NeXpy: A Python Toolbox for Interactive Data Analysis

http://www.nexusformat.org/NeXpy

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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

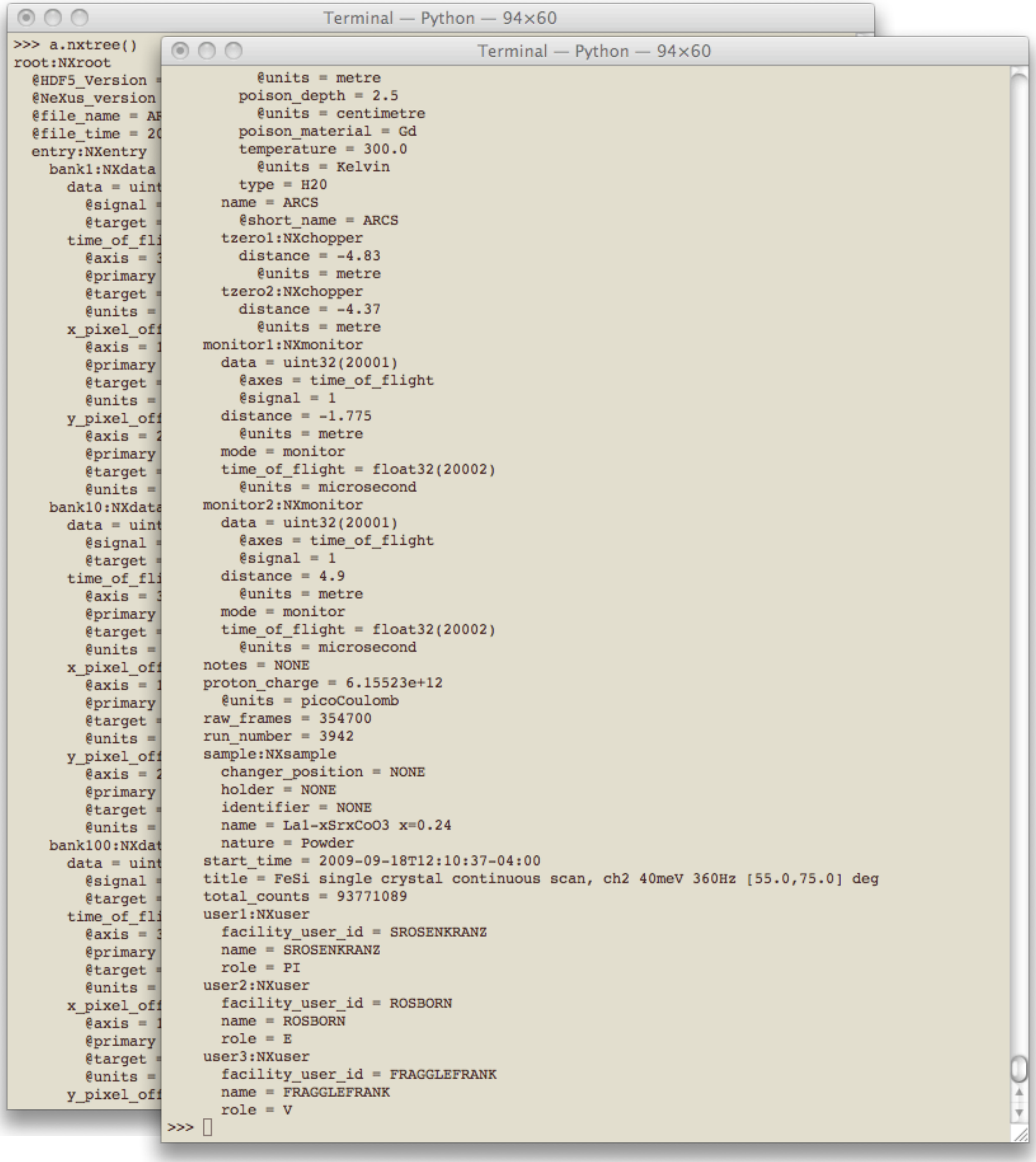
Python API

- 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 E
>>> 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.title
MgB2 PDOS 43.37g 8K 120meV E0@240Hz T0@120Hz
```

ARCS/SNS Data



```
>>> a.nxtree()
root:NXroot
 @HDF5_Version =
 @NeXus_version
 @file_name = AR
 @file_time = 20
 entry:NXentry
  bank1:NXdata
   data = uint
    @signal =
    @target =
   time_of_fli
    @axis = 3
    @primary
    @target =
    @units =
   x_pixel_off
    @axis = 1
    @primary
    @target =
    @units =
   y_pixel_off
    @axis = 2
    @primary
    @target =
    @units =
  bank10:NXdata
   data = uint
    @signal =
    @target =
   time_of_fli
    @axis = 3
    @primary
    @target =
    @units =
   x_pixel_off
    @axis = 1
    @primary
    @target =
    @units =
   y_pixel_off
    @axis = 2
    @primary
    @target =
    @units =
  bank100:NXdat
   data = uint
    @signal =
    @target =
   time_of_fli
    @axis = 3
    @primary
    @target =
    @units =
   x_pixel_off
    @axis = 1
    @primary
    @target =
    @units =
   y_pixel_off
```

```
     @units = metre
    poison_depth = 2.5
     @units = centimetre
    poison_material = Gd
    temperature = 300.0
     @units = Kelvin
    type = H2O
   name = ARCS
    @short_name = ARCS
   tzero1:NXchopper
    distance = -4.83
     @units = metre
   tzero2:NXchopper
    distance = -4.37
     @units = metre
  monitor1:NXmonitor
   data = uint32(20001)
    @axes = time_of_flight
    @signal = 1
   distance = -1.775
    @units = metre
   mode = monitor
   time_of_flight = float32(20002)
    @units = microsecond
  monitor2:NXmonitor
   data = uint32(20001)
    @axes = time_of_flight
    @signal = 1
   distance = 4.9
    @units = metre
   mode = monitor
   time_of_flight = float32(20002)
    @units = microsecond
  notes = NONE
  proton_charge = 6.15523e+12
   @units = picoCoulomb
  raw_frames = 354700
  run_number = 3942
  sample:NXsample
   changer_position = NONE
   holder = NONE
   identifier = NONE
   name = La1-xSrxCoO3 x=0.24
   nature = Powder
  start_time = 2009-09-18T12:10:37-04:00
  title = FeSi single crystal continuous scan, ch2 40meV 360Hz [55.0,75.0] deg
  total_counts = 93771089
  user1:NXuser
   facility_user_id = SROSENKRANZ
   name = SROSENKRANZ
   role = PI
  user2:NXuser
   facility_user_id = ROSBORN
   name = ROSBORN
   role = E
  user3:NXuser
   facility_user_id = FRAGGLEFRANK
   name = FRAGGLEFRANK
   role = V
>>> 
```

Features of NeXus tree interface

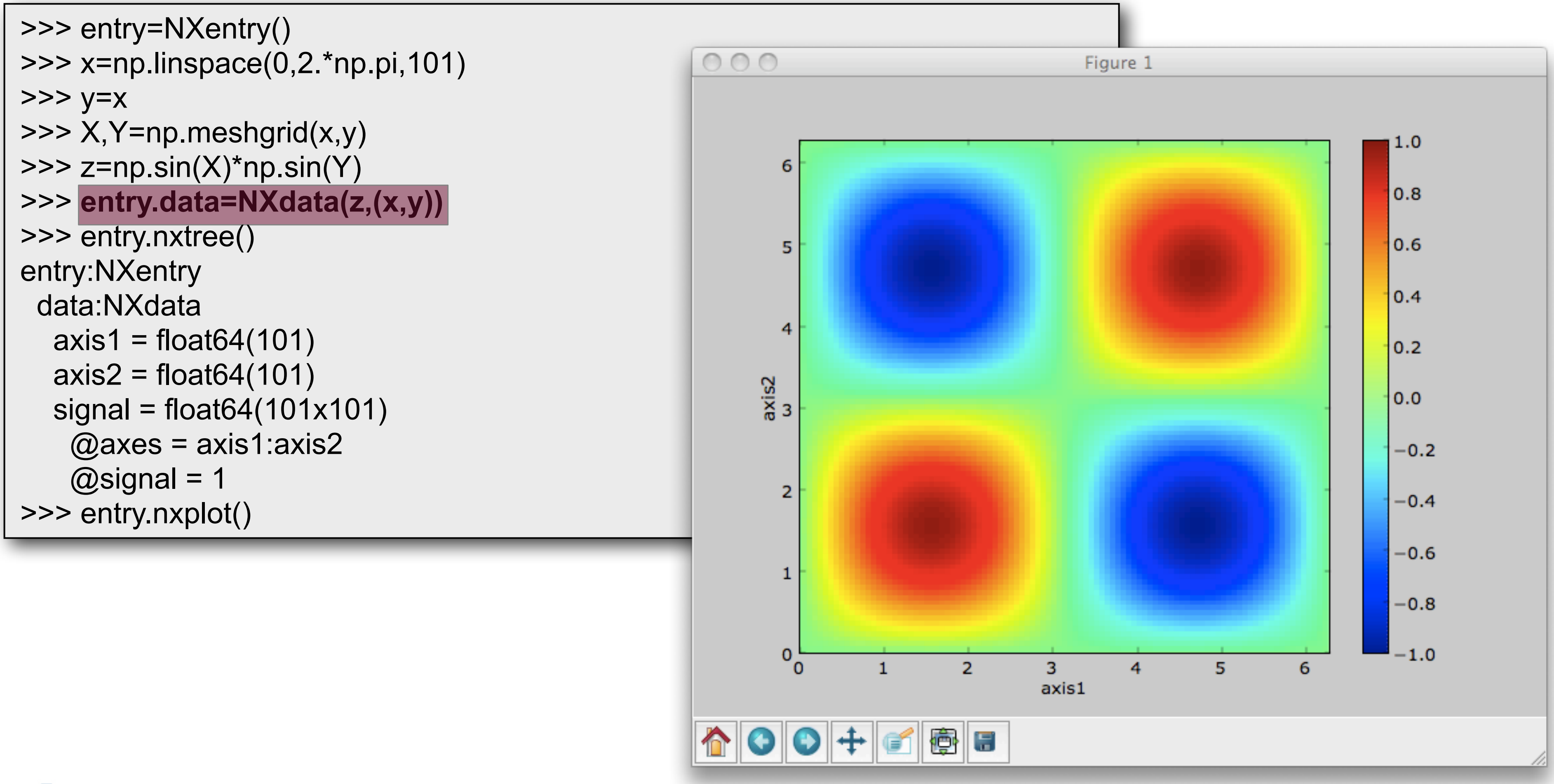
- The entire tree structure of a NeXus file can be loaded with a single command
  - The data values are not read until directly referenced
- NeXus objects can be created by simple assignments

```
>>> sample = NXsample()
>>> sample.temperature=40.0
>>> sample.temperature.units='K'
>>> entry = NXentry(sample)
>>> entry.nxtree()
entry:NXentry
  sample:NXsample
    temperature = 40.0
      @units = K
```

- Note: Command-line assignments automatically convert Numpy data into NeXus objects
  - *e.g.*, typing "entry.sample.temperature=40.0" converts the temperature into valid NeXus data
- All objects of the same class can easily be listed
  - *e.g.*, entry.NXdata[0], entry.NXdata[1], ...

Interactive manipulation of NeXus data

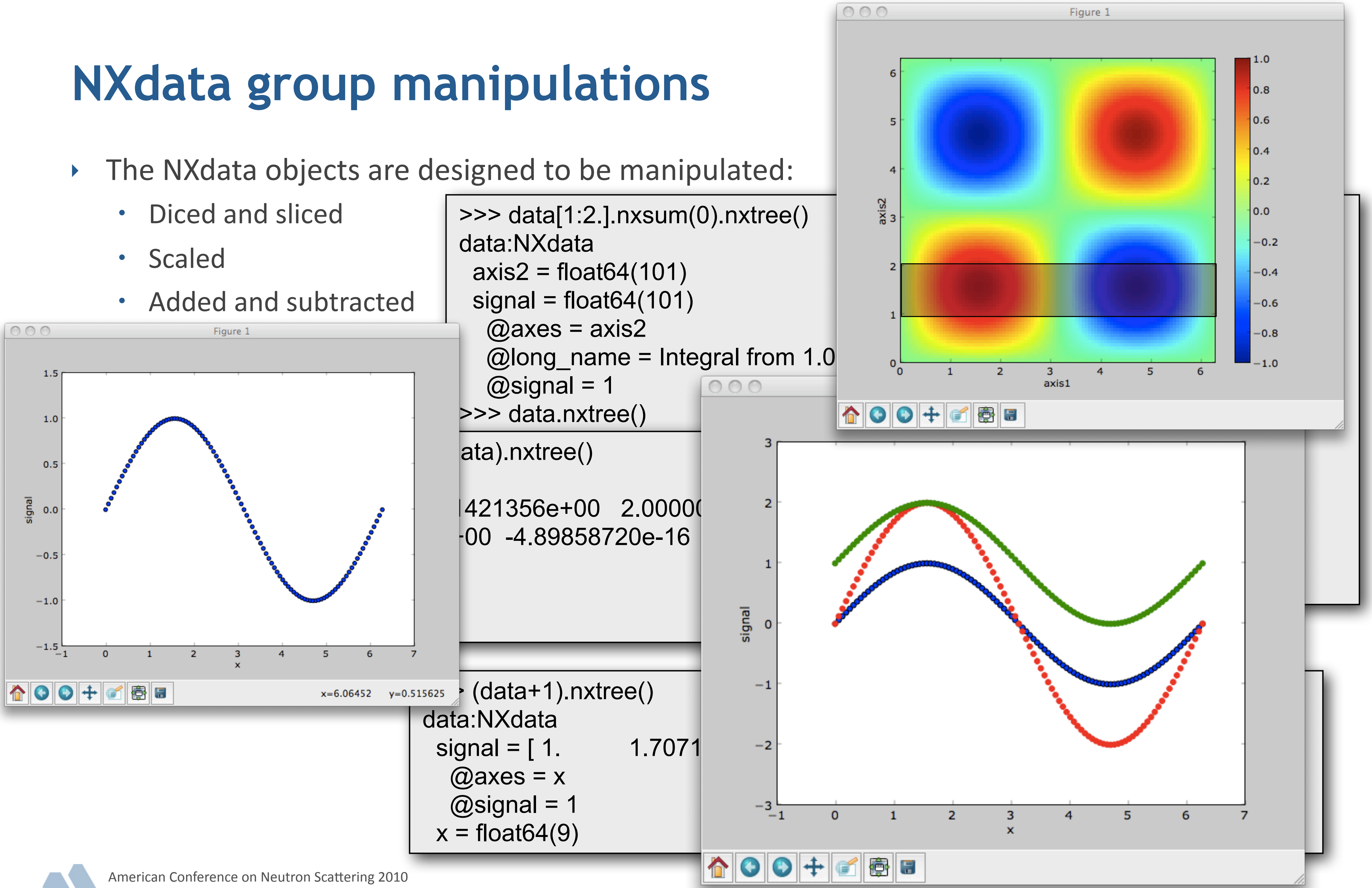
- The syntax makes the creation of standard-conforming NeXus data structures simple



```
>>> 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
    axis1 = float64(101)
    axis2 = float64(101)
    signal = float64(101x101)
      @axes = axis1:axis2
      @signal = 1
>>> entry.nxplot()
```

NXdata group manipulations

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



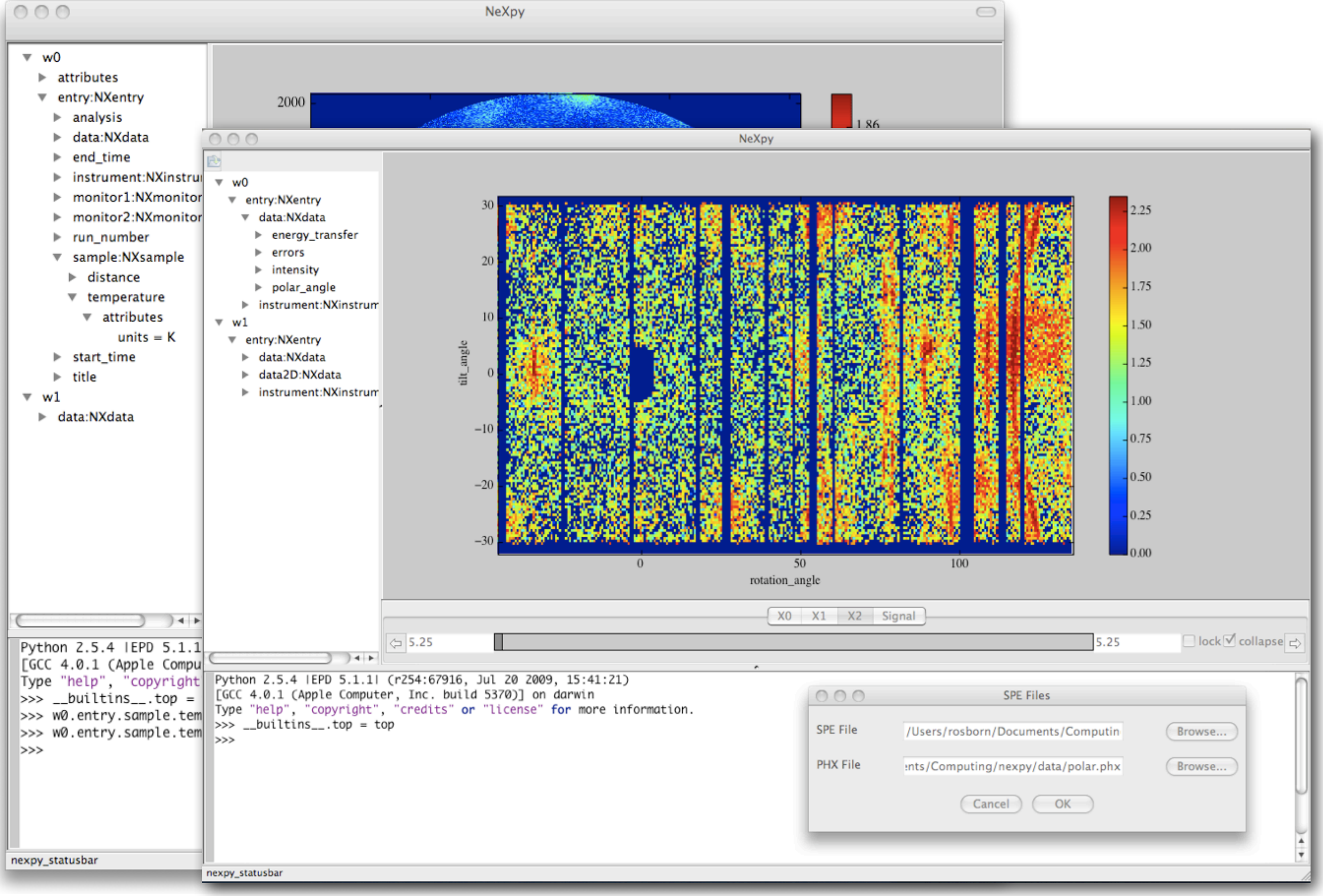
```
>>> data[1:2.].nxsum(0).nxtree()
data:NXdata
  axis2 = float64(101)
  signal = float64(101)
    @axes = axis2
    @long_name = Integral from 1.0
    @signal = 1
>>> data.nxtree()
```

```
ata).nxtree()

1421356e+00   2.0000(
-00  -4.89858720e-16
```

```
> (data+1).nxtree()
data:NXdata
  signal = [ 1.          1.7071
    @axes = x
    @signal = 1
  x = float64(9)
```

NeXpy GUI



```
Python 2.5.4 |EPD 5.1.1
[GCC 4.0.1 (Apple Compu
Type "help", "copyright
>>> __builtins__.top =
>>> w0.entry.sample.tem
>>> w0.entry.sample.tem
>>>
```

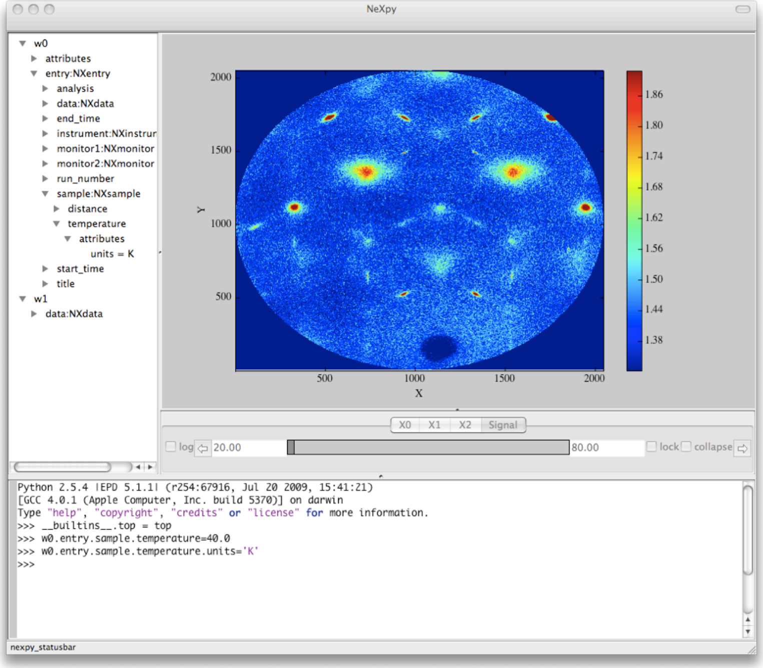
```
Python 2.5.4 |EPD 5.1.1| (r254:67916, Jul 20 2009, 15:41:21)
[GCC 4.0.1 (Apple Computer, Inc. build 5370)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> __builtins__.top = top
>>>
```

SPE File /Users/rosborn/Documents/Computin

PHX File nts/Computing/nexpy/data/polar.phx

Features of NeXpy GUI

- Persistent data
- Comprehensive access to metadata
- File-based memory management
  - Each data object maps directly to a valid NeXus file
- Non-proprietary language (*i.e.*, Python)
- Flexibility to do whatever you want to the data
  - No well-defined algorithms



```
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'
>>>
```

On the To-Do List (near-term)

- Adding a data editor
- Incorporating generalized coordinate transformations
- Incorporating Open GL modules to improve current Matplotlib speeds
- Expanded use of parallelization, including GPUs
- Adding full 3D plotting
  - Using Mayavi
- Adding a fitting pane
  - Using the DANSE *MYSTIC/PARK* framework
- Installing NeXpy as a standard part of the NeXus distribution
- Create a version for the iPad

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