A Python-based approach to interactive x-ray and neutron data analysis

How an ex-programming scientist recovered his mojo

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with special thanks to
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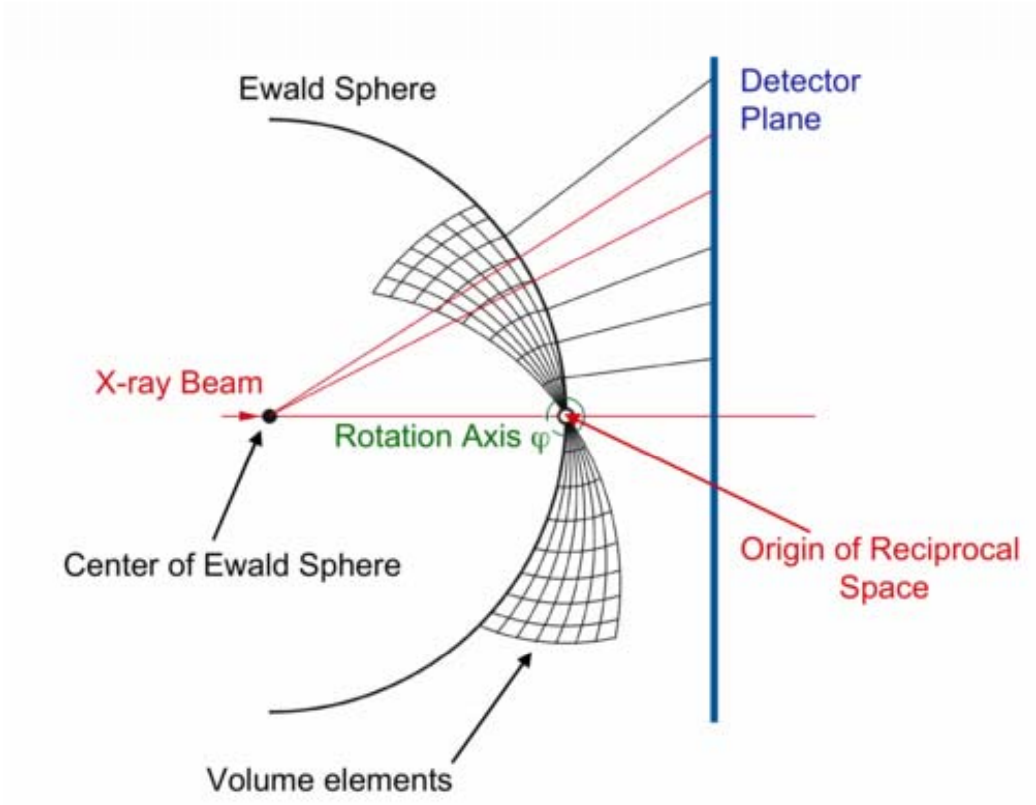
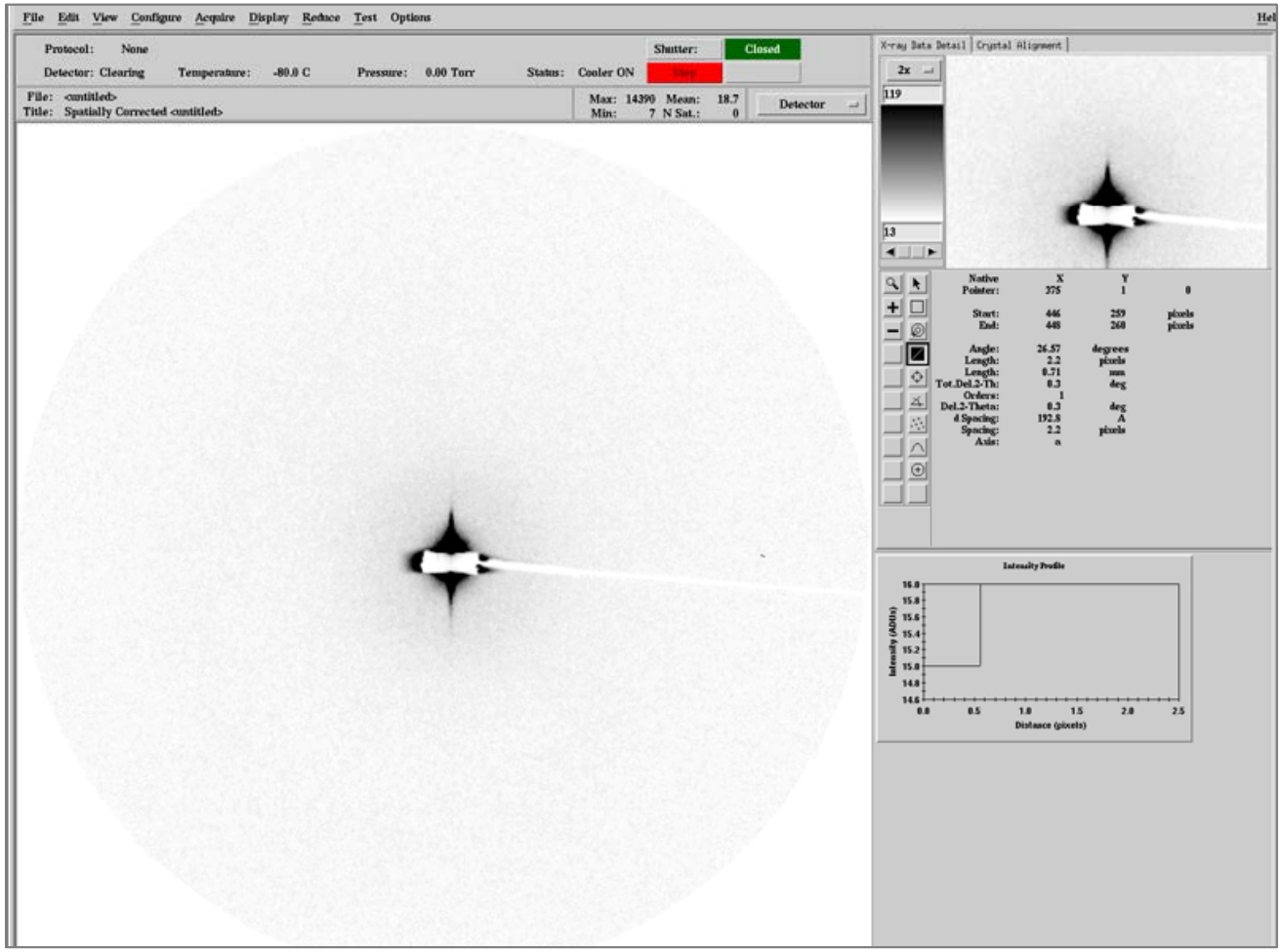
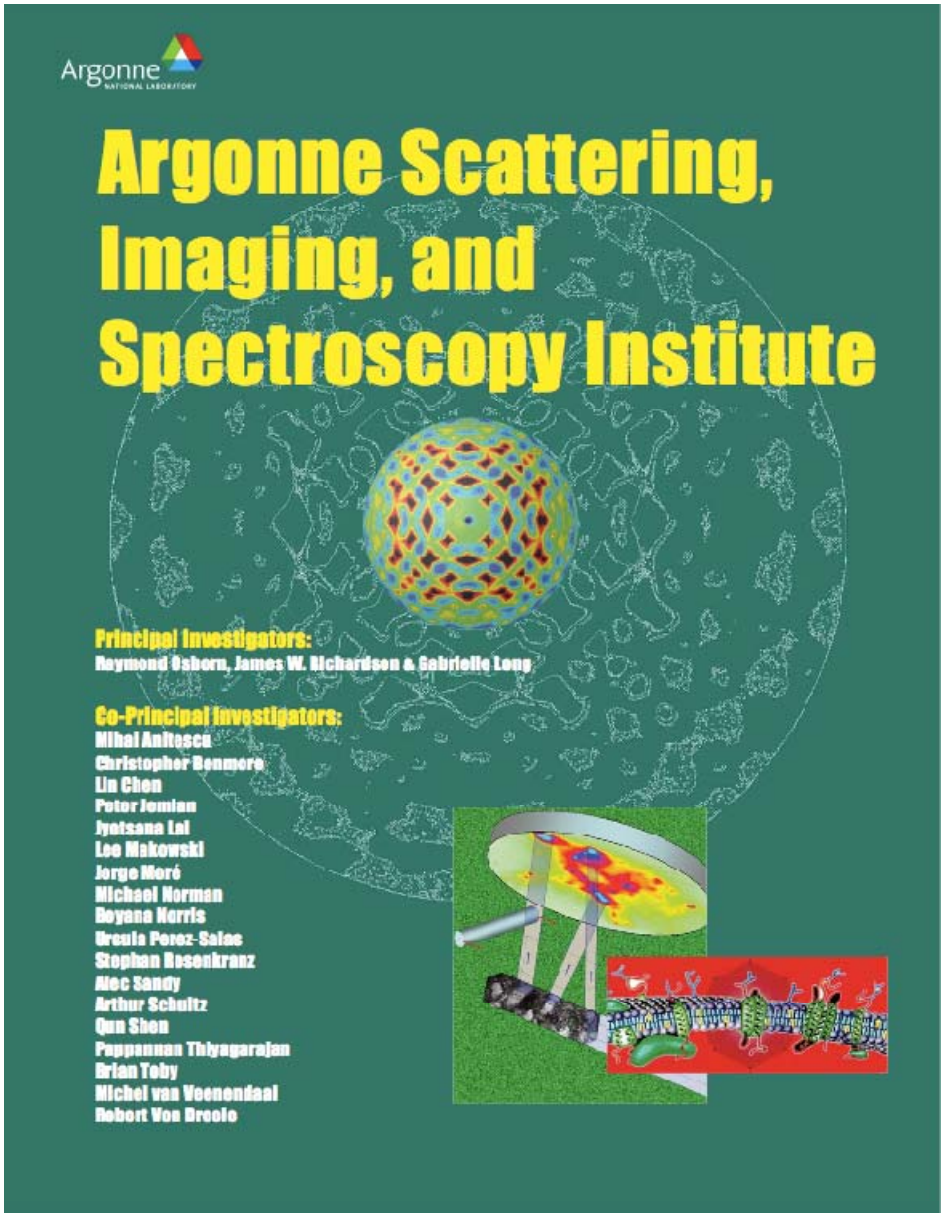
Where we want to be



QuickTime™ and a
Microsoft Video 1 decompressor
are needed to see this picture.

Where we are


File Edit View Configure Acquire Display Reduce Test Options
Protocol: None
Shutter: Closed
Detector: Clearing Temperature: -80.0 C Pressure: 0.00 Torr Status: Cooler ON
File: <untitled>
Title: Spatially Corrected <untitled>
Max: 14390 Mean: 18.7
Min: 7 N Sat.: 0
Detector
X-ray Data Detail
Crystal Alignment
2x
119
13
Intensity Profile
Intensity (ADUs)
Distance (pixels)


Argonne
NATIONAL LABORATORY
Argonne Scattering, Imaging, and Spectroscopy Institute
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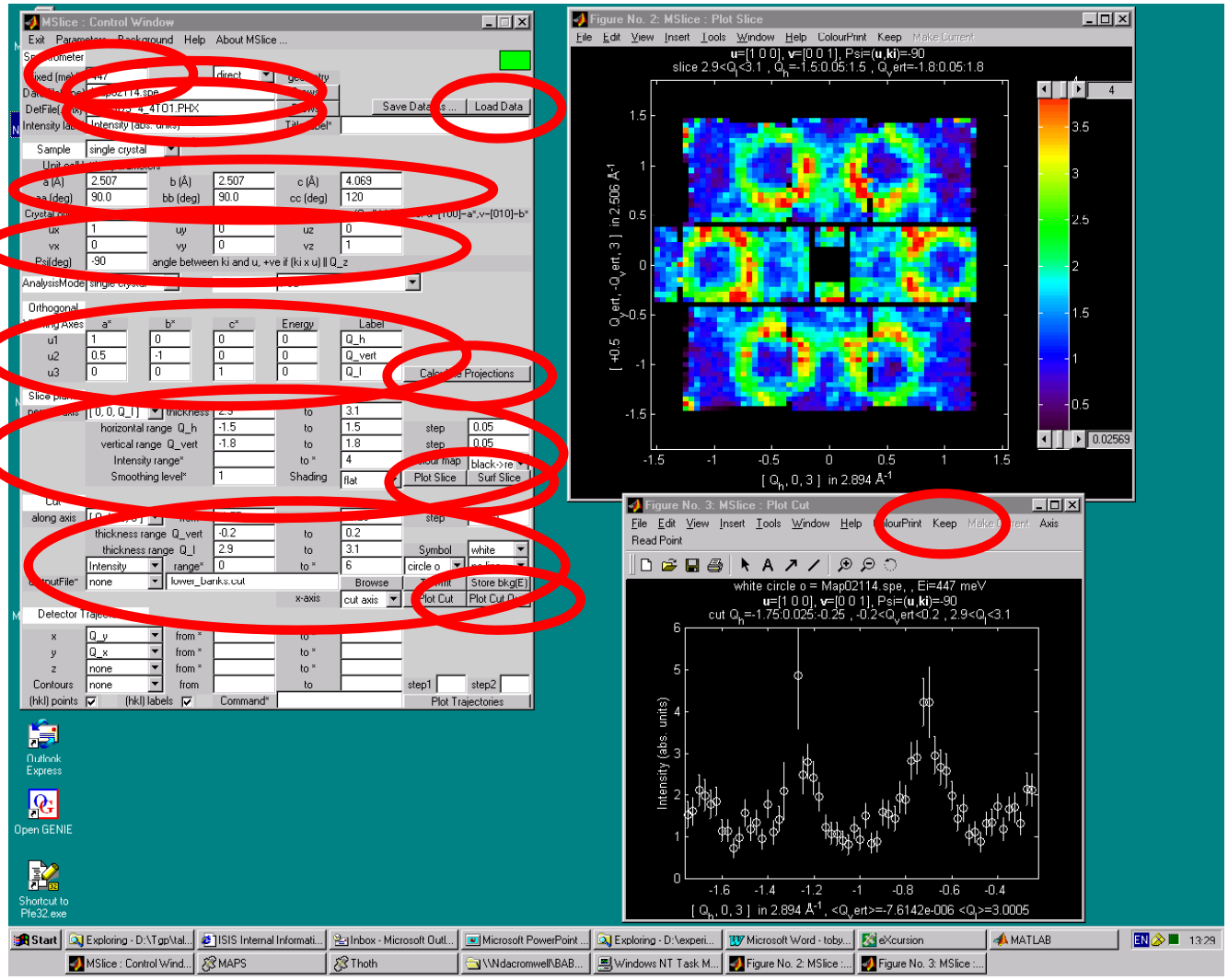
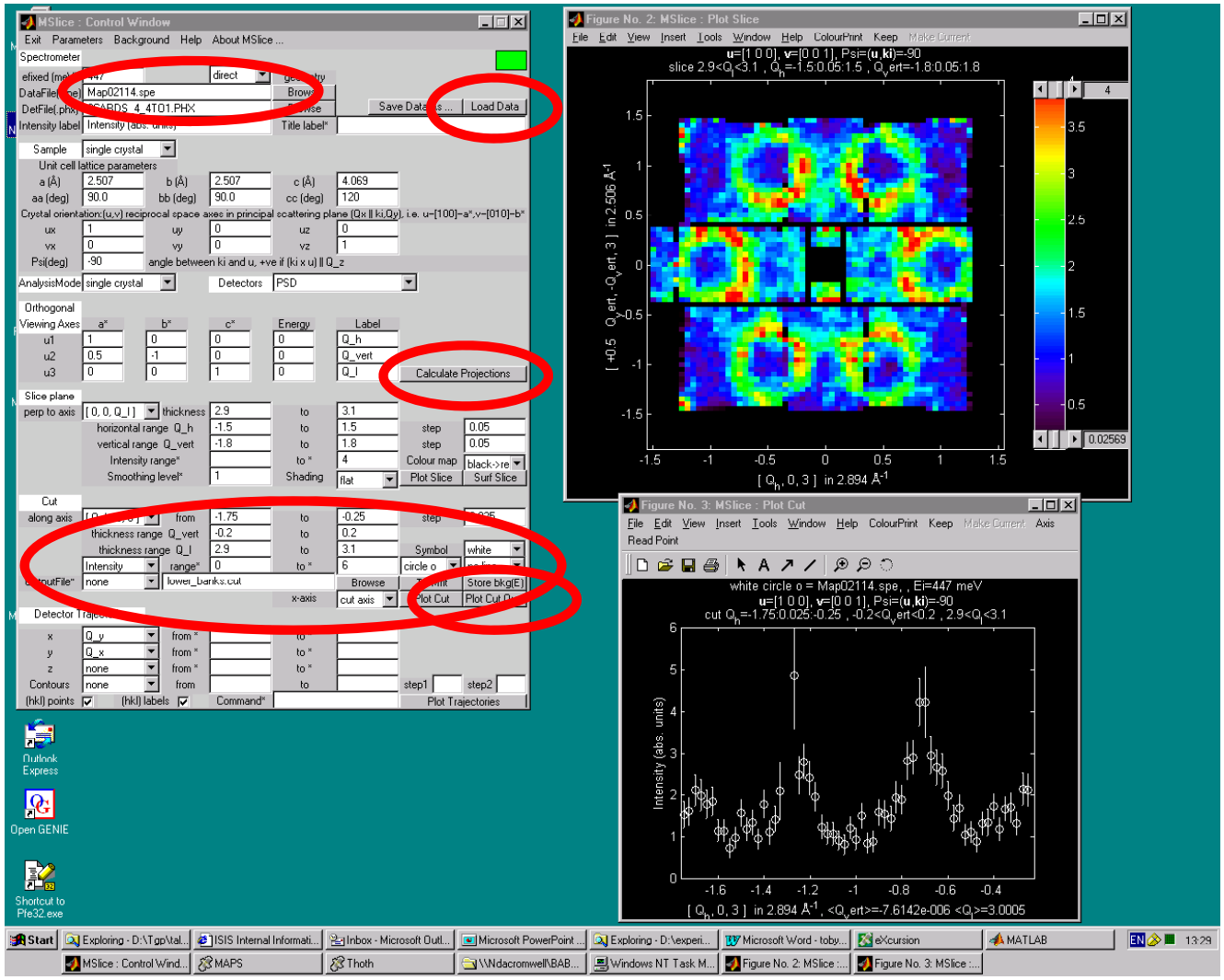
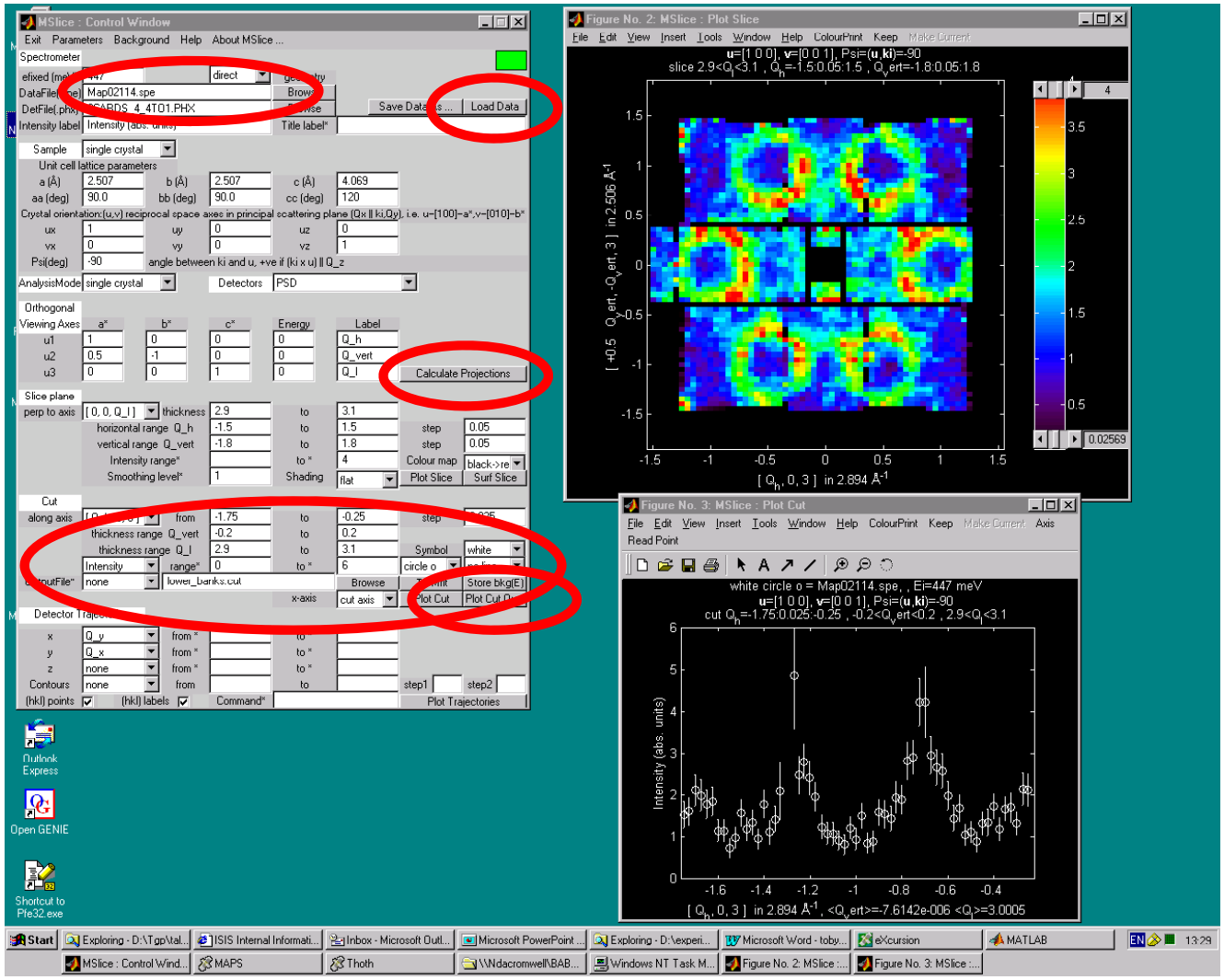
Interactive Friction



Interactive Friction (Take II)



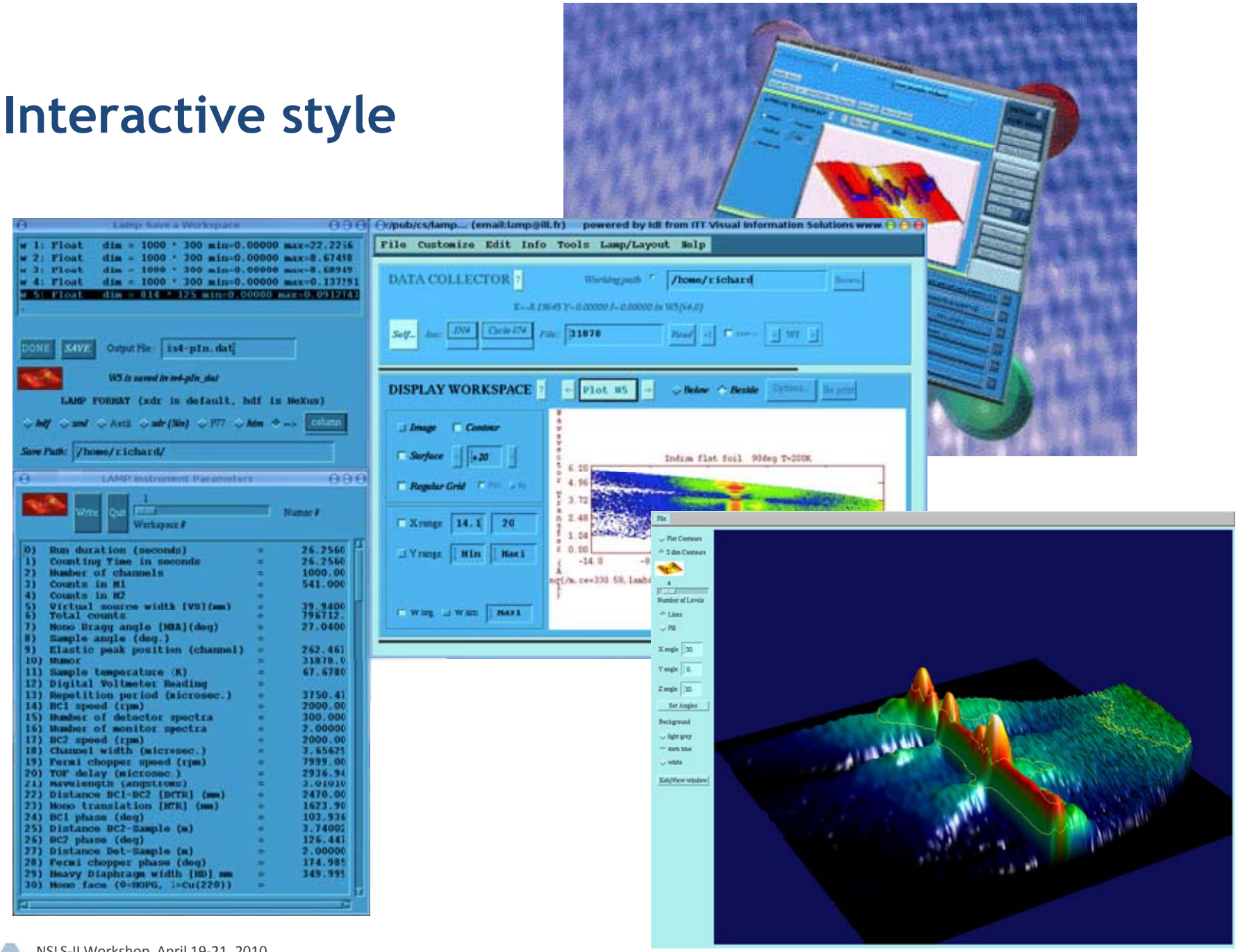
Interactive Friction (Take III)



Issues

- Repetitive workflow
- Insufficient data persistence
- Poor integration with previous analysis (or operating system)
- Lack of automation (scripting)
- No memory management
- Use of proprietary language

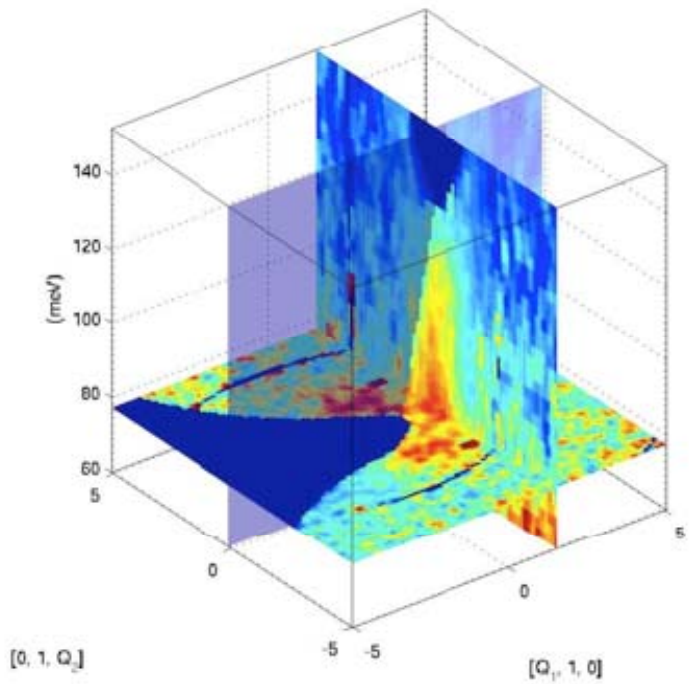
Interactive style



Issues

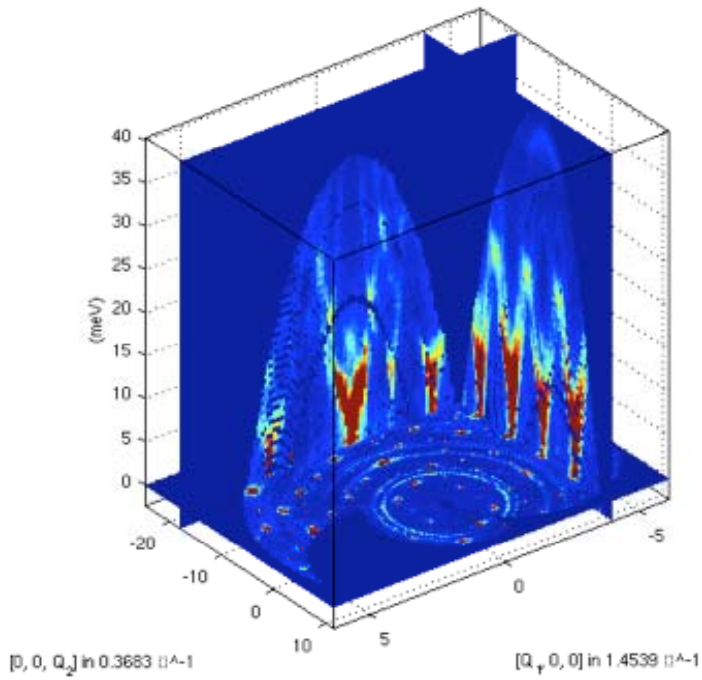
- Inadequate data model
- Insufficient and inconsistent access to instrumental metadata
- Use of proprietary language

Measurements of S(Q,ω) at ISIS (Horace-mode)



Magnetic Fluctuations in MnSi

R.A.Ewings, T.G.Perring (ISIS) unpublished



Lattice vibrations in calcite ($CaCO_3$)

Beth Cope, Martin Dove (Cambridge) unpublished

Issues

- Never, ever, define a “temporary” file format.

Problems to address

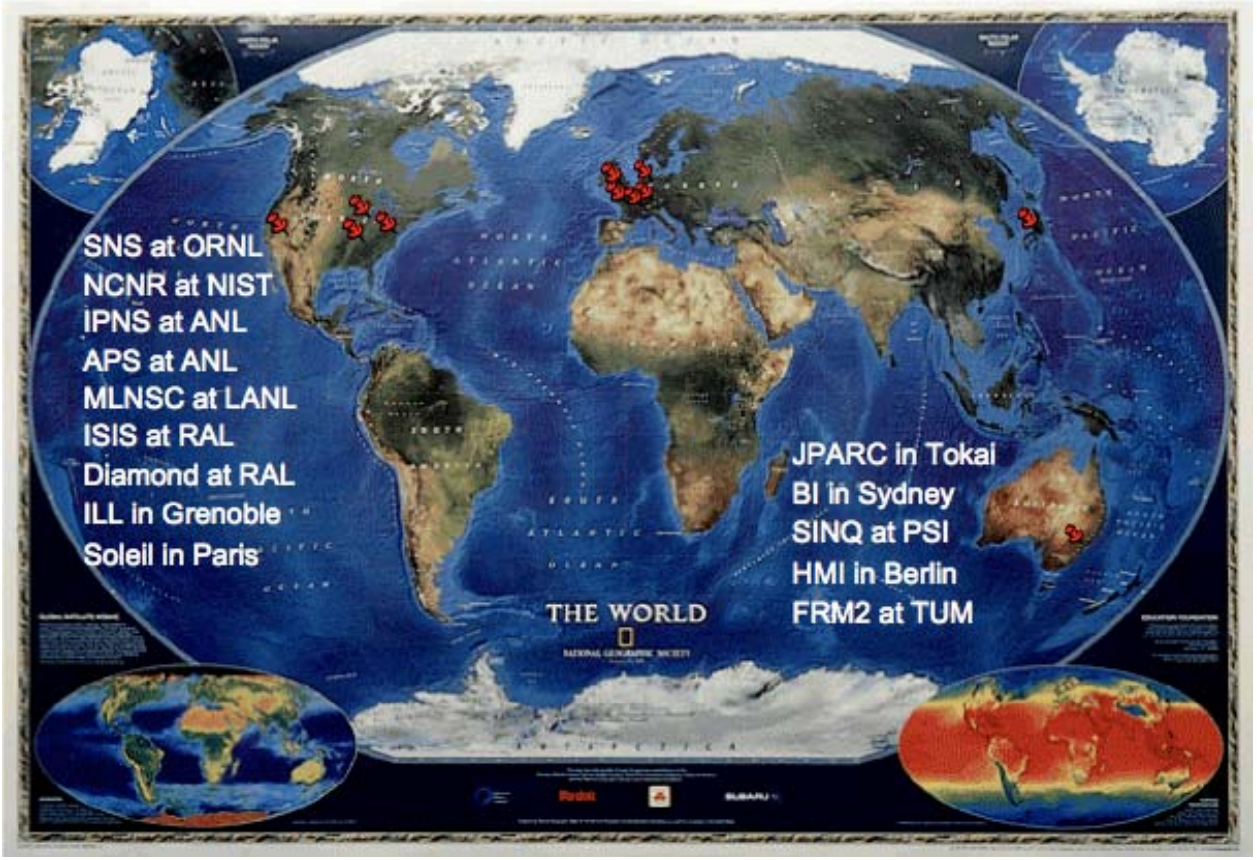
- Ensure that the workflow does not actively discourage data analysis
- Store the results of data analysis as long as needed (not limited by memory)
- Ensure that all relevant instrumental metadata is carried with the analysis
- Allow all repetitive actions to be scripted by the user
- Do not use proprietary languages and packages unless the functionality really demands it

NeXpy - a Python-based approach

- What NeXpy is not:
  - a comprehensive solution to all the issues so far raised
  - particularly sophisticated or novel
- What NeXpy is:
  - a toolbox for manipulating and visualizing arbitrary NeXus data
  - a possible scripting engine for GUI applications
  - a demonstration of the value of combining:
    - a flexible data model
    - a powerful scripting language

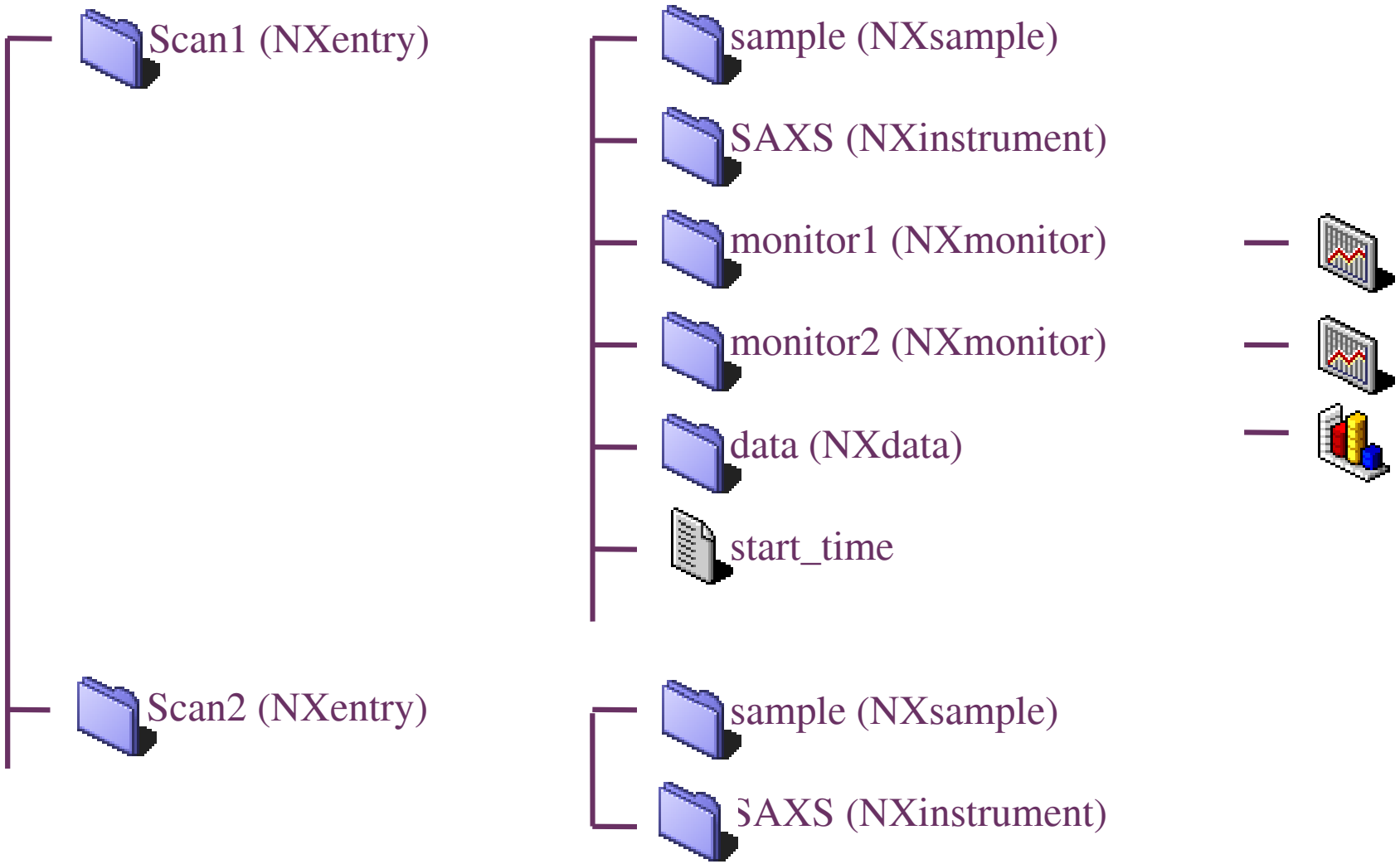
NeXus + NumPy

NeXus



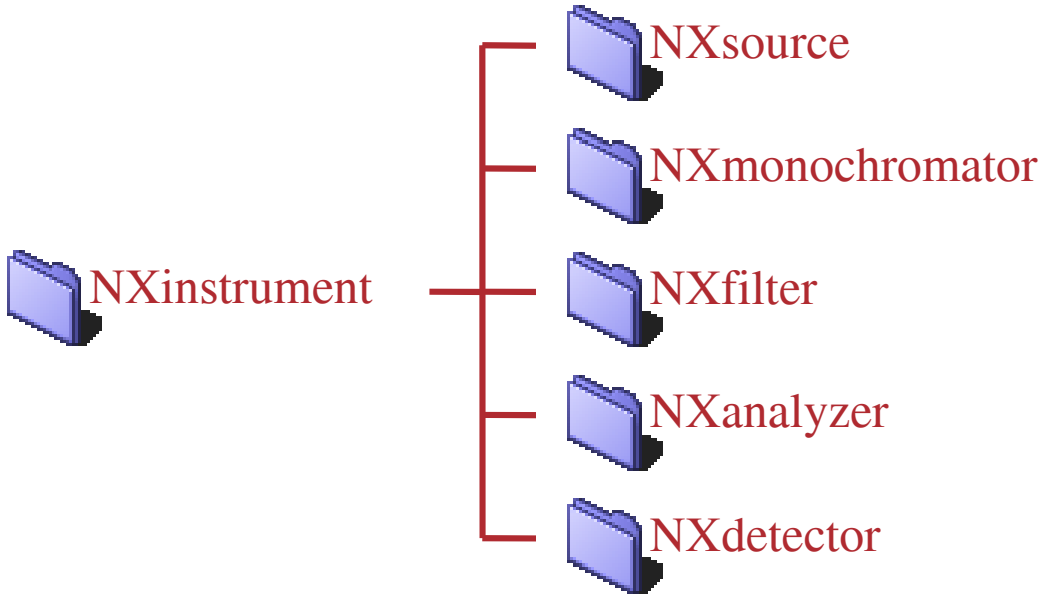
- The NeXus International Advisory Committee represents 16 international facilities and institutions
- If you want to use HDF5, there is no reason not to use the NeXus design principles
- If there are deficiencies in NeXus, join the NeXus mailing list and make a nuisance of yourself

NeXus Hierarchy

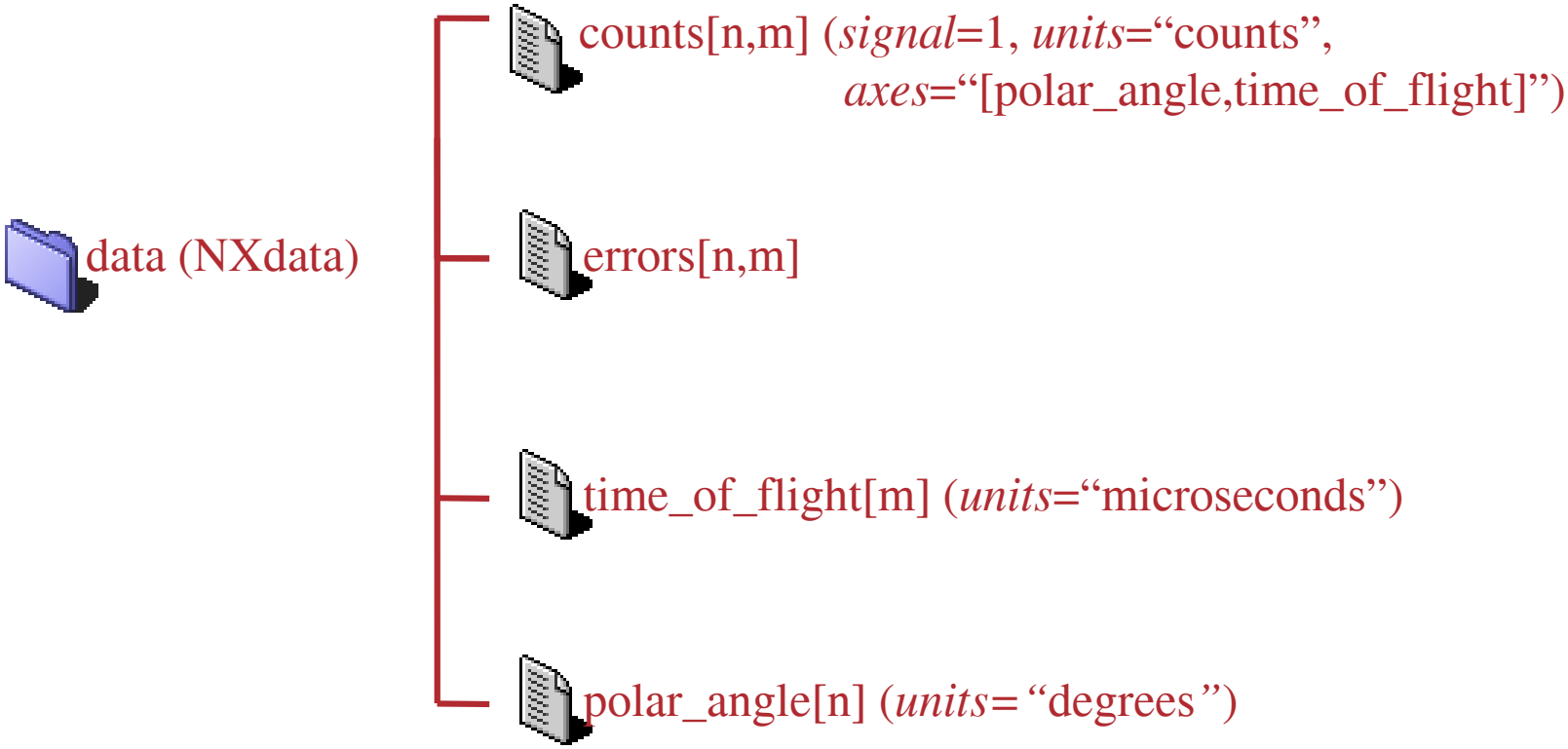


Simplest NeXus File

NXinstrument



NXdata Structures



Numpy

Array manipulation routines — NumPy v1.5.dev8106 Manual (DRAFT)

http://docs.scipy.org/doc/numpy/reference/routines.array-manipulation.html

numpy

Numpy and Scipy Documentation » NumPy Reference » Routines »

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Array manipulation routines

Changing array shape

reshape(a, newshape[, order])	Gives a new shape to an array without changing its data.
ravel(a[, order])	Return a flattened array.
ndarray.flat	A 1-D iterator over the array.
ndarray.flatten([order])	Return a copy of the array collapsed into one dimension.

Transpose-like operations

rollaxis(a, axis[, start])	Roll the specified axis backwards, until it lies in a given position.
swapaxes(a, axis1, axis2)	Interchange two axes of an array.
ndarray.T	Same as self.transpose(), except that self is returned if self.ndim < 2.
transpose(a[, axes])	Permute the dimensions of an array.

Changing number of dimensions

atleast_1d(*arys)	Convert inputs to arrays with at least one dimension.
atleast_2d(*arys)	View inputs as arrays with at least two dimensions.
atleast_3d(*arys)	View inputs as arrays with at least three dimensions.
broadcast	Produce an object that mimics broadcasting.
broadcast_arrays(*args)	Broadcast any number of arrays against each other.
expand_dims(a, axis)	Expand the shape of an array.
squeeze(a)	Remove single-dimensional entries from the shape of an array.

Changing kind of array

asarray(a[, dtype, order])	Convert the input to an array.
asanyarray(a[, dtype, order])	Convert the input to a ndarray, but pass ndarray subclasses through.
asmatrix(data[, dtype])	Interpret the input as a matrix.
asfarray(a[, dtype])	Return an array converted to a float type.
asfortranarray(a[, dtype])	Return an array laid out in Fortran order in memory.
asscalar(a)	Convert an array of size 1 to its scalar equivalent.
require(a[, dtype, requirements])	Return an ndarray of the provided type that satisfies requirements.

Table Of Contents

Array manipulation routines
- Changing array shape
- Transpose-like operations
- Changing number of dimensions
- Changing kind of array
- Joining arrays
- Splitting arrays
- Tiling arrays
- Adding and removing elements
- Rearranging elements

Previous topic

numpy.bmat

Next topic

numpy.reshape

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Enter search terms or a module, class or function name.

```
!
!Determine Ei from monitors 2 and 3
!
    subroutine get_Ei (Ei, a_M, s_M, t_M, b_M, d_M)

    include 'GET_SOURCES:COMCON.INC'
    include 'GET_SOURCES:COMFOR.INC'
    include 'GET_SOURCES:COMRUN.INC'
    include 'GET_SOURCES:COMINS.INC'
    include 'GET_SOURCES:COMTCB.INC'
    include 'GET_SOURCES:COMRAW.INC'
    real*4 y_t(MAX_CHAN), e_t(MAX_CHAN), a_M(3), s_M(2:3), t_M(2:3), b_M(2:3), d_M(2:3)
    real*4 t_min, t_max, fwhm
    parameter (c = 2286.26, pi = 3.1415927)

!Initialize peak search range
    if (Ei .gt. 0.0)) then
        t_M(2) = c * d_M(2) / sqrt (Ei)
        t_min = 0.9 * t_M(2)
        t_max = 1.1 * t_M(2)
    else
        t_min = 400
        t_max = 12000
    end if
!Loop over two monitors
    do i_m = 2,3
!Input Monitor data
        call get_tcb_time (timr(m_det(i_m)))
        call get_rawdata (1, spec(m_det(i_m)), 1)
        do i = 1,n_tc
            dt = tc(i+1) - tc(i)
            y_t(i) = rawdata(i) / dt
            e_t(i) = rawdata(i) / dt**2
        end do
!Determine peak centres from a moment analysis
        call get_moments (n_tc, tc, y_t, e_t, t_min, t_max, a_M(i_m)
b_M(i_m))
        if (i_m .eq. 2) then
            t_M(3) = t_M(2) * d_M(3) / d_M(2)
            t_min = 0.95 * t_M(3)
            t_max = 1.05 * t_M(3)
        end if
    end do
!Perform energy calculation
    Ei = ((c * (d_M(3)-d_M(2))) / (t_M(3) - t_M(2))) ** 2

    return
    end
```

```
    subroutine get_moments (n_tc, t, y_t, e_t, t_min, t_max, area, centre, sigma, fwhm, bkgd)
!
!  Modified:
!   10/11/94  T.G.Perring
!
!
    include 'GET_SOURCES:COMCON.INC'

    real*4 t(MAX_CHAN), y_t(MAX_CHAN), e_t(MAX_CHAN), t_min, t_max, centre, sigma, area, bkgd
    real*4 h, xp, xm, deriv, error, dtp, dtm, dt, xmin, x, dx, y, a0, a1, a2, a3
    integer*4 n_tc, i, imax, ip, im, nbkgd

!Determine peak position - assume it lies between t_min and t_max
    i = 1
    do while (i .lt. n_tc .and. t(i) .lt. t_min)
        i = i + 1
    end do
    h = 0.0
    do while (i .lt. n_tc .and. t(i) .lt. t_max)
        if (y_t(i) .gt. h) then
            h = y_t(i)
            imax = i
        end if
        i = i + 1
    end do
!Determine width of peak
    ip = imax
    do while (ip .lt. n_tc-2 .and. y_t(ip) .gt. h/2)
        ip = ip + 1
    end do
    if (y_t(ip-1) .ne. y_t(ip)) then
        xp = t(ip) - (((h/2) - y_t(ip)) * (t(ip) - t(ip-1)) / (y_t(ip-1) - y_t(ip)))
    else
        xp = 0.5 * (t(ip-1) + t(ip))
    end if
    im = imax
    do while (im .gt. 2 .and. y_t(im) .gt. h/2)
        im = im - 1
    end do
    if (y_t(im+1) .ne. y_t(im)) then
        xm = t(im) + (((h/2) - y_t(im)) * (t(im+1) - t(im)) / (y_t(im+1) - y_t(im)))
    else
        xm = 0.5 * (t(im) + t(im+1))
    end if
    fwhm = xp - xm
!Determine time range for moment analysis - use derivatives to define peaks
    deriv = -1000
    error = 0.0
    do while (ip .le. n_tc-2 .and. deriv .lt. -error)
        dtp = 0.5 * (t(ip+2) - t(ip))
        dtm = 0.5 * (t(ip+1) - t(ip-1))
        deriv = 0.5*(((y_t(ip+1) - y_t(ip)) / dtp) + ((y_t(ip) - y_t(ip-1)) / dtm))
```

Python API

- There are two levels to the Python API
  - A one-to-one mapping of the C-API returning Numpy arrays (napi.py)
  - A one-to-one mapping of the NeXus data objects into Python classes (tree.py)

```
>>> f=nexus.open("data/chopper.nxs")>>> f.opengroup("entry","NXentry")>>>
f.opendata("title")>>> f.getdata()'MgB2 PDOS 43.37g 8K 120meV E0@240Hz
T0@120Hz'
>>> f.closedata()
>>> f.closegroup()
>>> f.close()
```

```
>>> a=nexus.load("data/chopper.nxs")>>> a.entry.data.nxtree()data:NXdata  data =
int32(148x750)    @axes = polar_angle:time_of_flight    @long_name = Neutron
Counts    @signal = 1    @units = counts  polar_angle = float32(148)
@long_name = Polar Angle [degrees]    @units = degrees  time_of_flight = [ 1900.
1902.  1904. ...,  3396.  3398.  3400.]    @long_name = Time-of-Flight
[microseconds]    @units = microseconds  title = MgB2 PDOS 43.37g 8K 120meV
E0@240Hz T0@120Hz>>> print a.entry.data.titleMgB2 PDOS 43.37g 8K 120meV
E0@240Hz T0@120Hz
```

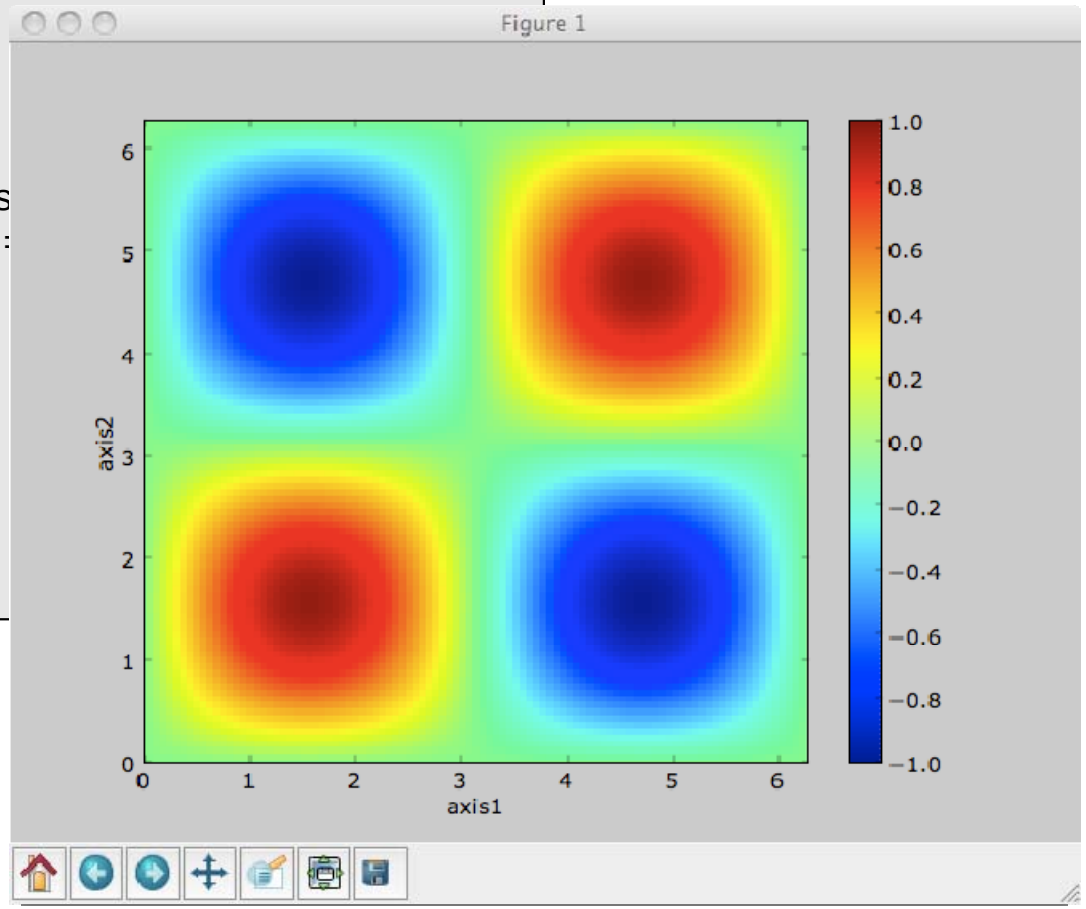
Features of NeXus tree interface

- The entire tree structure of a NeXus file can be loaded with a single command
- The data values are not read unless directly referenced
- Each NeXus object is a sub-class of the class NXnode
  - NeXus data have class SDS
  - NeXus groups have class NXgroup, with subclasses for each group class
    - e.g., NXentry, NXdata, NXsample ...
- All objects of the same class can easily be listed
  - e.g., entry.NXdata[0], entry.NXdata[1], ...
- All data attributes have a class NXattr
  - e.g., entry.data.polar_angle.units="K"
- Command-line assignments automatically convert Numpy data into NeXus objects
  - e.g., typing "entry.sample.temperature=40.0" converts the temperature into a valid SDS object
  - this is achieved by customizing __setattr__

Interactive manipulation of NeXus data

- The syntax makes the creation of standard-conforming NeXus data structures simple

```
>>> entry=NXentry()>>> x=np.linspace(0,2.*np.pi,101)
>>> y=x
>>> X,Y=np.meshgrid(x,y)
>>> z=np.sin(X)*np.sin(Y)
>>> entry.data=NXdata(z,(x,y))
>>> entry.nxtree()entry:NXentry  data:NXdata   axis
float64(101)   signal = float64(101x101)     @axes =
>>> entry.nxplot()
```



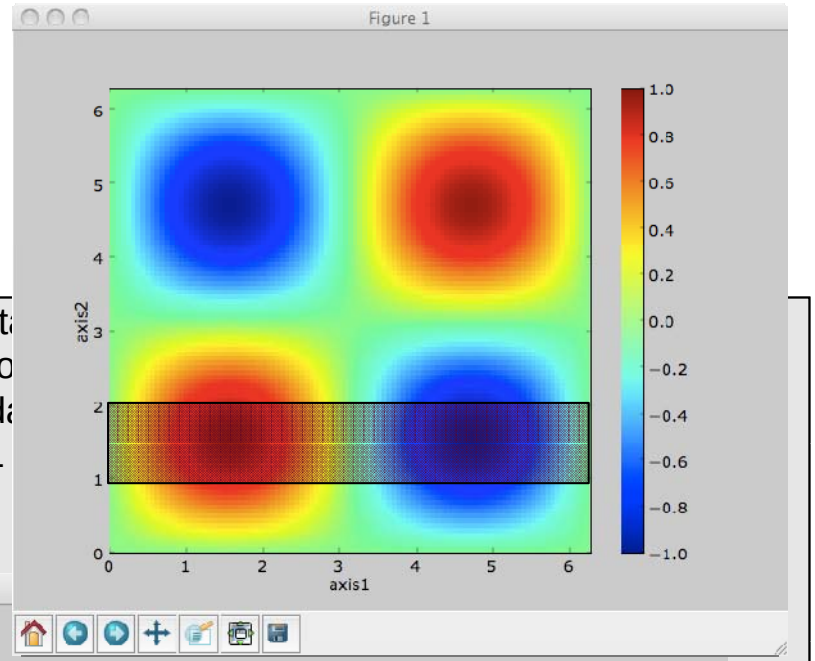
NXdata group manipulations

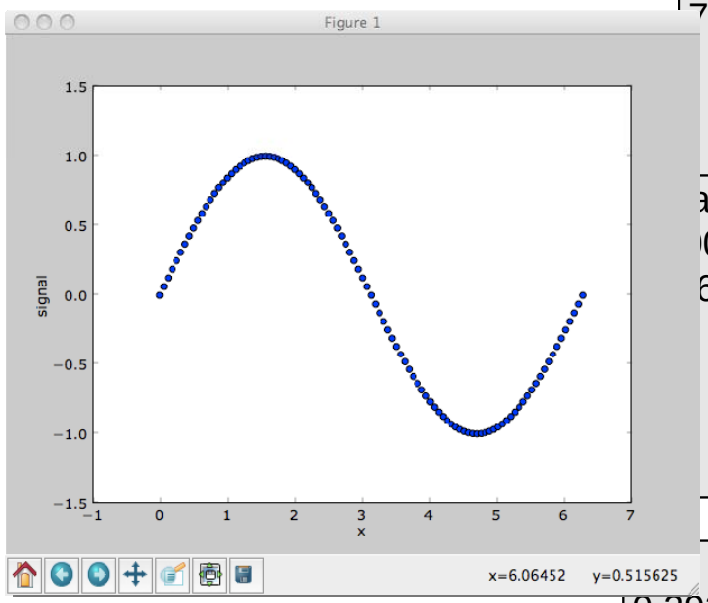
- The NXdata objects are designed to be manipulated:
  - Diced and sliced
  - Scaled
  - Added and subtracted

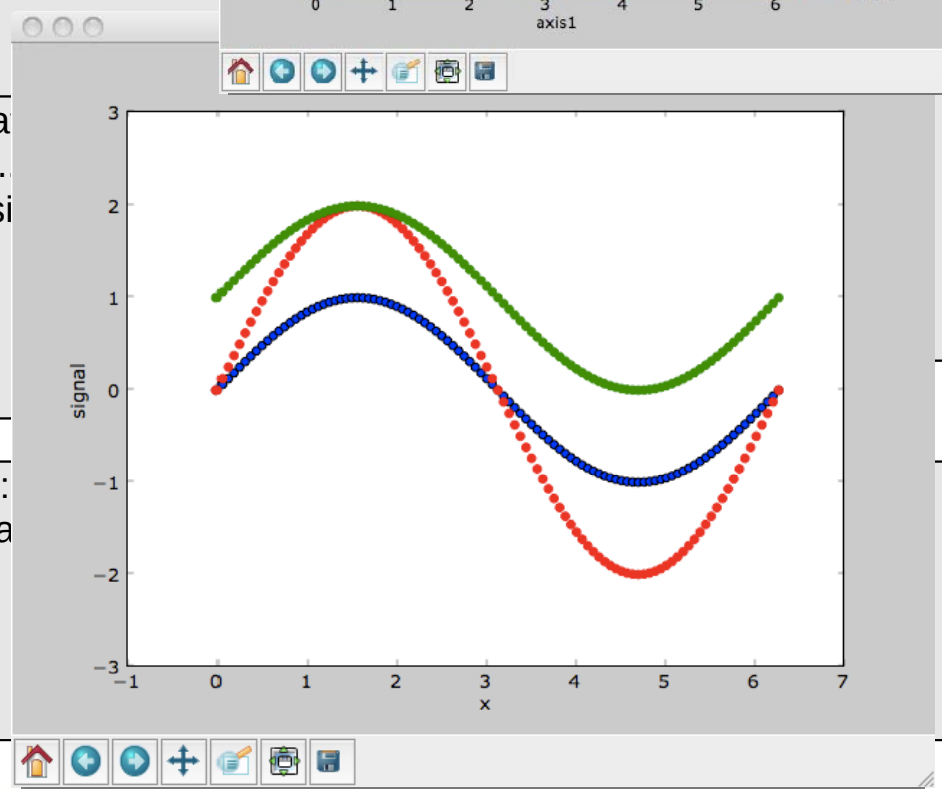
```
>>> data[1:2.].nxsum(0).nxtree()dat
float64(101)    @axes = axis2    @lo
2.0106192983    @signal = 1>>> da
0.00000000e+00   7.07106781e-01
7.07106781e-01  -2.44929360e-16
```

```
ata).nxtree()data:NXda
0   2.00000000e+00 ..
6 ]    @axes = x    @si
```

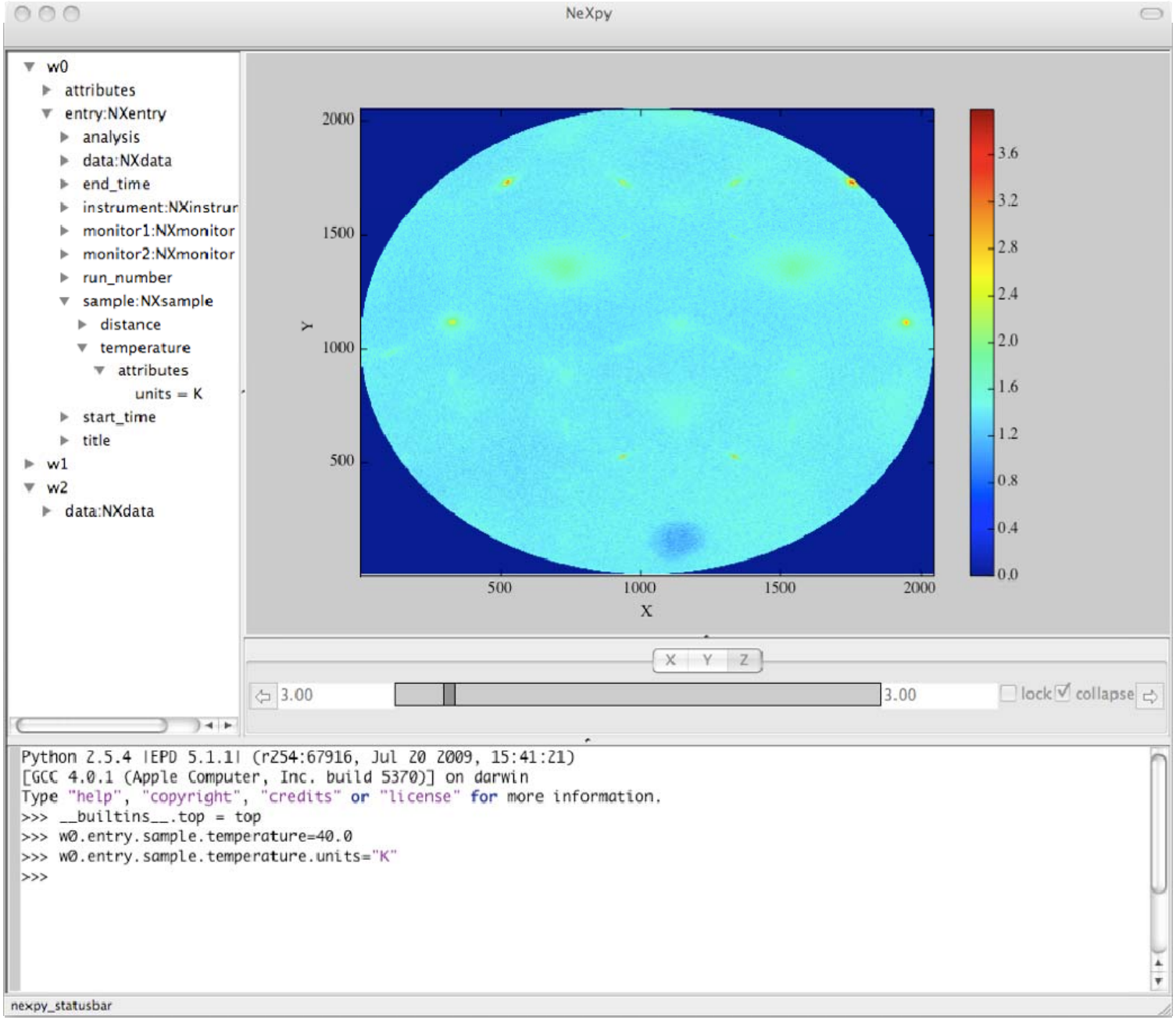
```
(data+1).nxtree()data:
0.29289322  1.        ]    @a
```







NeXpy GUI


NeXpy
w0
attributes
entry:NXentry
analysis
data:NXdata
end_time
instrument:NXinstrur
monitor1:NXmonitor
monitor2:NXmonitor
run_number
sample:NXsample
distance
temperature
attributes
units = K
start_time
title
w1
w2
data:NXdata
2000
1500
1000
500
Y
500
1000
1500
2000
X
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
X Y Z
3.00
3.00
lock
collapse
Python 2.5.4 |EPD 5.1.1| (r254:67916, Jul 20 2009, 15:41:21)
[GCC 4.0.1 (Apple Computer, Inc. build 5370)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> __builtins__.top = top
>>> w0.entry.sample.temperature=40.0
>>> w0.entry.sample.temperature.units="K"
>>>
nexpy_statusbar

On the To-Do List (near-term)

- Adding a data editor
- Incorporating generalized coordinate transformations
- Incorporating Open GL modules to improve over current Matplotlib speeds
- Adding full 3D plotting
  - Using Mayavi
- Adding a fitting pane
  - Using Paul Kienzle's PARK framework
- Installing it as a standard part of the NeXus distribution