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BASIS User Manual

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Section 1. Introduction

The purpose of this User Guide is to provide guidelines for collection and reduction of neutron scattering data from the SNS backscattering spectrometer, BASIS. The information included in this Guide should be sufficient for the BASIS users to reduce the data independently. Because the data reduction process may be reviewed and improved periodically, there may be updates that have not been included in the present version of the Guide; such instances will be indicated in the text, and you should consult the instrument personnel.

Section 2. Description of the SNS Backscattering Spectrometer, BASIS

The BASIS is an acronym that stands for **Ba**ckscattering **Si**licon **S**pectrometer. BASIS is an indirect geometry spectrometer located on BeamLine 2 (BL2) at the Spallation Neutron Source (SNS). It has a sample position located in an external building (see Figure 1) some 84 m from the top upstream decoupled (and poisoned) liquid H_2 moderator. The beam is transported to the sample position (inside the instrument tank; see Figures 1 and 2) through a system of guides located along the corridor connecting the BASIS external building with the main target building.

Figure 1. Top, left: BASIS external building. Top, right: BASIS overall schematics. Bottom, left: BASIS tank view (with the door open) from the corridor connecting the BASIS external building to the main target building. Top, right: BASIS tank view from the floor of the BASIS external building.

Figure 2. Inside the BASIS tank, view from the open tank door. Shown are the incident beam guide (enclosed in the shielding) and the crystal analyzer panels.

BASIS is used for high-energy resolution (typically 3.0 to 3.5 μeV, FWHM, at the elastic line) measurements with a relatively wide, variable energy transfer range, and the momentum transfer of $0.2\ \text{Å}^{-1} < Q < 2.0\ \text{Å}^{-1}$, with Q-resolution that varies between 0.05 and 0.10 Å^{-1}. BASIS experiments usually measure quasielastic scattering (due to diffusion or relaxational motions on the pico- to nano-second time scale), or low-energy inelastic scattering. An example of an experiment that probes both quasielastic and inelastic scattering is shown in Figure 3.

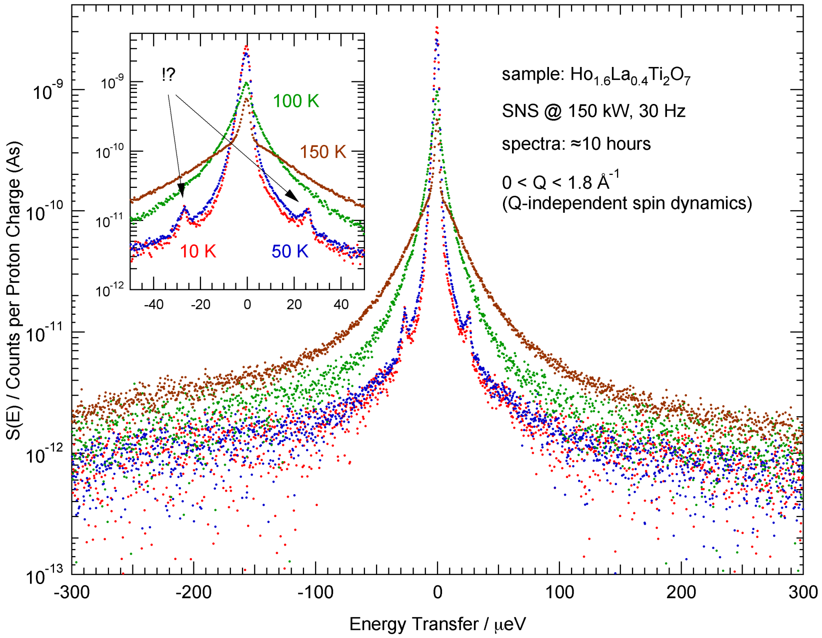

Figure 3. Quasielastic scattering and inelastic excitations measured simultaneously on BASIS.

The important parameters of the Beamline 2 are as follows.

<u>Moderator-to-sample distance:</u> 84.000 m. On the way to the sample, neutrons pass though the incident bandwidth-defining choppers (at 7.000, 9.250, and 50.000 m) and the incident beam monitor (at 83.766 m, or 0.234 m upstream the sample position).

Sample-to-analyzers distance: 2.500 m (for a point sample)

Analyzers-to-detectors distance: variable, from 2.710 m to 2.729 m. Each detector pixel row has its unique analyzer-to-detector distance, defined by the Bragg reflection geometry of the analyzers, as we will discuss below. The data reduction routine takes this spread into account. Assuming a single analyzer-to-detector distance (thus, neglecting the actual spread) leads to the energy resolution degraded by about 50 %. Furthermore, the Bragg-reflected wavelength is also a function of the pixel row: it varies slightly between 6.2671 Å to 6.2678 Å. The detailed explanation of the pixilation of the BASIS linear position-sensitive detectors will be given in the next Sections.

Section 3. The Indirect Geometry Method - General

In general, on a TOF spectrometer, the scattering intensity is measured as a function of energy transfer, $E = E_i - E_f$, where E_i and E_f is the incident and final (detected) neutron energy, respectively. In the indirect (or inverted) TOF geometry, the E_f is fixed (for example, defined by a filter or an analyzer crystal), whereas the E_i is variable, and can be determined from the neutron TOF. In the extreme case of a backscattering TOF spectrometer, the E_f is known very precisely by means of utilizing back reflection from analyzer crystals. Thus, the energy transfer, E, can also be measured very precisely, if one knows the E_i with equally good precision. Usually, the precision of measuring E (the energy resolution) of the inverted geometry backscattering spectrometer is higher compared to that of a direct geometry spectrometer. For example, a typical BASIS spectrum collected from an incoherently scattering vanadium standard is shown in Figure 4.

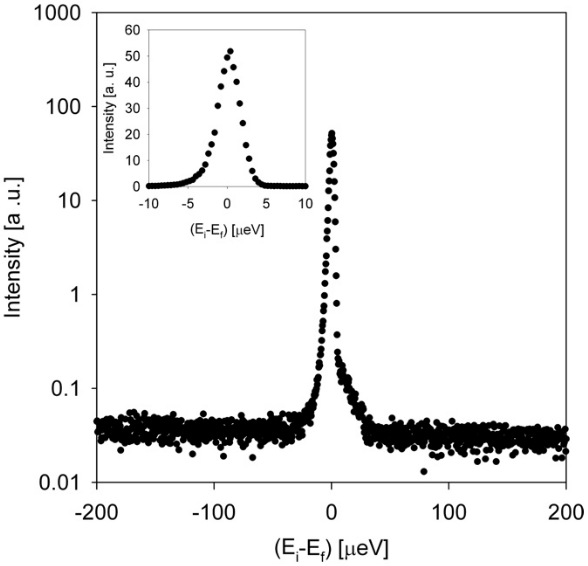

Figure 4. Q-averaged spectrum collected from a 10 % scattering annular vanadium standard showing the energy resolution of the BASIS of about 3.5 μeV, FWHM.

Another important feature of the inverted geometry spectrometer is the access to a generally wider (compared to direct geometry spectrometers) range of neutron energy loss side (see Figure 5 for the range accessible on the BASIS).

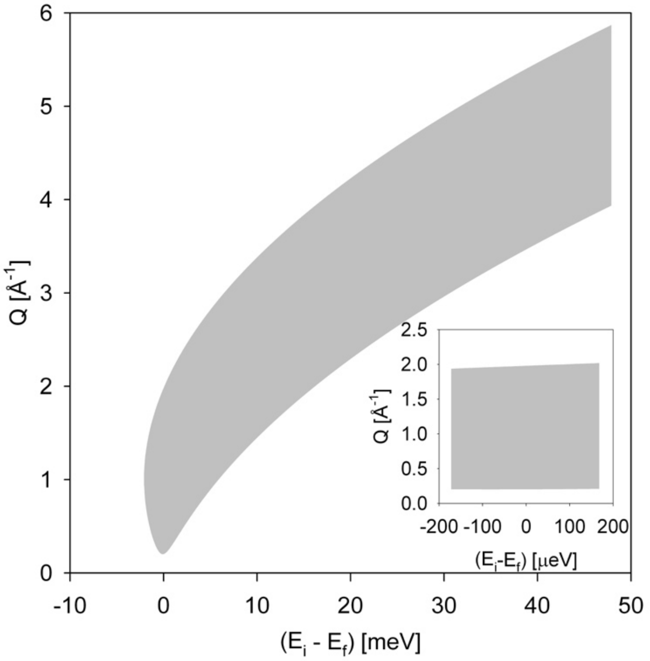

Figure 5. Q-E region accessible on the BASIS (note: it will require several measurements with different choppers settings to cover the entire range shown). Inset: typical Q-E coverage in the quasielastic measurement regime at 60 Hz.

A disadvantage of the indirect geometry spectrometers is a generally higher level of the lowest attainable background, which is a direct consequence of admitting a relatively wide incident wavelength band inside the spectrometer, as opposed to just a single wavelength at a direct geometry spectrometer.

Section 4. Specifics of the Indirect Geometry Method on BASIS

How do we measure scattering on the BASIS? Schematically, BASIS works as follows. For each accelerator pulse, the system of choppers transmits a wavelength band of neutrons of about 0.5 Å wide (when the choppers are operated at 60 Hz) that travel from the moderator to the sample through the neutron guide. Alternatively, the choppers can be operated at a sub-harmonic frequency (e.g., 30 Hz); in such a mode, the incident wavelength band is extended, albeit at the expense of missing some accelerator pulses.

The list of "corrections" that need to be applied to reduce BASIS data are as follows

- For the variation of the moderator emission time $T0(E_i)$ as a function of E_i
- For the variation of the incident flux $\Phi(E_i)$ as a function of E_i
- The variation of the final (analyzing) energy and flight path distance for different detector pixels because of the spherical symmetry of the analyzer crystals
- The variation of the solid angle subtended by different detector pixels (via the analyzer crystals) at the sample position
- The variation of the detector efficiency does **not** need to be taken into account (unlike for the incident beam monitor) because single wavelength gets registered at the detectors
- The variation of the analyzer crystal reflectivity across the analyzer panels and from analyzer panel to analyzer panel
- The masking out of noisy or inaccessible (via Bragg scattering from the analyzer crystals) detector pixels

Moderator Emission Time Variation T(Ei)

It takes some time after the prompt pulse for the moderated neutron pulse to get emitted from the moderator; the faster neutrons have shorter emission times. In the BASIS data reductions, the emission times are assumed to be linearly dependent on the incident wavelength: $t_0 = t_{0,slope}\lambda_i + t_{0,offse}$. The slope and offset parameters are updated depending on the state of the moderator.

Variation of the Incident Flux Distribution $\Phi(E_i)$

The incident band is non-uniform in intensity as a function of wavelength. At each value of the incident wavelength, the intensity is a product of the moderator output, transmission through the guide, and absorption in the thin aluminum windows that separate multiple sections of the guide. To measure the wavelength distribution of the incident spectrum, the incident beam monitor (IBM) is positioned upstream the sample position. As a result, the TOF spectrum at the IBM is shifted toward shorter TOFs, and also has a slightly shorter TOF span compared to the detector spectrum (Figure 6).

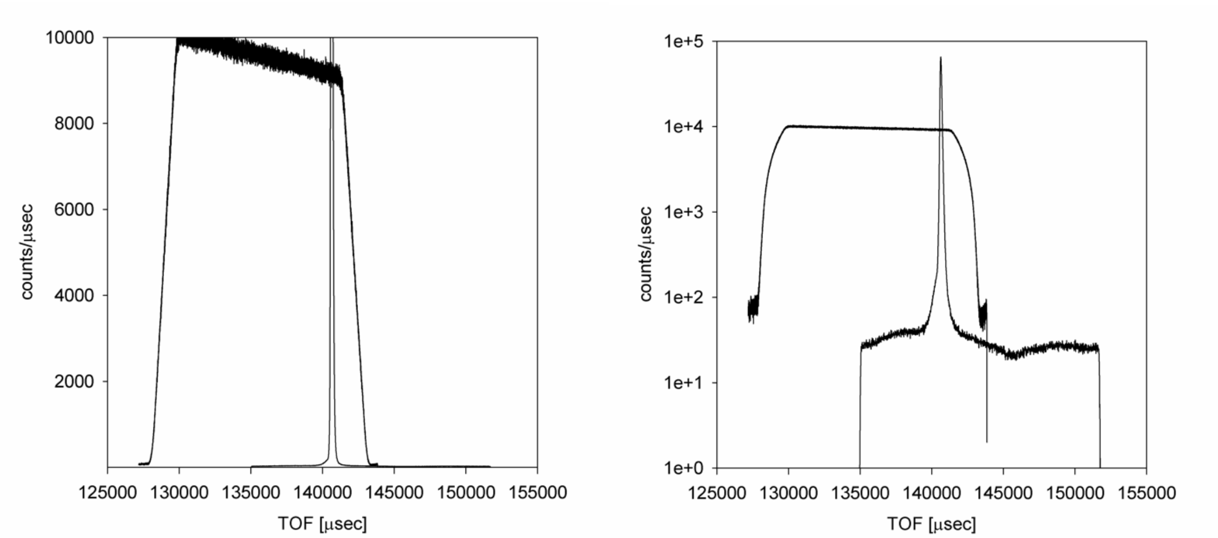

Figure 6. TOF signal from a sample measured at the detectors (with the elastic peak at about 140,600 μsec) and the incident beam monitor. Left: linear scale. Right: logarithmic scale.

Therefore, the counts need to be expressed in the unit of incident wavelength rather than TOF before normalization to the IBM can be performed.

Variation of the Final Flight Energy and Flight Path

The neutrons are scattered by the sample, elastically or inelastically, in all directions. Those intercepted by the analyzer crystal panels (see Figure 7) have a chance of being reflected to the detectors, but only if their final wavelength assumed in the process of getting scattered by the sample happens to be 2.627 Å, which is a Si(111) Bragg reflection wavelength at 88 degrees. Thus, in theory, the time-of-flight (TOF) for all the detectable neutrons in known for the path from the sample to the analyzer crystals to the detectors. In practice, however, the detected signal can be contaminated by spurious scattering due to neutrons that have a wavelength different from 6.267 Å after getting scattered by the sample, and, therefore, cannot be Bragg-reflected properly, yet manage to find their way into the detectors. Another complication is that, even for the properly Si(111) Bragg-reflected neutrons, the Bragg angle (thus, the reflected wavelength) and, more importantly, the distance traveled by the reflected neutrons from the analyzer panels to the detectors, vary slightly as a function of the vertical coordinate of the neutron reflection point on the analyzer panels (see Appendix 1). This vertical coordinate is tied to a particular pixel row in the BASIS detectors; thus, there will be its own flight-path and wavelength for neutrons detected in the particular pixel row. Analyzers-to-detectors distance varies from 2.710 m to 2.729 m. The Bragg-reflected wavelength varies from 6.2671 Å to 6.2678 Å.

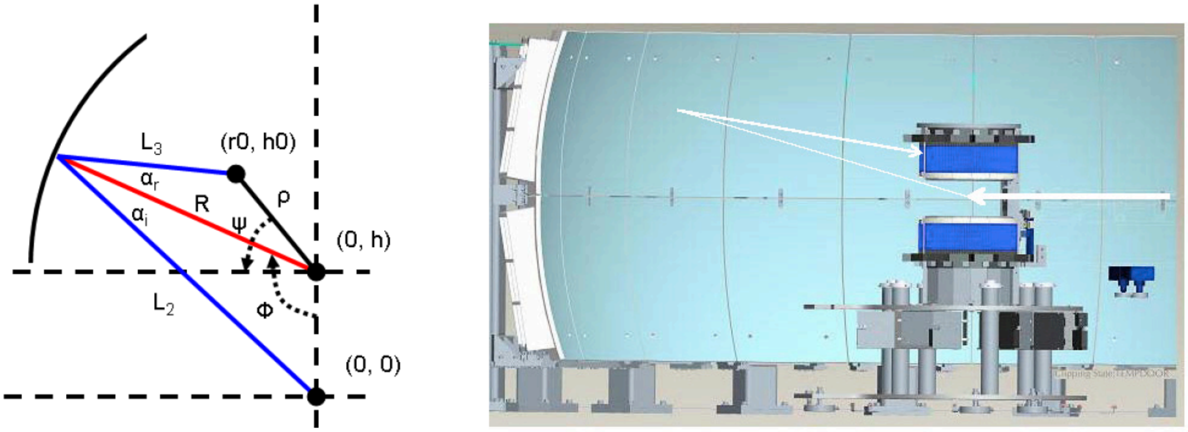

Figure 7. Schematics of scattered neutron trajectories Bragg-reflected from the crystal analyzer panels into the detectors. Note that the panels are split in the middle to preserve the energy resolution; hence, two detector banks with a gap in the middle.

The Solid Angle Variation for Each Pixel

Each pixel of the BASIS detectors accepts Bragg-reflected neutrons from a certain area of the crystal analyzer panels. In turn, such area accepts neutrons scattered by the sample into a certain solid angle, $d\Omega$. The data reduction routine uses a pre-computed array of the solid angles associated with each detector pixel.

Analyzer Reflectivity and Detector Pixel Efficiency

As one can see in Figure 8, the distribution of the "raw" intensities shows that the pixels are not illuminated uniformly, even when a nominally "isotropic" sample such as incoherently scattered vanadium are used. Some variations in the intensities are expected, because of the (1) variations of the associated solid angles among the pixels and (2) possible variations of the pixels detection efficiencies. However, Figure 8 reveals the dominant role of the more systematic variations; namely, the scattering pattern approximately reflects the geometry of the analyzer crystal scattering panels; 9 two-dimensional intensity maxima in each the top and bottom detector banks correspond to the 9 panels in each the top and bottom banks of the crystal analyzer panels. Thus, while the correction for the solid angle can be computed and applied explicitly, the correction for the pixel efficiency of the detectors and the reflectivity efficiencies of the analyzers needs to be applied as a pixel-by-pixel division by the elastic line of the scattering intensity pattern obtained from an isotropically scattering sample, such as a vanadium standard.

Masking of Noisy Pixels

At users' discretion, a mask can be applied to any group(s) of chosen pixels. For example, noisy pixels, or the pixels with intensities dominated by contributions from Bragg peaks, can be masked out. Such pixels are then disregarded by the data reduction routines.

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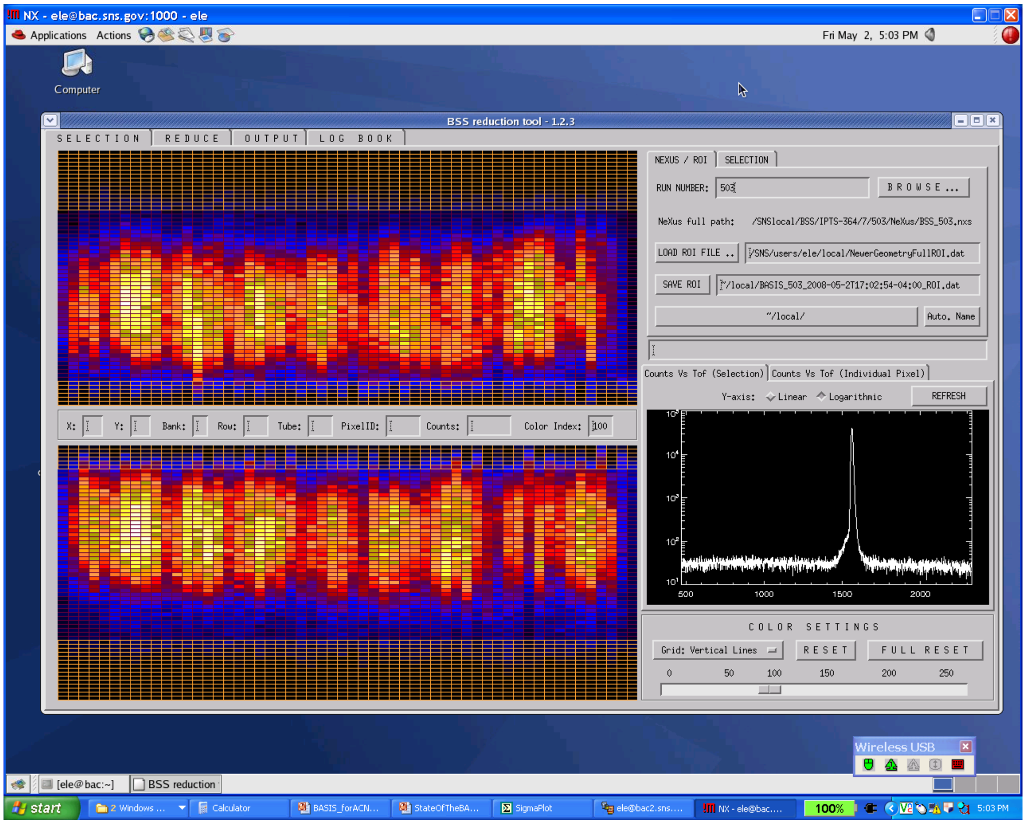


RUN NUMBER: 503

NeXus full path: /SNSlocal/BSS/IPTS-364/7/503/NeXus/BSS_503.nxs

LOAD ROI FILE .. /SNS/users/ele/local/NewerGeometryFullROI.dat

SAVE ROI ~/local/BASIS_503_2008-05-2T17:02:54-04:00_ROI.dat

~/local/ Auto. Name

Color Index: 100

Figure 8. A typical snapshot of the BASIS data view for an isotropically scattering sample such as a vanadium standard.

A typical pixel view, as presented in Figure 8, consists of two dimensional colored intensity map that represent the pixilated total (summed over all TOF channels) intensities registered in the BASIS detectors. There are two detector banks, top and bottom, each consisting of 56 He-3 tubes. Each tube is a vertically pixilated linear position-sensitive detector; hence, two-dimensional intensity distribution. The plot on the right is the TOF signal summed over all non-masked pixels.

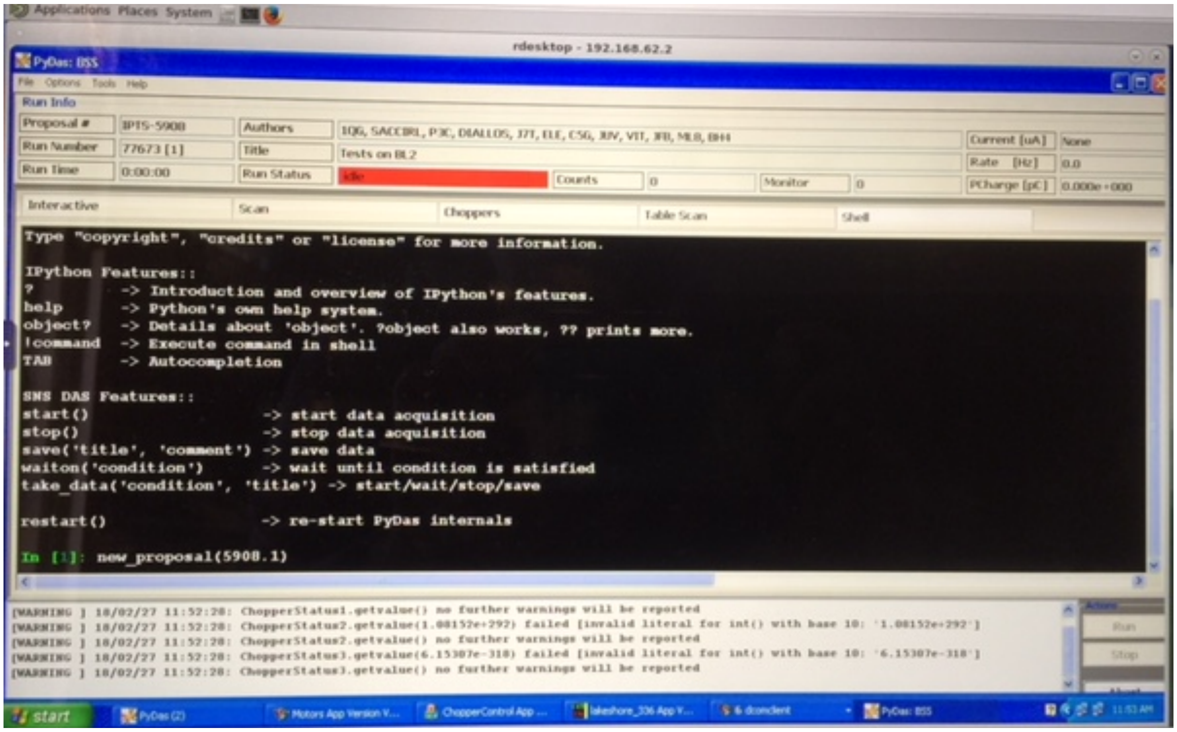
Section 5. Data Collection

Setting up the instrument

PyDas

When starting an experiment at BASIS, to set up all the necessary variables, double click the PyDas icon on the desktop of the control computer (Figure 9). The necessary applications to set up and run an experiment at BASIS will be launched. First set the correct IPTS number from the PyDas/shell (see Figure 10). This should populate the fields for proposal number, authors, and title for the experiment and give the users access to their data that will be measured and stored under the proposal number.

Figure 9. PyDas icon.



Proposal # IPTS-5908
Run Number 77673 [1]
Run Time 0:00:00
Authors IQG, SACCBRL, P3C, DIALLOS, J7T, ELE, C5G, JUV, VIT, JFB, MLB, BHH
Title Tests on BL2
Run Status Idle
Counts 0
Monitor 0
Current [uA] None
Rate [Hz] 0.0
PCharge [pC] 0.000e+000

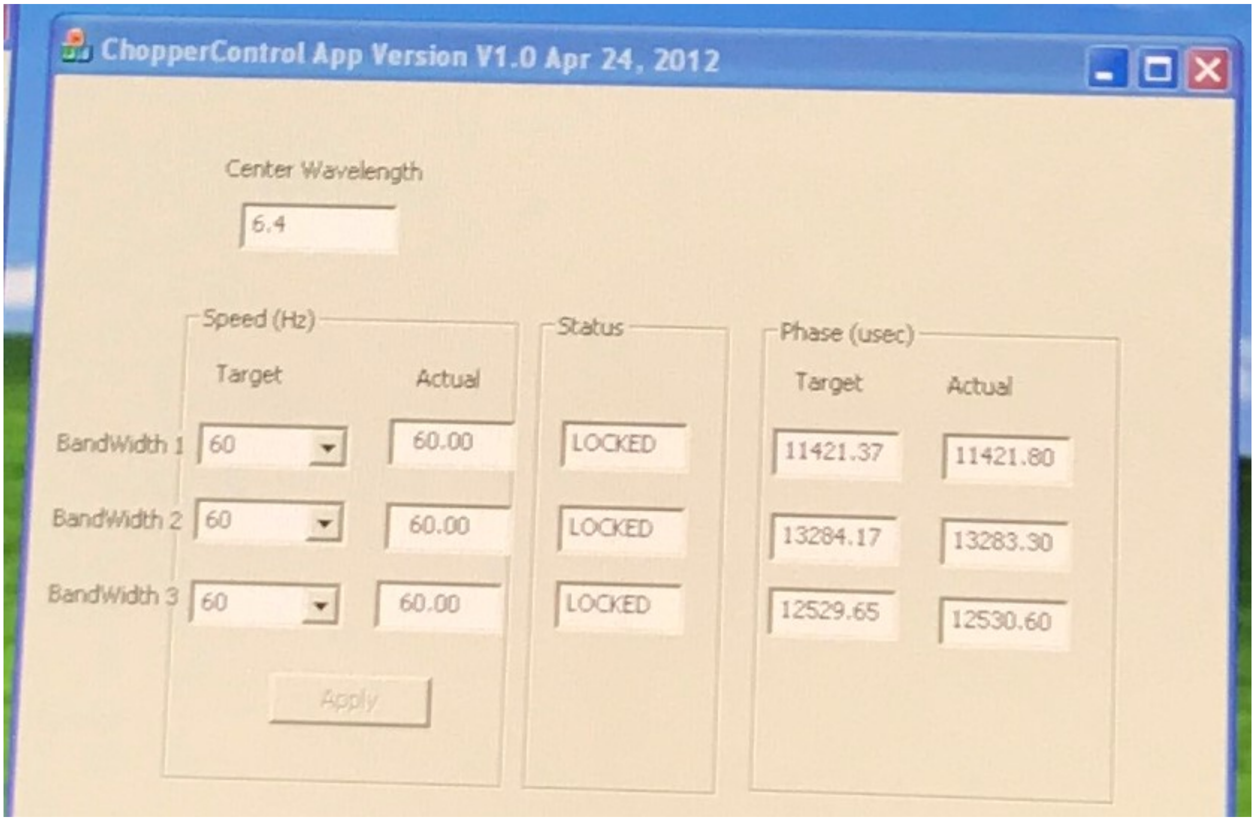
```
Type "copyright", "credits" or "license" for more information.

IPython Features::
?         -> Introduction and overview of IPython's features.
help      -> Python's own help system.
object?   -> Details about 'object'. ?object also works, ?? prints more.
!command  -> Execute command in shell
TAB       -> Autocompletion

SNS DAS Features::
start()                    -> start data acquisition
stop()                     -> stop data acquisition
save('title', 'comment') -> save data
waiton('condition')        -> wait until condition is satisfied
take_data('condition', 'title') -> start/wait/stop/save

restart()                  -> re-start PyDas internals

In [1]: new_proposal(5908.1)
```

```
[WARNING ] 18/02/27 11:52:28: ChopperStatus1.getvalue() no further warnings will be reported
[WARNING ] 18/02/27 11:52:28: ChopperStatus2.getvalue(1.08152e+292) failed [invalid literal for int() with base 10: '1.08152e+292']
[WARNING ] 18/02/27 11:52:28: ChopperStatus2.getvalue() no further warnings will be reported
[WARNING ] 18/02/27 11:52:28: ChopperStatus3.getvalue(6.15307e-318) failed [invalid literal for int() with base 10: '6.15307e-318']
[WARNING ] 18/02/27 11:52:28: ChopperStatus3.getvalue() no further warnings will be reported
```

Figure 10. PyDas /shell.

Choppers

To set up the desired instrumental configuration, one needs to choose first whether to use the Si111 or the Si311 analyzers. Si111 analyzers cover ¾ of the instrument, and Si311 analyzers cover ¼ of the instrument. Therefore, the counting statistics when using the Si311 analyzers are lower. Si111 configuration is the most commonly used, providing elastic energy resolution of about 3.5 μeV (FWHM), analyzable energy transfer range of about ±100 μeV, and Q range from 0.2 to 2.0 $Å^{-1}$. When using this configuration, wavelength is centered usually to 6.4 Å, and the choppers are set to 60 Hz (sometimes, to 30 Hz, in order to access ±200 μeV energy transfer range with the same energy resolution, but half of the measurement statistics). Configuration using Si311 analyzers has coarser resolution function, about 15 μeV (FWHM), energy range of about ±660 μeV (at 60 Hz choppers operation) or about ±1700 μeV (at 30 Hz choppers operation). The available Q range is from 0.4 to 3.7 $Å^{-1}$. The wavelength for Si311 measurements is centered to 3.35 Å. The 30 Hz choppers operation options should be discussed with the instrument scientists, if extended energy transfer range is desired at the expense of the flux at the sample. Oftentimes, the choppers frequency change cannot be set at the control computer and needs to be assisted by an instrument staff member.


ChopperControl App Version V1.0 Apr 24, 2012

Center Wavelength: 6.4

	Speed (Hz) Target	Speed (Hz) Actual	Status	Phase (usec) Target	Phase (usec) Actual
BandWidth 1	60	60.00	LOCKED	11421.37	11421.80
BandWidth 2	60	60.00	LOCKED	13284.17	13283.30
BandWidth 3	60	60.00	LOCKED	12529.65	12530.60

Figure 11. Chopper application at the control computer. The values set for the standard configuration for Si111 analyzers.

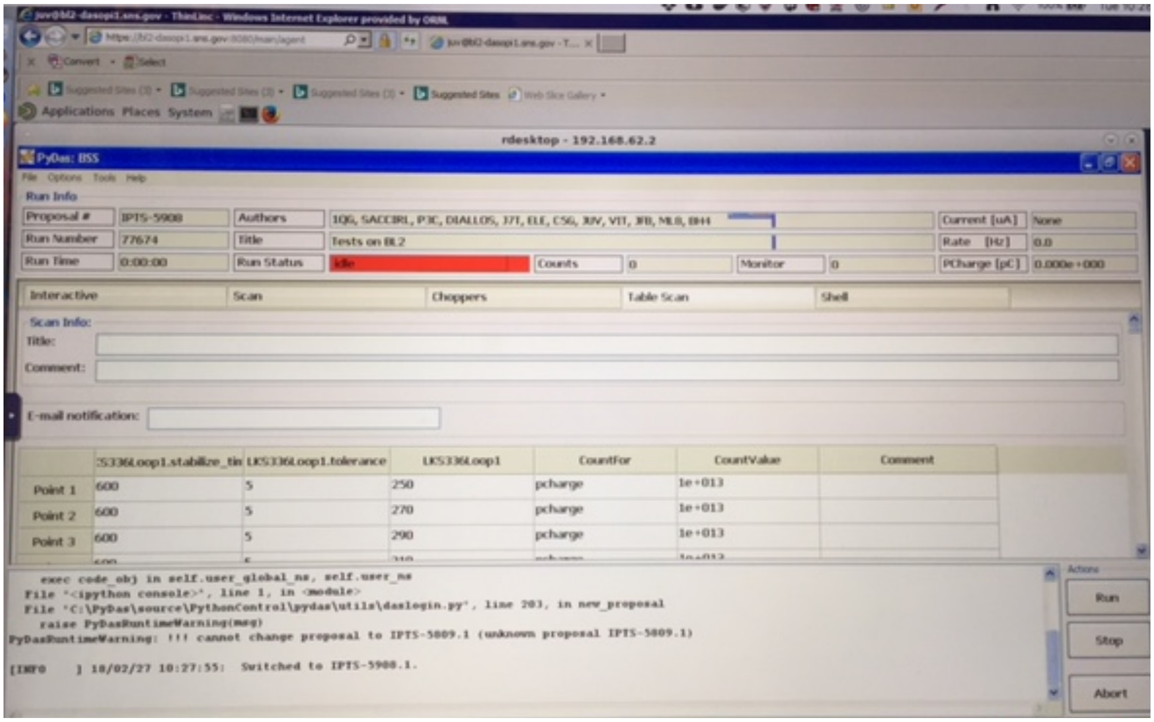
Slits
The motors application can be used to adjust the beam size at BASIS. When using the cylindrical annular sample cans, the beam size is typically set to 30 mm x 30 mm. The corresponding slit values are given as follows:

s1left	3.75	s1bottom	-21.25
s1right	-3.75	s1top	-1.75

If the sample size is different, the motors application is able to calculate the correct values for given width and height (S1HWidthRequest, and S1VHeigthRequest) in mm units. (**Note: Slits are very delicate in nature, therefore, only the instrument scientists have an authority to adjust them).**

Tablescan
To set up scripts for a series of measurements, the tablescan option under the PyDas can be used. Number of columns with different variables can be chosen to fulfill the requirements of the experiment. Below, in figure 12, those variables are:

1. *Stabilization time,* time (in seconds) to be waited before progressing with the measurement after the requested temperature within the given tolerance is reached.
2. *Tolerance*, the temperature variation allowed around the requested temperature.
3. *LKSLoop1*, the temperature point request, in Kelvin.
4. *CountFor*, choose to count for statistics (pcharge) or for time (s). Counting for equal statistics is preferred, since the source power is not constant all the time.
5. *CountValue*, give value for certain statistics / time; when this value is reached, the measurement will progress to the next line in the table scan.



Run Info
Proposal # IPTS-5908
Run Number 77674
Run Time 0:00:00
Title Tests on BL2
Run Status Idle
Counts 0
Monitor 0
Current [uA] None
Rate [Hz] 0.0
PCharge [pC] 0.000e+000

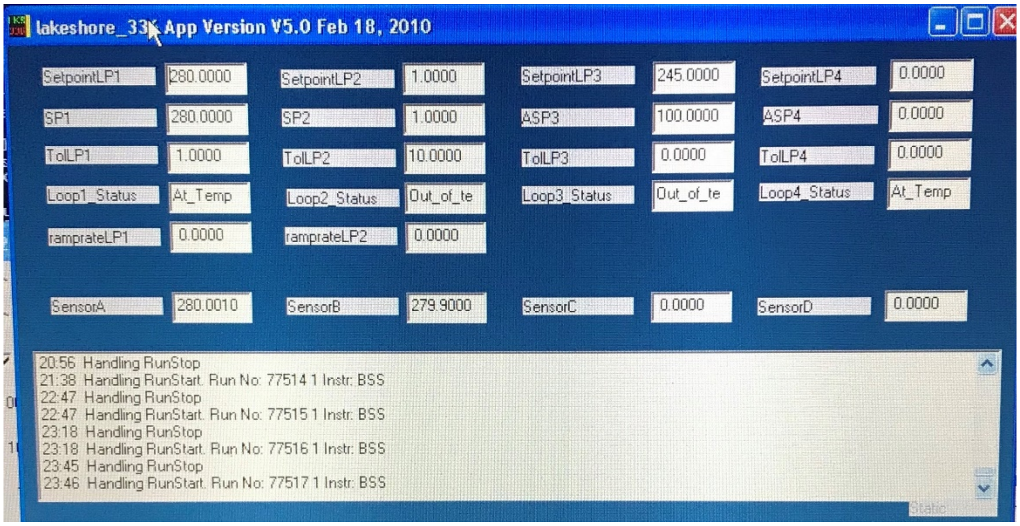
Scan Info:
Title:
Comment:
E-mail notification:

	:S336Loop1.stabilize_tin	LKS336Loop1.tolerance	LKS336Loop1	CountFor	CountValue	Comment
Point 1	600	5	250	pcharge	1e+013	
Point 2	600	5	270	pcharge	1e+013	
Point 3	600	5	290	pcharge	1e+013	

```
    exec code_obj in self.user_global_ns, self.user_ns
  File "<ipython console>", line 1, in <module>
  File "C:\PyDas\source\PythonControl\pydas\utils\daslogin.py", line 203, in new_proposal
    raise PyDasRuntimeWarning(msg)
PyDasRuntimeWarning: !!! cannot change proposal to IPTS-5809.1 (unknown proposal IPTS-5809.1)

[INFO    ] 18/02/27 10:27:55:  Switched to IPTS-5908.1.
```

Figure 12. PyDas tablescan to set script for number of measurements.

Lakeshore
The temperature of the sample environment is controlled with the Lakeshore application at the control computer. The required temperature can be given in the temperature request field. If table scan option is used, the value for this field will be automatically communicated from the current given value at the table scan. The actual value can be typically read at the channel A, which is the closest measured point to the sample. The other channels show the temperatures at various points inside the CCR.



SetpointLP1 280.0000
SP1 280.0000
TolLP1 1.0000
Loop1_Status At_Temp
ramprateLP1 0.0000

SetpointLP2 1.0000
SP2 1.0000
TolLP2 10.0000
Loop2_Status Out_of_te
ramprateLP2 0.0000

SetpointLP3 245.0000
ASP3 100.0000
TolLP3 0.0000
Loop3_Status Out_of_te

SetpointLP4 0.0000
ASP4 0.0000
TolLP4 0.0000
Loop4_Status At_Temp

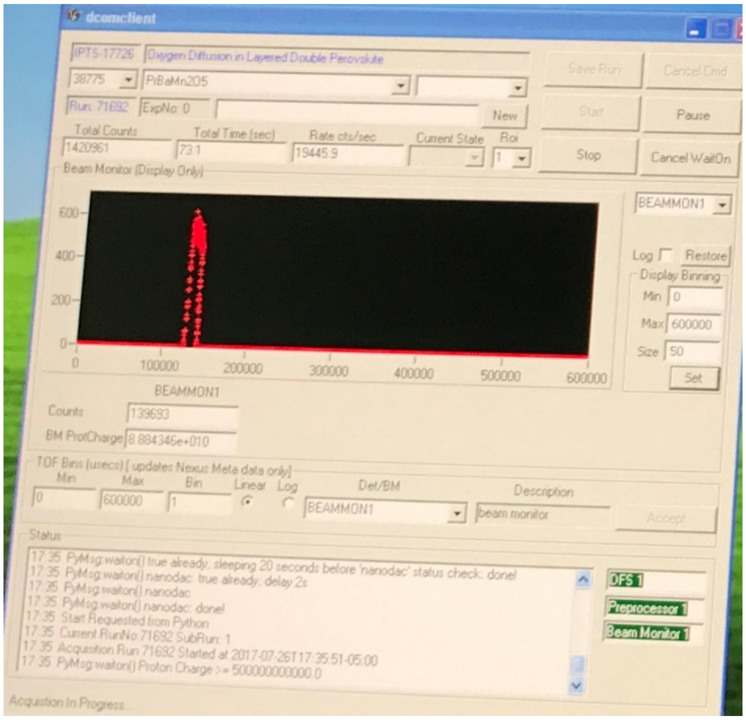
SensorA 280.0010
SensorB 279.9000
SensorC 0.0000
SensorD 0.0000

```
20:56  Handling RunStop
21:38  Handling RunStart. Run No: 77514 1 Instr: BSS
22:47  Handling RunStop
22:47  Handling RunStart. Run No: 77515 1 Instr: BSS
23:18  Handling RunStop
23:18  Handling RunStart. Run No: 77516 1 Instr: BSS
23:45  Handling RunStop
23:46  Handling RunStart. Run No: 77517 1 Instr: BSS
```

Figure 13. Lakeshore application to set temperature

Starting and stopping measurements

One can use either dcomclient (see Figure 14 below), or PyDas /tablescan (see Figure 12 above) to start measurement at BASIS. When starting the measurement at dcomclient, a user needs to click the ***start***, and the measurement will progress until the user manually stops the measurement by clicking the ***stop***. The measurement time and statistics are displayed at the dcomclient window. If the measurement is started at tablescan window, by clicking ***run,*** then the measurement will progress line by line until the last populated line is finished, or until the user stops it by clicking ***stop*** at the table scan window. When measurement is started, the detectors banks (Figure15) should show intensity at the quarters populated by the type of analyzers used for the current measurement. Each measurement will have associated run number, and the data will be stored automatically after each run is finished under the current IPTS number.



IPTS-17726 Oxygen Diffusion in Layered Double Perovskite

38775 PrBaMn2O5

Run: 71692 ExpNo: 0

Total Counts: 1420961
Total Time (sec): 73.1
Rate cts/sec: 19445.9
Current State:
Roi: 1

Beam Monitor (Display Only)

BEAMMON1

Log ☐

Display Binning
Min: 0
Max: 600000
Size: 50

BEAMMON1
Counts: 139693
BM ProtCharge: 8.884346e+010

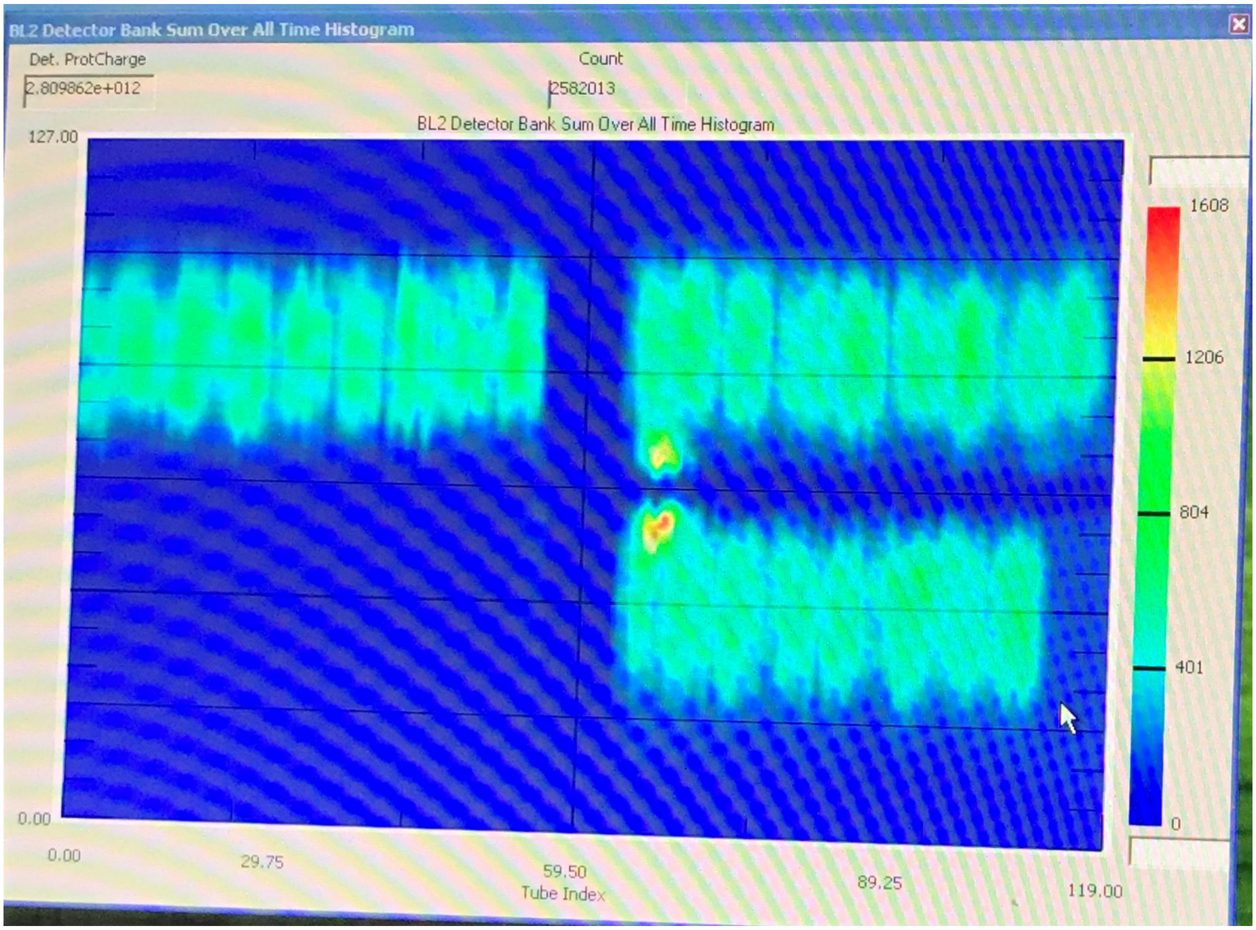
TOF Bins (usecs) [updates Nexus Meta data only]
Min: 0
Max: 600000
Bin: 1
Linear ● Log ○
Det/BM: BEAMMON1
Description: beam monitor

Status

```
17:35 PyMsg:waiton() true already; sleeping 20 seconds before 'nanodac' status check: done!
17:35 PyMsg:waiton() nanodac: true already; delay 2s
17:35 PyMsg:waiton() nanodac
17:35 PyMsg:waiton() nanodac: done!
17:35 Start Requested from Python
17:35 Current RunNo:71692 SubRun: 1
17:35 Acqusition Run 71692 Started at 2017-07-26T17:35:51-05:00
17:35 PyMsg:waiton() Proton Charge >= 500000000000.0
```

Acqustion In Progress...

Figure 14. dcomclient window to control the measurement at BASIS.



Det. ProtCharge 2.809862e+012

Count 2582013

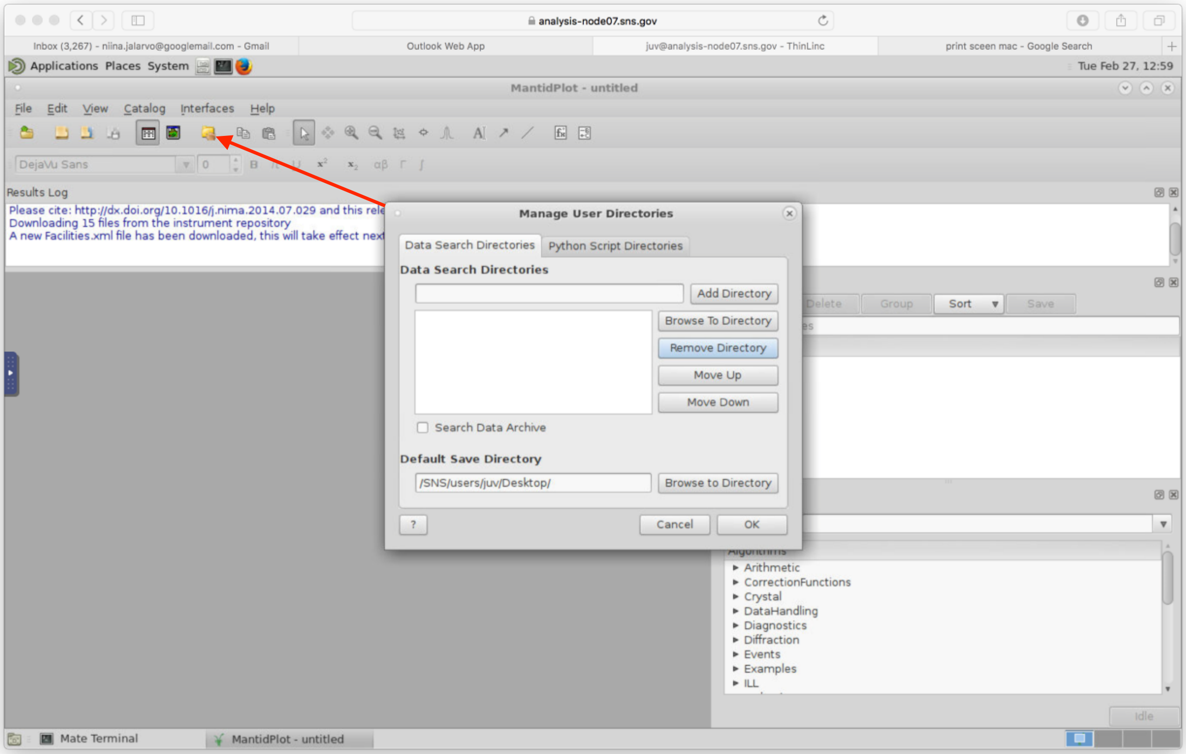
Figure 15. Detector banks at BASIS. The intensity in this case is distributed over the 3 quarters populated with the Si111 analyzers. The quarter without intensity (left side bottom) is covered with Si311 analyzers.

Section 6. Data Reduction

BASIS data can be reduced by using the bac or bac2 computers located at the BASIS control hut, or from other locations by connecting to analysis.sns.gov. BASIS users can login to these computers using their ucams or xcams accounts. When logged in, MantidPlot first needs to be launched.

Setup User Directory

To set up desired directory for reduced data, click the *Manage User Directories* symbol on the symbol bar (seventh from the left). A pop-up window will open allowing user to modify the save directory as wished (Figure 16). The input data will be automatically searched at the server.



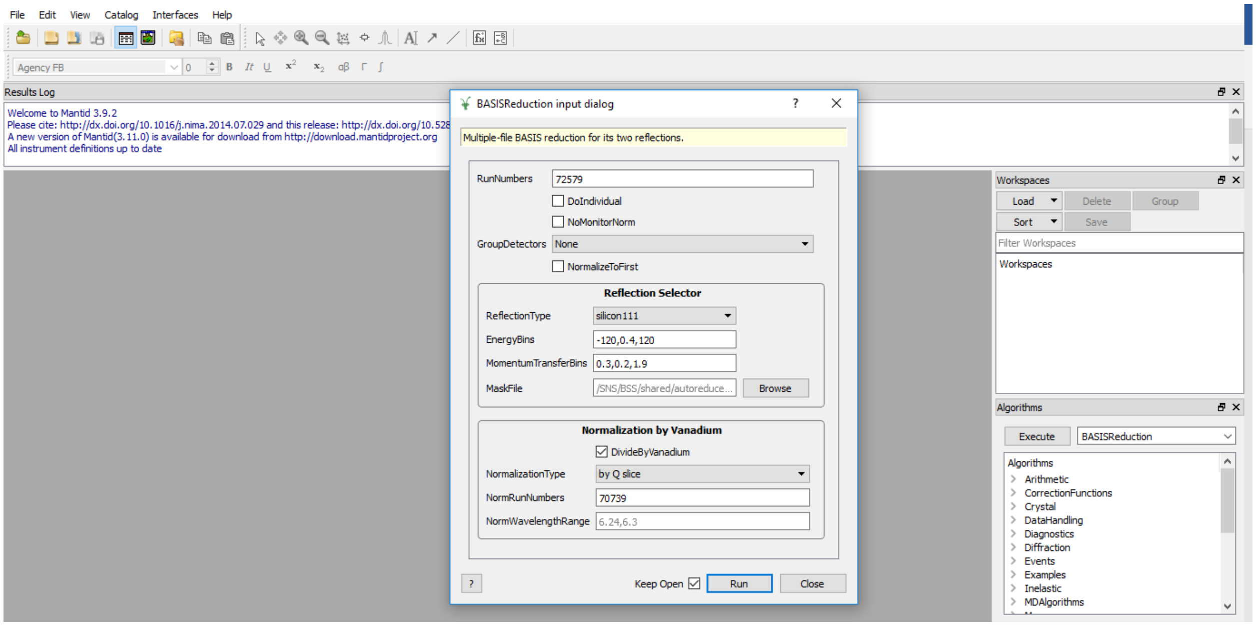
```
Please cite: http://dx.doi.org/10.1016/j.nima.2014.07.029 and this rele
Downloading 15 files from the instrument repository
A new Facilities.xml file has been downloaded, this will take effect next
```

Default Save Directory: /SNS/users/juv/Desktop/

Figure 16. MantidPlot setup user directories.

BASIS data reduction

- To *__launch BASISReduction__* algorithm, type BASISReduction to the line next to the execute-button (right hand side on the middle of the window), then click execute. BASISReduction pop-up window will open (Figure 17).
- *__Fill in the run number__* or run numbers to be reduced. If several runs are to be reduced, there is an option to reduce them so that they will be merged to one output file. Alternatively, each one of them can be reduced separately and the data will be saved in separate files. In the latter case, choose the DoIndividual option right below the given run numbers.
- Then move to the *__Reflection Selector part__*. Choose the analyzer type that was used for the measurement, either Si111 or Si311.
    - For Si111 analyzer the *EnergyBins* should be set up from -120 to +120 using step size of 0.4 (-120,0.4,120). *MomentumTransferBins* are set the same way, first will be given the average of the lowest Q bin value, then the step size and then the average of the highest Q bin value. Typically, data is grouped to 9 Q bins, with bin width of 0.2 A^{-1} (these values are displayed in Figure 17). Also, bin width of 0.1 A^{-1} is often used if the statistics of the data allows. In that case the given limits, would be 0.25 and 1.95 to reflect the average value of the lowest and highest Q bin. Then the correct *MaskFile* needs to be chosen. Mask_default_111 can be used to Si111 analyzers, and Mask_default_311 can be used for Si311 analyzers. These files can be found under shared directory (BSS/shared/autoreduce/new_masks_08-12-2015).
    - For Si311 input values for *EnergyBins* would be (-740, 1.6, 740) and for *MomentumTransferBins* (0.4, 0.3, 3.7).
- When possible, *__normalization by vanadium__* should be done. In this case, click the DividebyVanadium box, choose NormalizationType for *by Q slice,* and give the vanadium run number. If you did not measure vanadium, BASIS instrument staff member can provide the current vanadium run number for standard sample geometries.
- By clicking the ***run*** box on the bottom of the BASISReduction window, the data reduction will start. This will take some time, and when it is finished, reduced data files will be stored in the specified directory. Reduced data files will also appear in MandtidPlot as workspaces. Those can be viewed immediately (right mouse click the workspace and then choose *plot spectrum*).
- Data will be stored automatically in *.nxs and *.dat formats. The former is readable in MantidPlot, allowing also to visualize and work on the data within MandtidPlot. The dat format is a grouped ascii file, that has 3 columns (energy value, data point, error), and all the Q bins are written into these columns one after the other. This format is required by DAVE/PAN application that is often used to fit BASIS data at present time.



Welcome to Mantid 3.9.2
Please cite: http://dx.doi.org/10.1016/j.nima.2014.07.029 and this release: http://dx.doi.org/10.528
A new version of Mantid(3.11.0) is available for download from http://download.mantidproject.org
All instrument definitions up to date

BASISReduction input dialog

Multiple-file BASIS reduction for its two reflections.

RunNumbers 72579
☐ DoIndividual
☐ NoMonitorNorm
GroupDetectors None
☐ NormalizeToFirst

Reflection Selector

ReflectionType silicon111
EnergyBins -120,0.4,120
MomentumTransferBins 0.3,0.2,1.9
MaskFile /SNS/BSS/shared/autoreduce...

Normalization by Vanadium

☑ DivideByVanadium
NormalizationType by Q slice
NormRunNumbers 70739
NormWavelengthRange 6.24,6.3

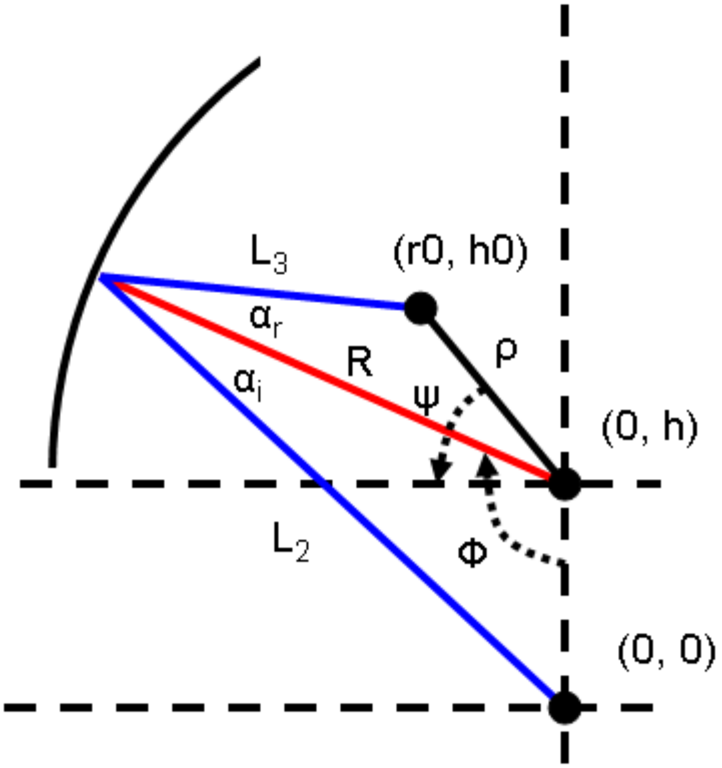
Keep Open ☑

Figure 17. MantidPlot; launching BASISReduction algorithm. The reduction here is done for Si111 analyzers, and for 9 Q bins.

Section 7. Data Output Formats

The standard output of the BASIS data reduction routine is a file compatible with the 3-column ASCII format used by the DAVE reduction software (energy transfer, intensity, intensity error). If the data are binned to more than one Q bin, the file format is known as DAVE Grouped ASCII (1 column of data for the energy transfers (same for all Qs), then 1 column of data for the Q values, then 2 columns of data for the intensity and intensity error for each Q value or "Group", beginning with Group 0, which corresponds to the first Q value). Note that DAVE may experience problems with loading a file that has a Grouped ASCII format, yet possesses only one Q bin. In such case, even if the data are intended to be reduced using just one Q bin (e.g., for the BASIS all-inclusive (in QENS regime) Q range of 0.2 Å^{-1} $< Q < 2.0$ Å^{-1}, for which - - mom-trans-bin = 0.2, 2.0, 1.8 command is utilized), users may add, for the sake of getting the output data loaded to DAVE quickly, a second, "dummy" Q bin (e.g., 0.2 Å^{-1} $< Q < 2.0$ Å^{-1} and 2.0 Å^{-1} $< Q < 3.8$ Å^{-1-}, for which - - mom-trans-bin = 0.2, 3.8, 1.8 command is utilized). It should be noted that not all versions of DAVE would accept a file containing one or more nan (not a number) values.

Appendix. Bragg reflections from the crystal analyzer panels.



- r_0, `rCylinder` - The radius of the cylinder that the detectors are on.
- R, `rSphere` - The radius of the sphere that the analyzer crystals are on.
- h, `sphereOffset` - The vertical offset to the focal point of the analyzer crystal.
- h_d, `cylinderOffset` - The vertical offset of the detector center.
- $h_0 = y_{off} + h_d$, `h0` - The position (height) of the pixel in global coordinates.
- ϕ, `phi` - The angle of elevation of the radius vector to where the neutron is scattered on the surface of the analyzer crystal measured from the negative y-axis.
- ψ, `psi` - The angle between the detector pixel position vector and the horizontal.
- α, `alpha` - The angle of reflection on the analyzer crystal measured from the surface normal.
- α_i, `alphaI` - The incident angle of reflection on the analyzer crystal measured from the surface normal.
- α_r, `alphaR` - The reflected angle of reflection on the analyzer crystal measured from the surface normal.
- x_{off}, `xOffset` - The arc position ($x_{off} = r_o\theta$) of the pixel in the local x-coordinate.
- y_{off}, `yOffset` - The position of the pixel in the local y-coordinate.

- θ_D, `thetaD` - The angle from the pole of the detector pixel constrained in the scattering plane.
- ρ, `rho` - The distance from the sphere center to the detector pixel.
- λ, `wavelength` - The wavelength of the scattered neutrons.
- λ_{off}, `wavelengthOffset` - Scale parameter of the scattered wavelength. It is the wavelength of the neutrons selected if they are scattered normal to the scattering plane.

The parameter ψ is described by

- $\psi = \arctan\left(\frac{h_0 - h}{r_0}\right)$

while the parameter ρ is

- $\rho = \sqrt{r_0^2 + (h_0 - h)^2}$

There are three values that all other information depends on. They are the secondary flight path (distance), polar angle, and azimuthal angle. The equations for these three entitees are:

- $distance = L_2 + L_3$
- $polar = \arccos\left[\frac{R}{L_2}\cos(\theta_D)\sin(\phi)\right]$
- $azimuthal = \arctan\left(\frac{h/R - \cos(\phi)}{\sin(\phi)\sin(\theta_D)}\right)$

In the equation for distance L2, the distance from sample to analyzer crystal, is calculated using

- $L_2 = \sqrt{R^2 + h^2 - 2Rh\cos(\phi)}$

L3, the distance from analyzer crystal to detector, is calculated using

- $L_3 = \sqrt{R^2 + \rho^2 + 2R\rho\sin(\psi - \phi)}$

The wavelength is calculated according to

- $\lambda = \lambda_{off}\cos(\alpha)$

Where α is calculated (the two alphas should be identical):

- $\alpha = \frac{\alpha_i + \alpha_r}{2}$

The incident angle of reflection is

- $\alpha_i = \arccos\left(\frac{R^2 + L_2^2 - h^2}{2RL_2}\right)$

The reflected angle of reflection is

- $\alpha_r = \arccos\left(\frac{R^2 + L_3^2 - \rho^2}{2RL_3}\right)$

The goodness of fit, the criteria for determining the value of ϕ is

- $fit = \cos(\alpha_i) - \cos(\alpha_r) \propto L_3\left(R^2 + L_2^2 - h^2\right) - L_2\left(R^2 + L_3^2 - \rho^2\right)$

A 'good' value of phi is found when this is zero.