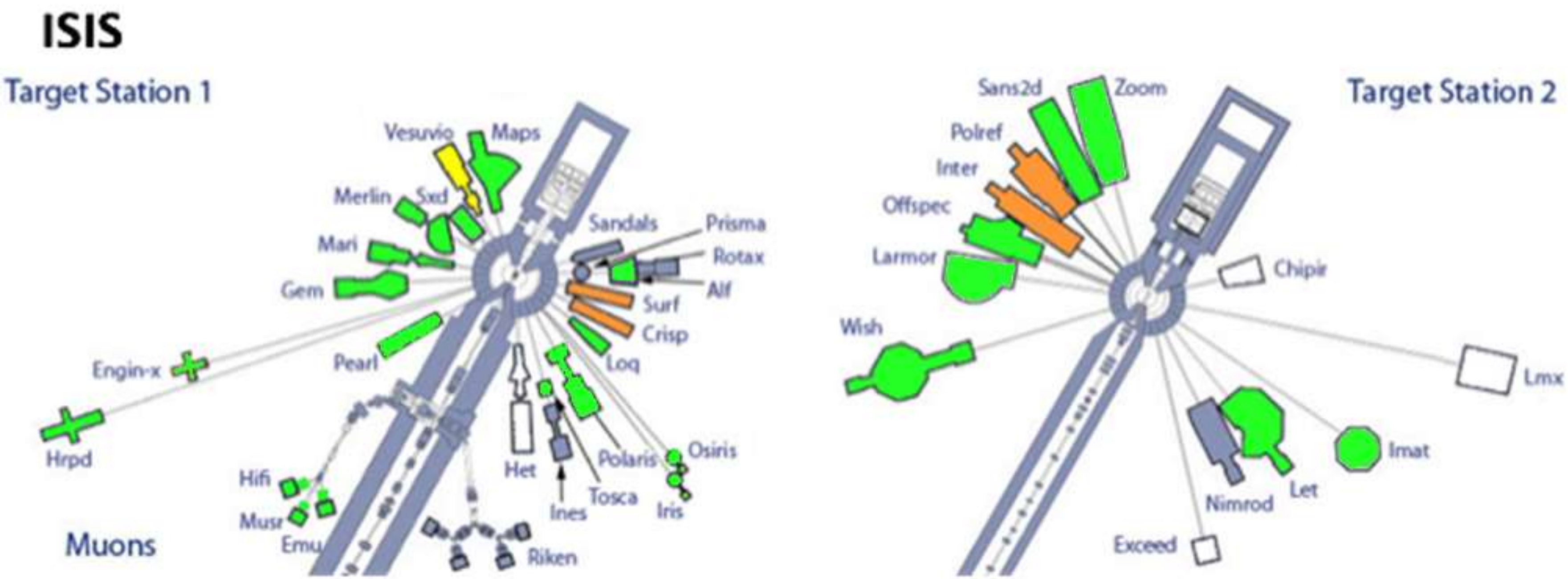
Partners and Contributors

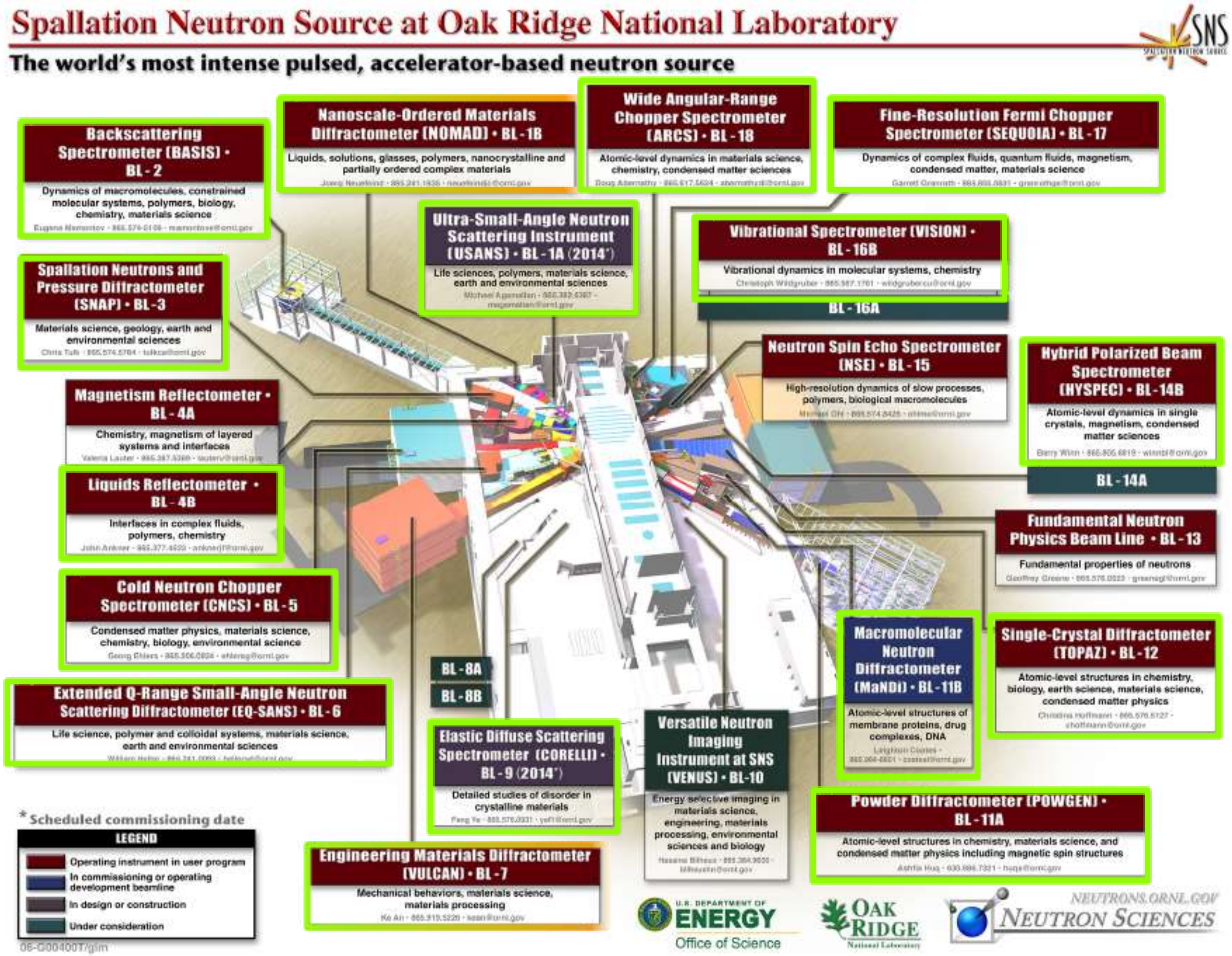
- Partners
  - ISIS
  - Oak Ridge National Laboratory | High Flux Isotope Reactor | Spallation Neutron Source
  - European Spallation Source — joining soon

- Contributors
  - Tessella Technology & Consulting
  - Paul Scherrer Institut PSI
  - ILL Neutrons for Science®
  - Orphée Laboratoire Léon Brillouin
  - McStas
  - FRM II Forschungs-Neutronenquelle Heinz Maier-Leibnitz
  - ansto
  - LANSCE Lujan Center Los Alamos National Laboratory

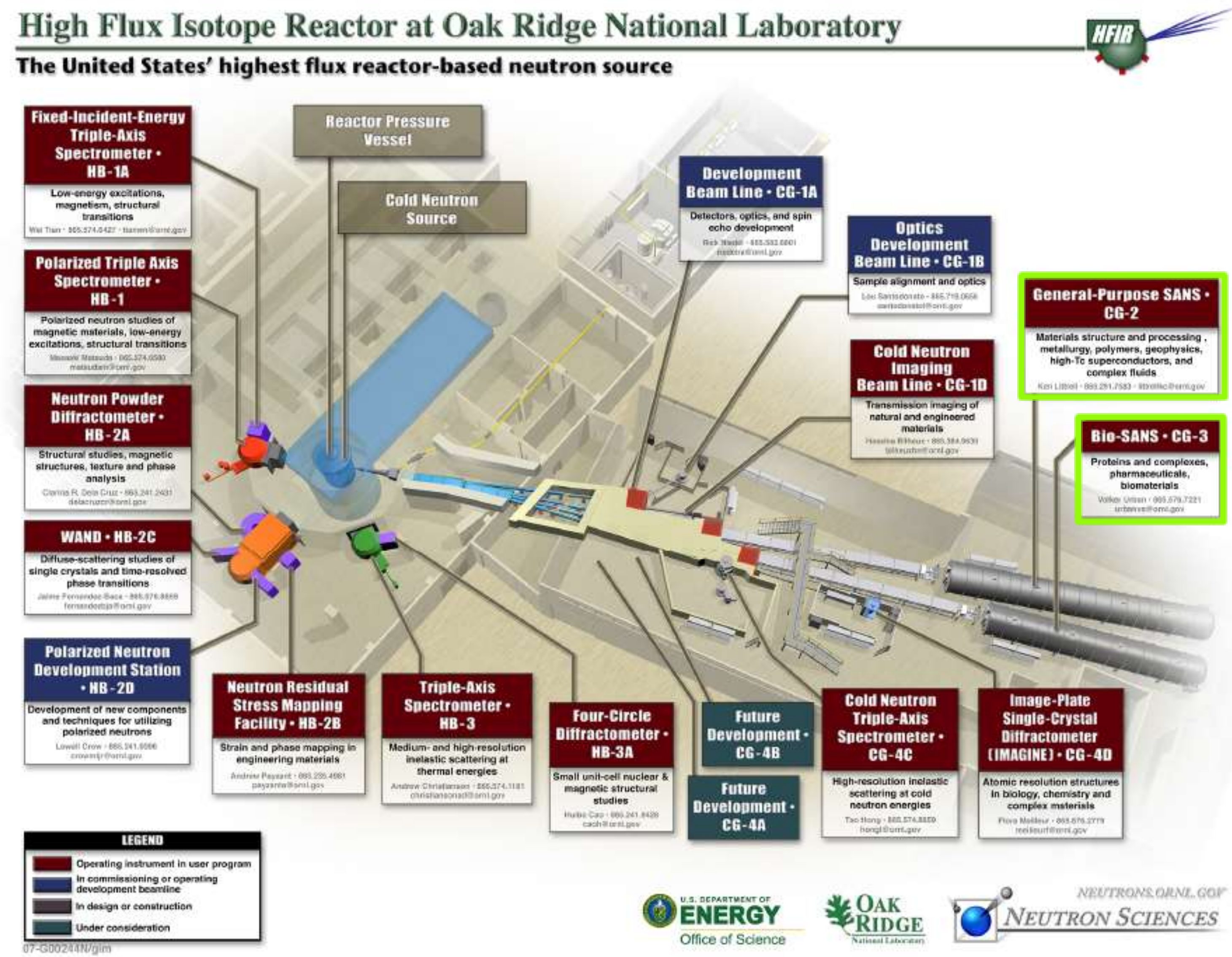
Deployment at ISIS



Deployment at SNS



Deployment at HFIR



Other instruments

- NMI3 supported evaluation
- IN4,5 & 6
- D33

- Focus
- Poldi

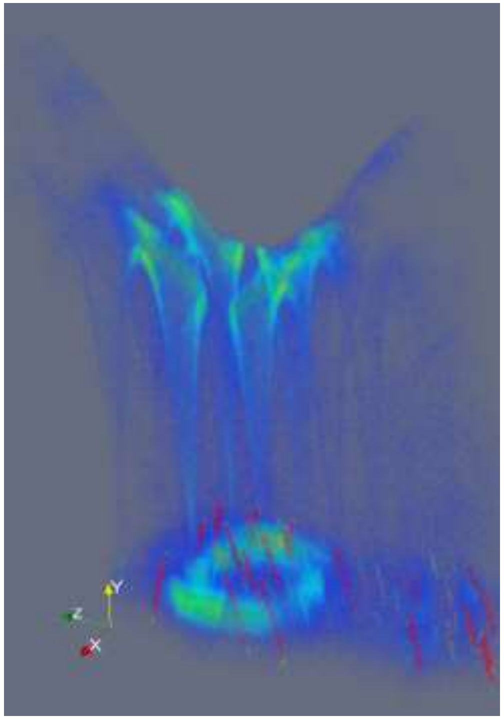
- Mibemol

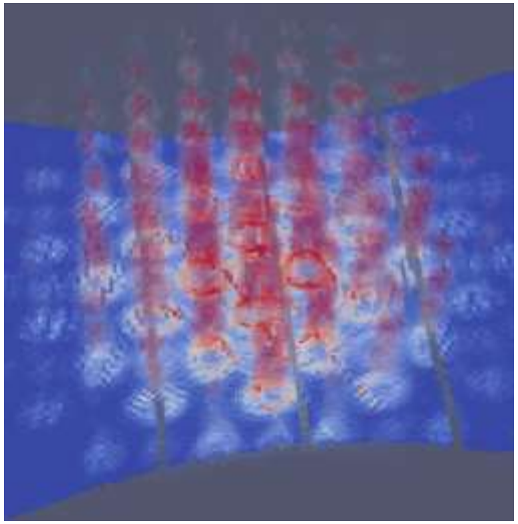
- TofTof

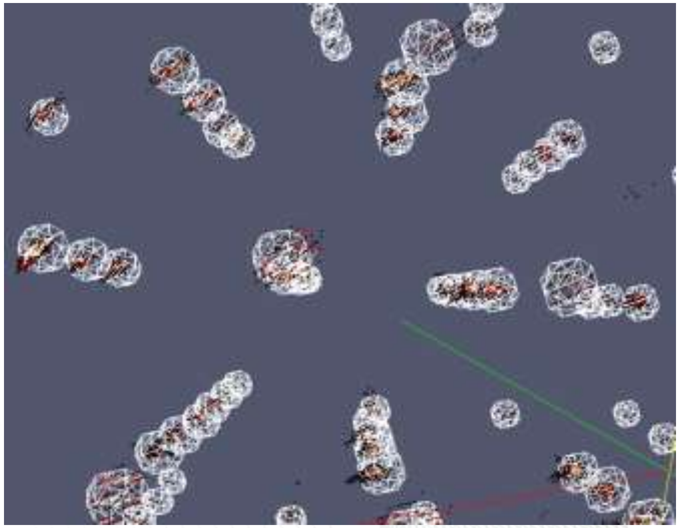
- Pelican
- Bilby

Advanced Visualization

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



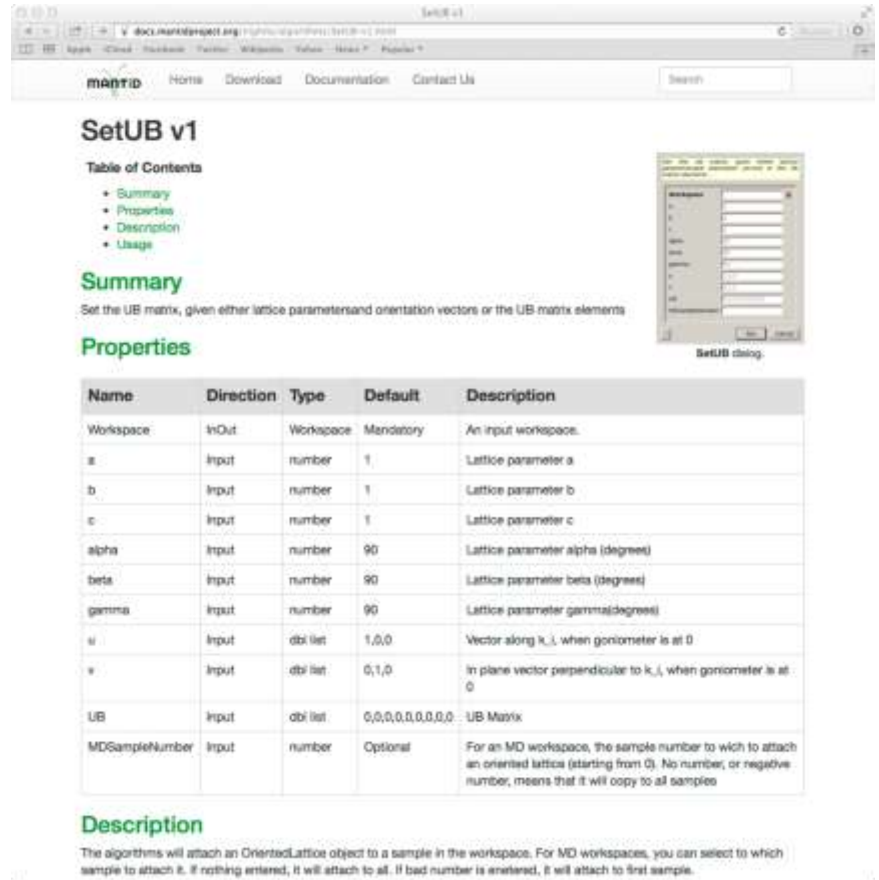




Improved Sphinx based documentation

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::
```



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SetUB v1

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Summary

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

SetUB dialog.

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.

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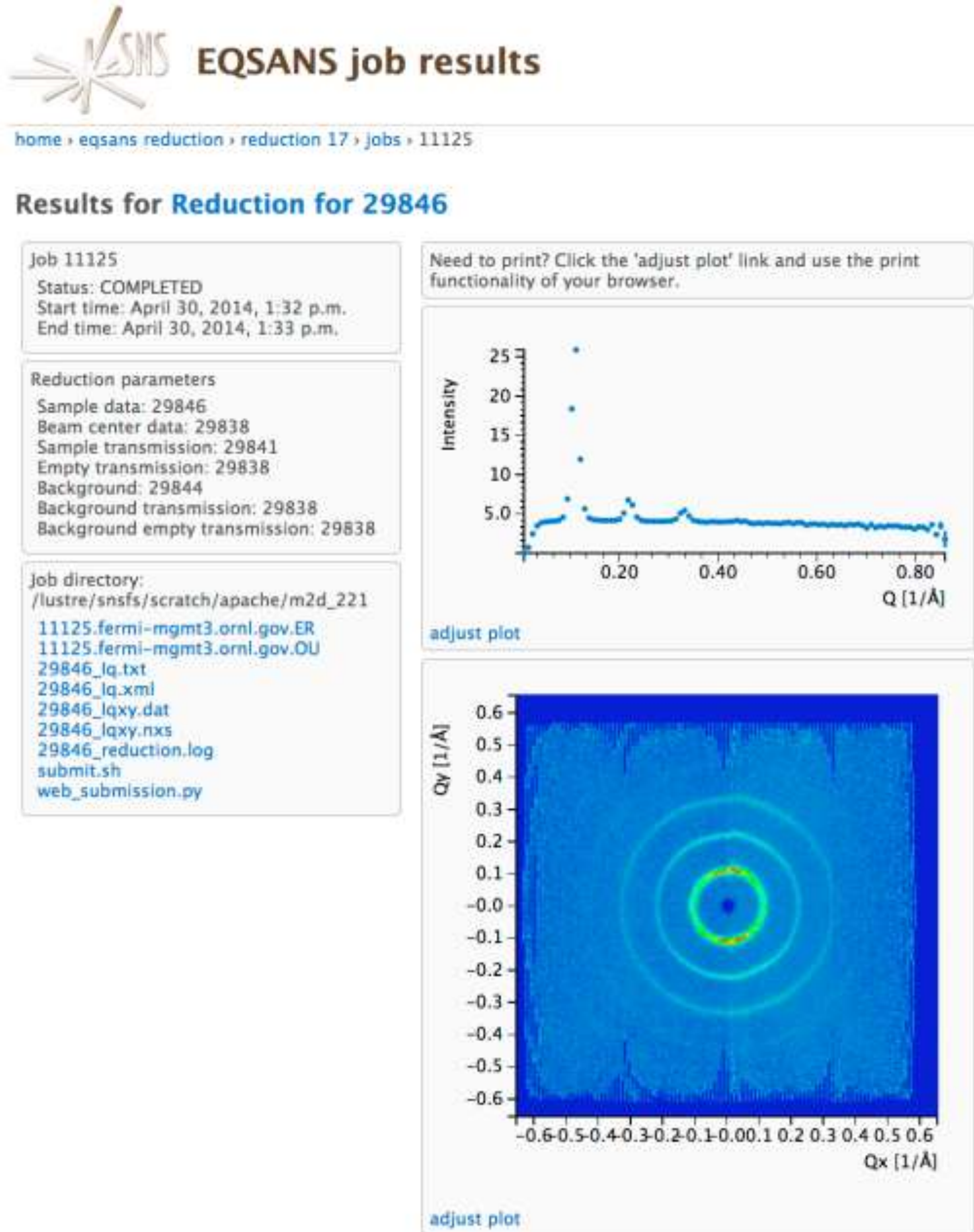
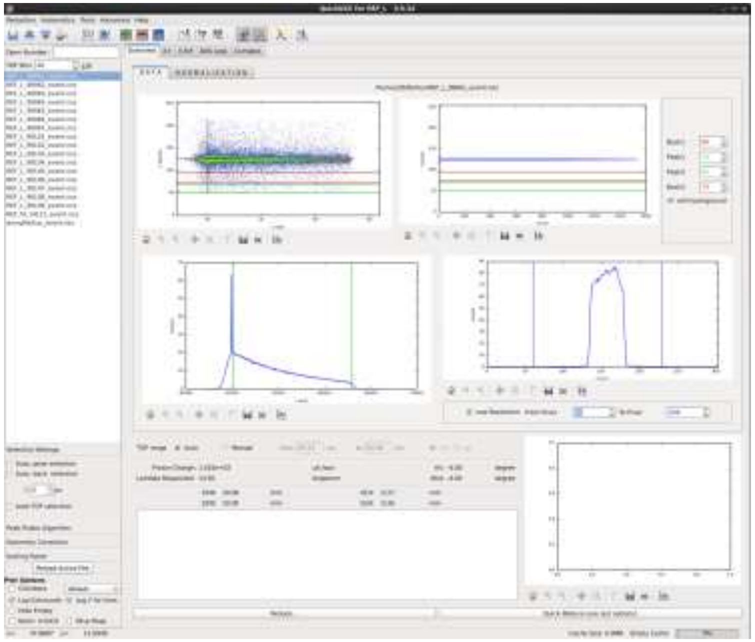
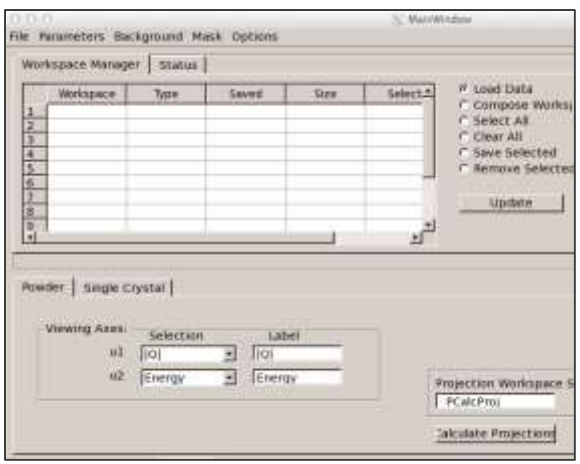
Python API - auto reduction

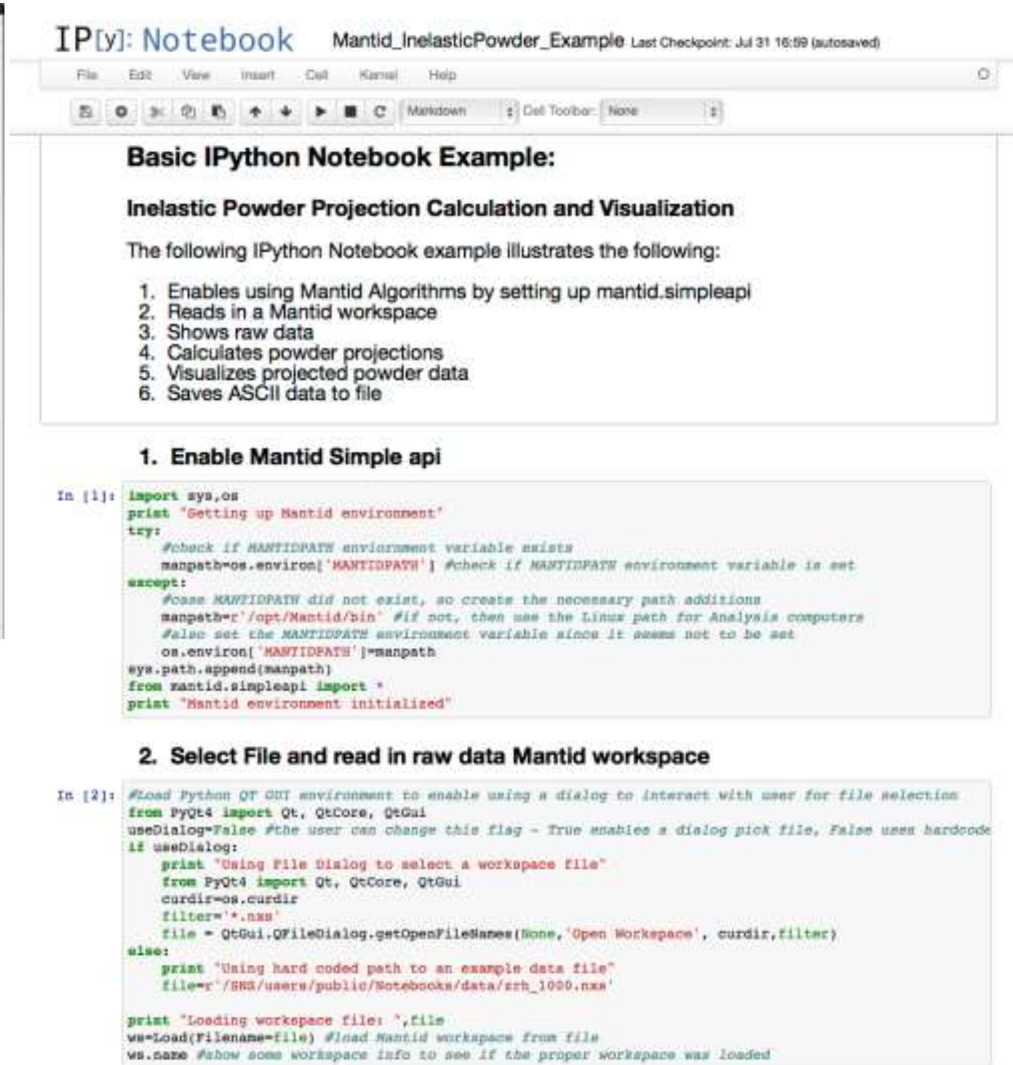


- Simple shell driven script after a run completes
- Introduced as a help
- Users now expect autoreduction to work.
- Prototyping web driven reduction

Python API – use your favorite interface







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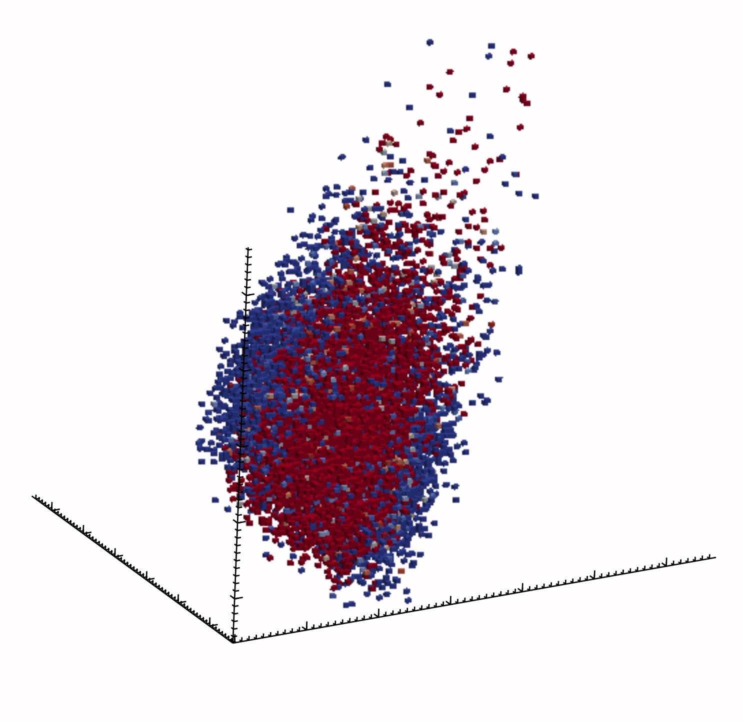
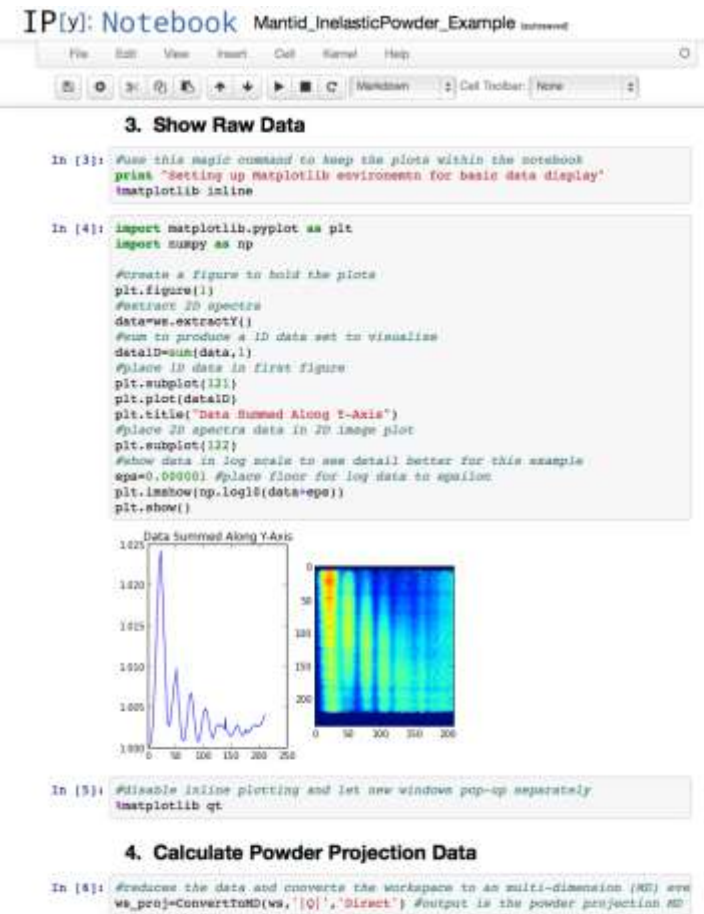
Python API - get data in and out





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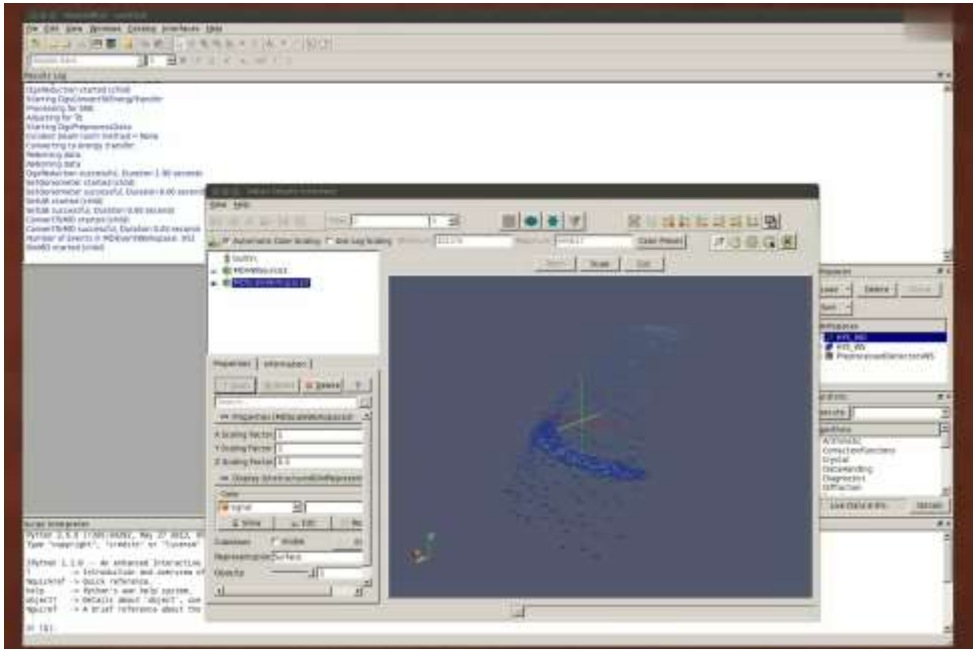
Live Data

- 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
- Currently working through normalization of different statistic runs
  - Some algorithms can be challenging
- Allows for pump probe filter experiments

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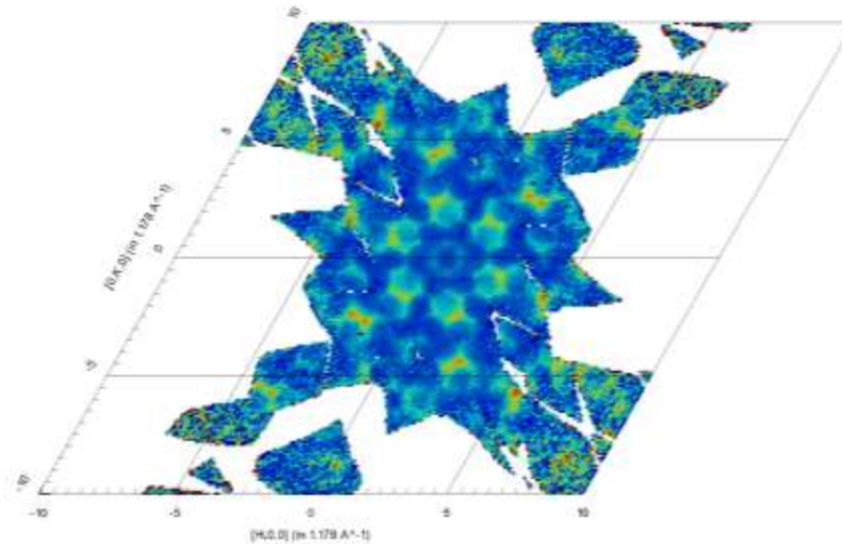
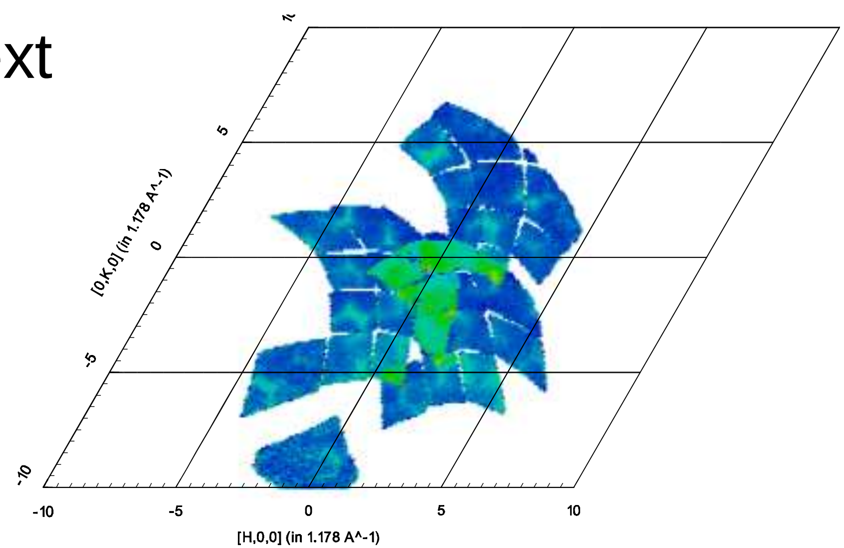
Event Diffraction Data Normalization

- Most Challenging for diffraction
  - Different Incident flux for every incident wavelength /time bin

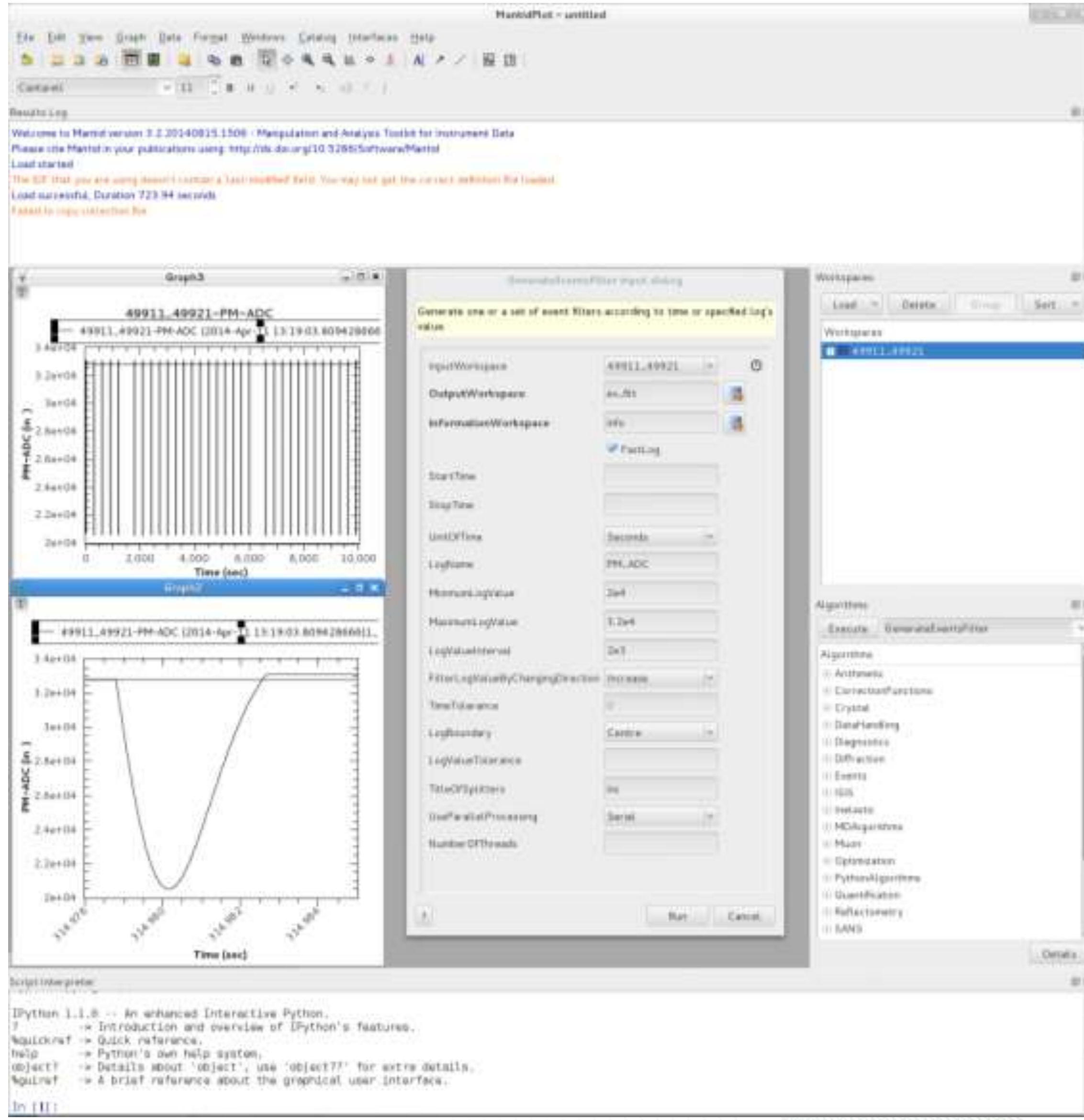


- Moving to inelastic next
  - Much faster than histograms



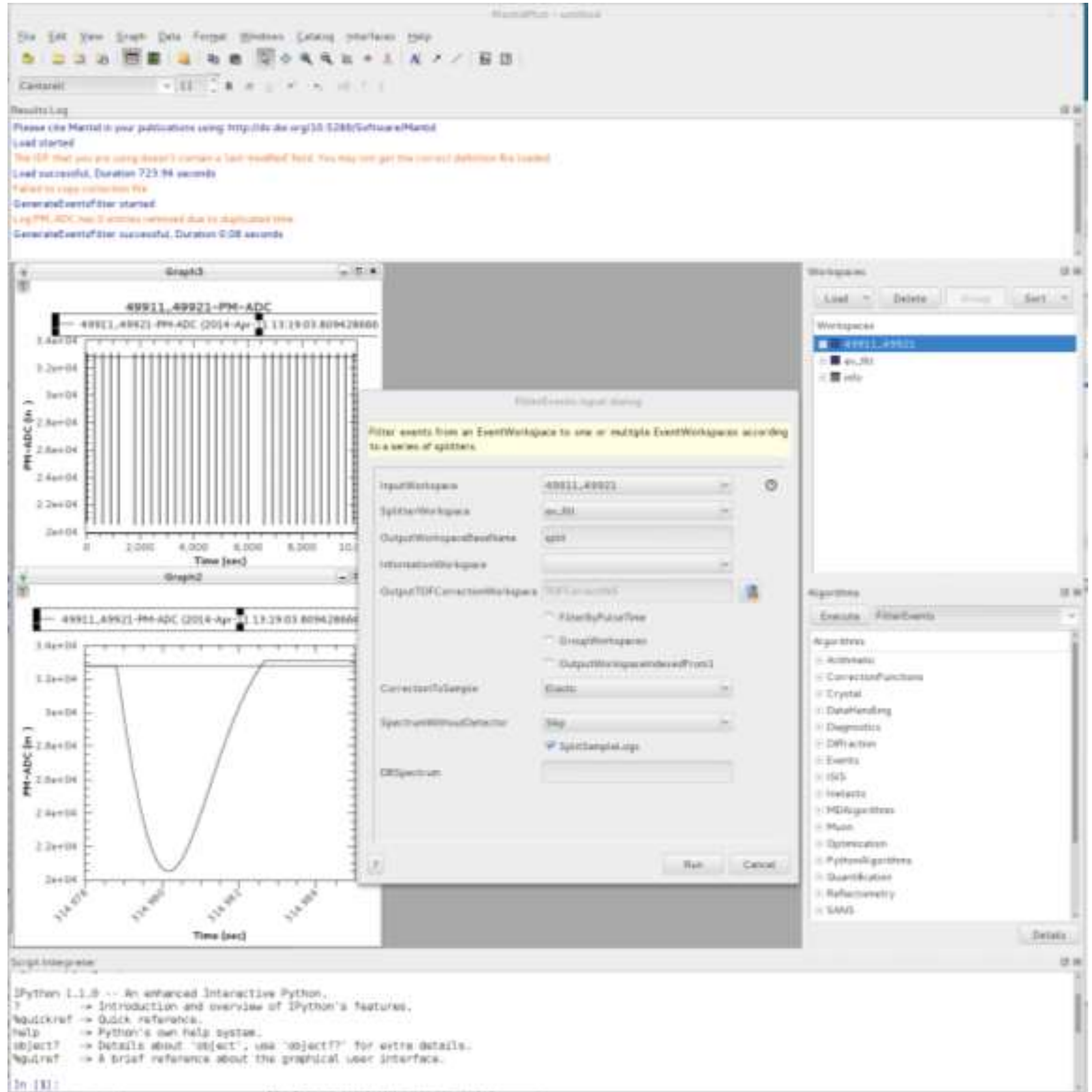
Filter fast logs – a use case

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

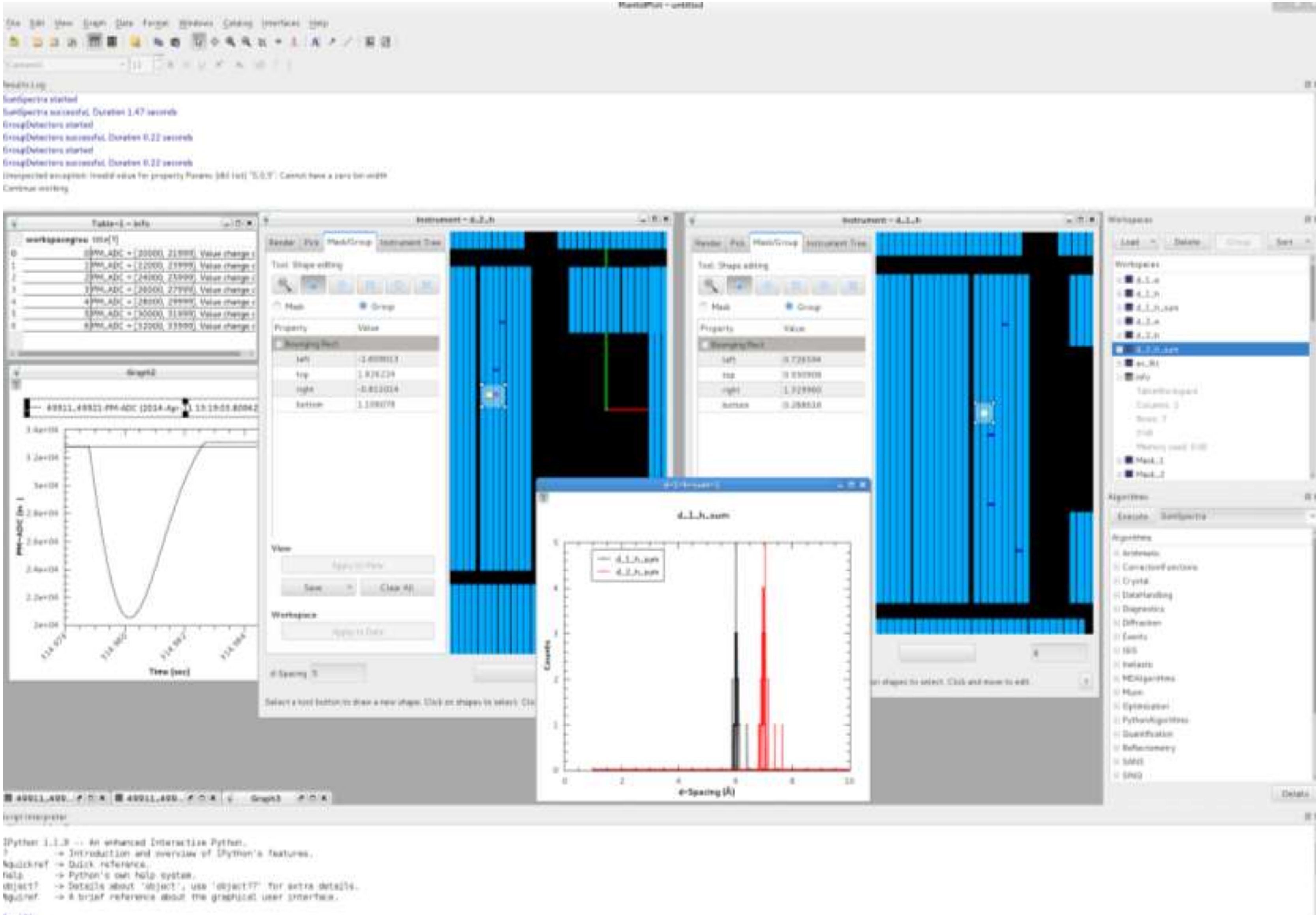


Filter fast logs – a use case

- Interface to perform the filtering



Filter fast logs – a use case



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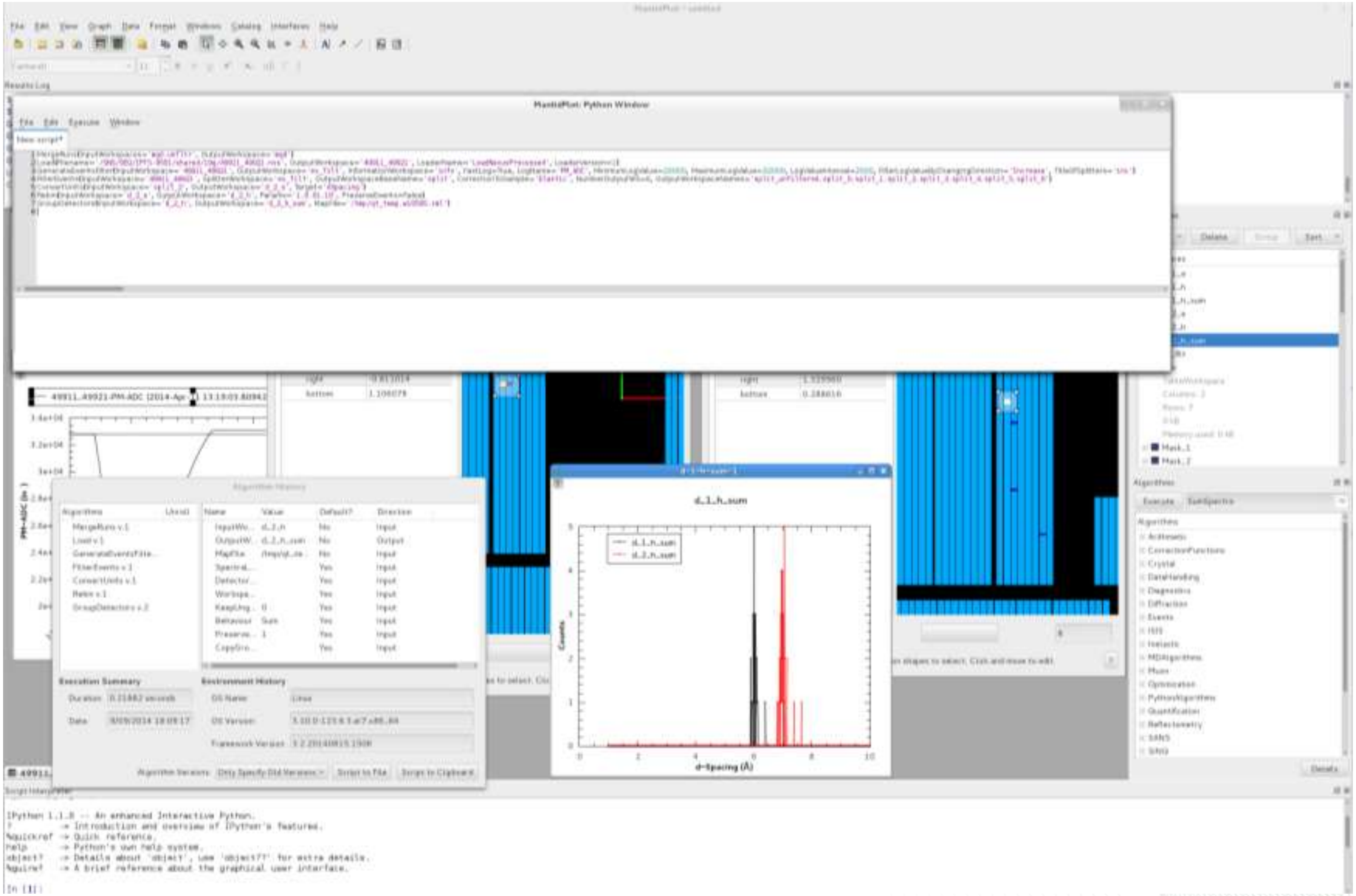
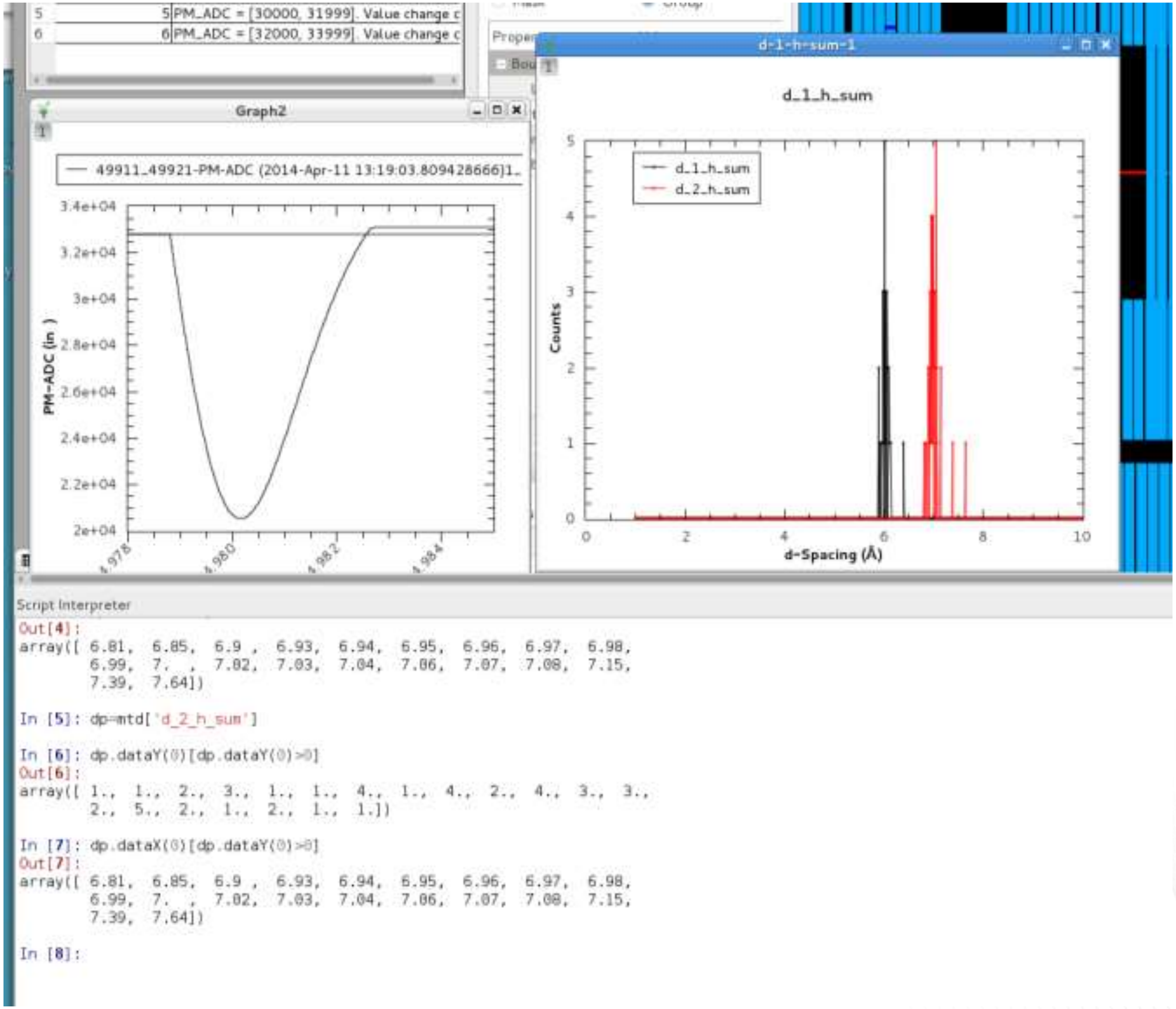


Filter fast logs – a use case



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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 an interface useful for developing scientific workflows in Mantid.