Contents

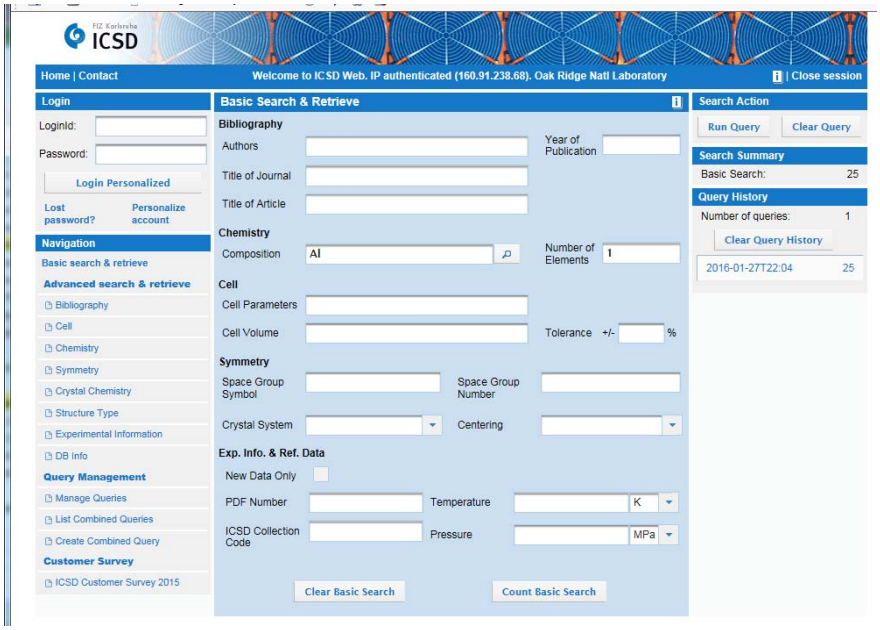
1. Propose an experiment

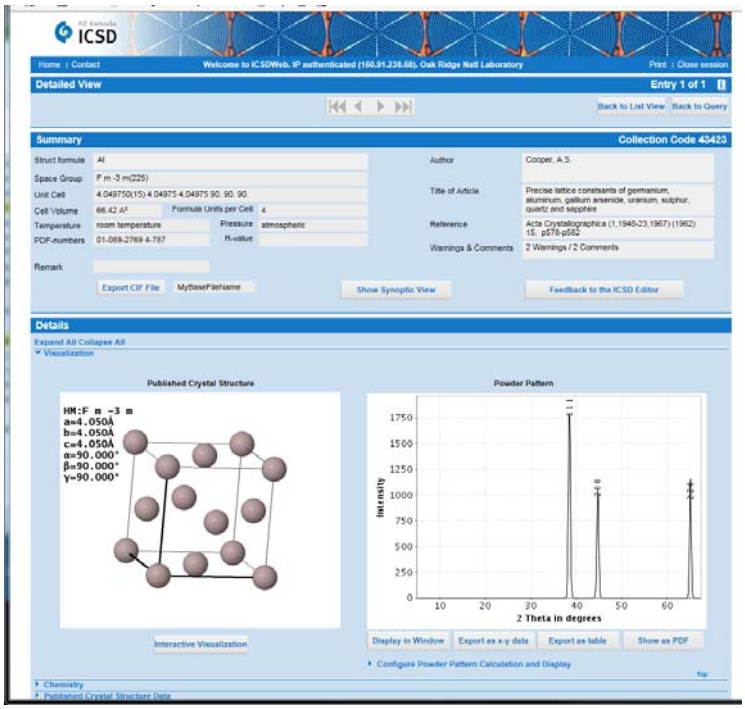
a. Choose an instrument
    i. Basic decisions
        1. Elastic or spectroscopy?
        2. Energy resolution desired? (TAX, DGS / VISION, backscattering, NSE)
        3. Type of measurement (parameter in narrow Q is better for TAX)
        4. Energy transfer range & Q desired? (ARCS/SEQ or CNCS/HYSPEC)
    ii. HYSPEC is NOT a typical Direct Geometry Spectrometer
        1. Our strength is NOT out-of-horizontal-plane scattering, so don't bother lining up on the c-axis to measure the AB-scattering.
        2. Instead, just like at a TAX, align any single crystal with the desired scattering plane in the horizontal plane.
        3. Yes, we also do powders.
        4. Vertical focusing washes out our vertical Q resolution. Most users prefer the flux.
    iii. Recommended papers to read to understand HYSPEC's niche:
        1. "Recent progress on HYSPEC, and its polarization analysis capabilities", EPJ Web of Conferences, **83**, 03017(2015)
        2. "A comparison of four direct geometry time-of-flight spectrometers at the Spallation Neutron Source", Review of Scientific Instruments, **85**, 4, 045113 (2014).
    iv. Communicate with instrument scientists about your experimental needs
        1. Ovi Garlea: garleao@ornl.gov
        2. Barry Winn: winnbl@ornl.gov
b. Consider instrument configuration (see section 7 below) in advance
    i. NOW THAT'S THINKING AHEAD!
c. IPTS 101
    i. The links under 'Become a User' at http://neutrons.ornl.gov/users are helpful.
    ii. Instructions on using IPTS in general???
    iii. HYSPEC specific: Special questions for polarization analysis and for being considered for the HYSPEC IDT proposal review.

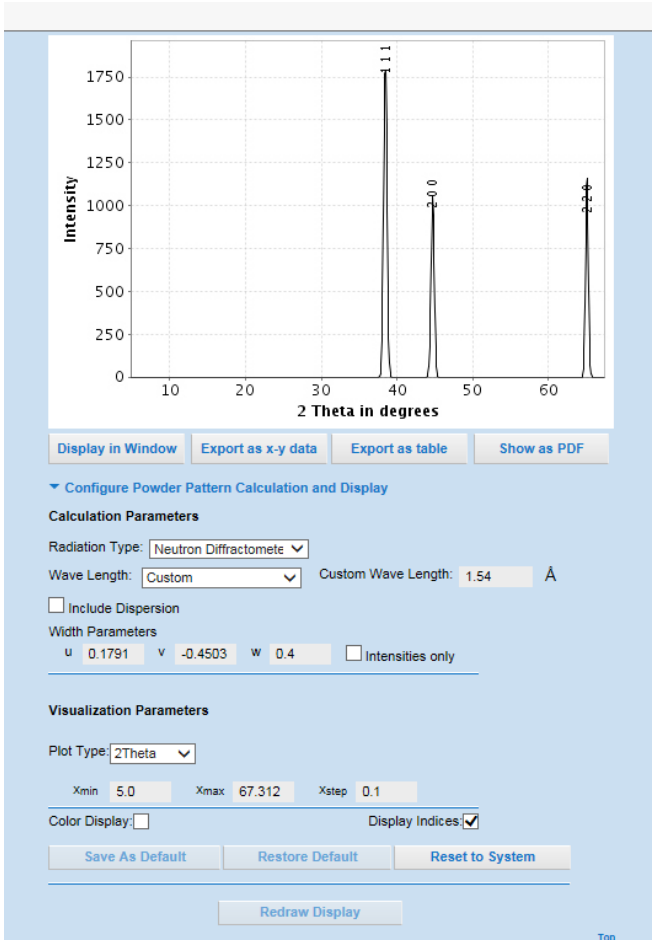
2. Before you travel to HYSPEC

a. Know your sample

i. ICSD 101 (for Bragg peak locations and neutron scattered intensities)
https://icsd.fiz-karlsruhe.de/search/basic.xhtml





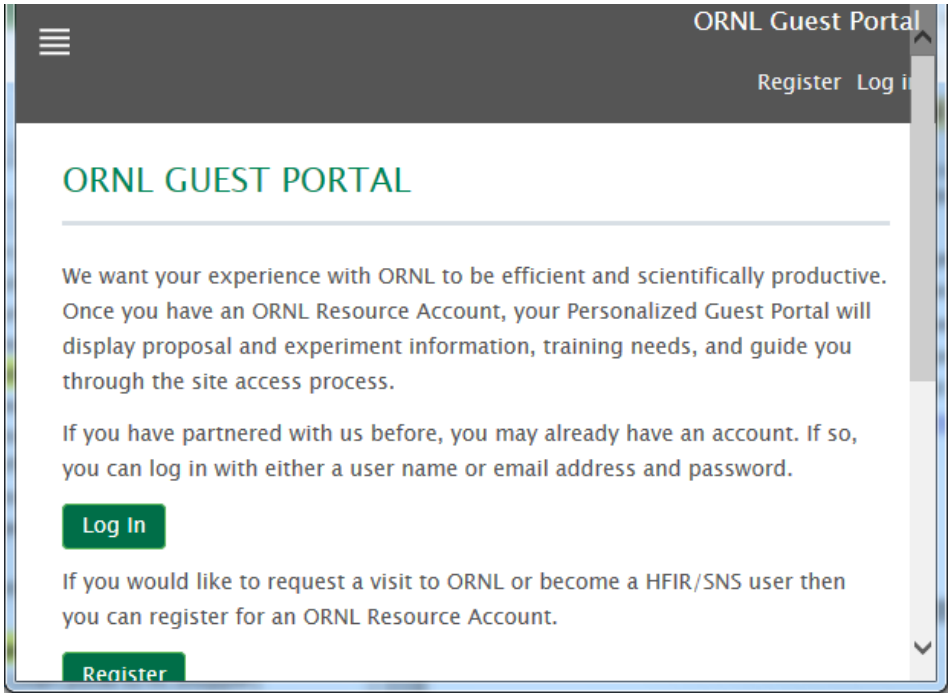


ii. Users are expected to know the crystal lattice structure and dimensions prior to arriving. You need to know the basis cell dimensions and angles, and if it's a

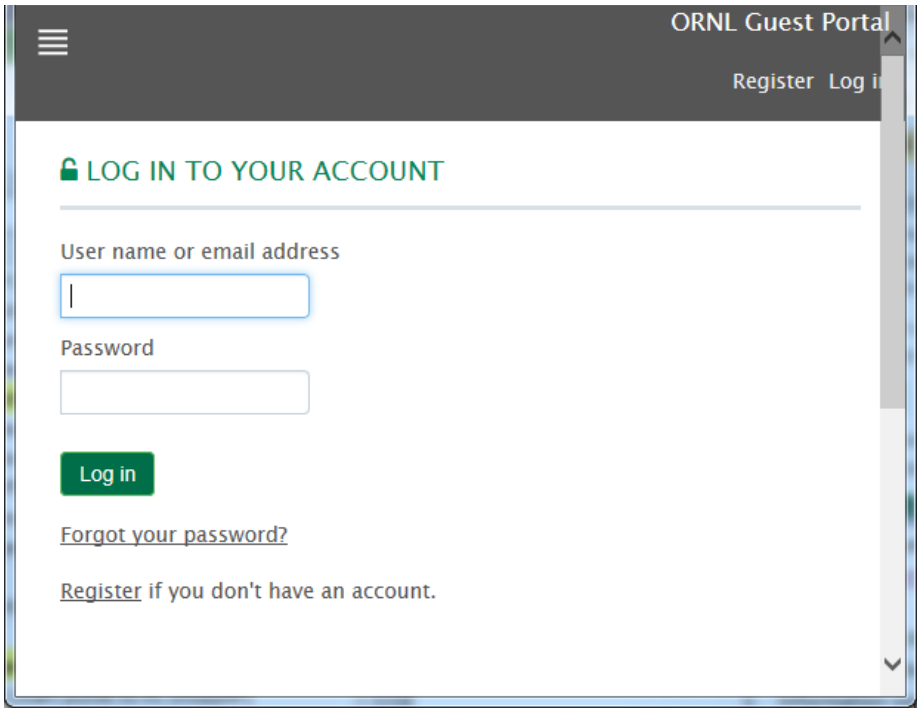
single crystal you also need to know which scattering plane you intend to study, in terms of key symmetry directions in reciprocal lattice unit dimensions (r.l.u). These directions often correspond to Bragg peaks visible in that plane.

b. Preparing for data

   i. You must have an XCAMS account in order to do several things, including the web-based training required prior to entry. You also need this account in order to access your experimental data and to use ORNL's computing resources to process / analyze the data.

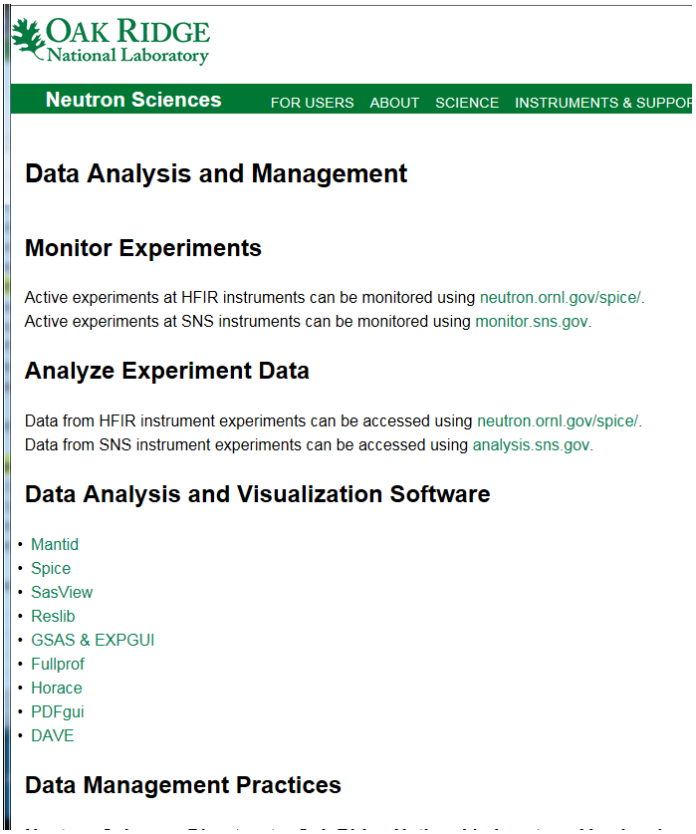


If you do not yet have an account, go to the guest portal at https://user.ornl.gov/ to register.



Not to worry; there is a link at https://user.ornl.gov/Account/Login for those many users who have once again forgotten their passwords.

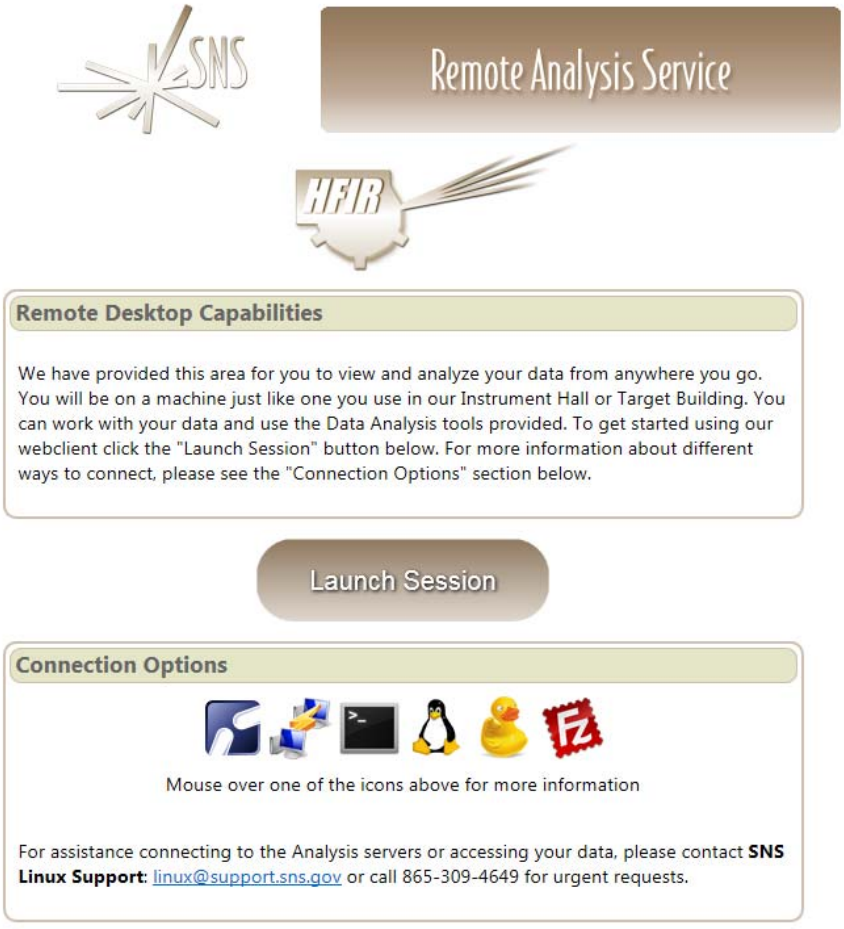
ii. Information concerning data analysis for HYSPEC and other neutron scattering instruments at ORNL can be found at http://neutrons.ornl.gov/users/data-mgmt.



If you are unfamiliar with analysis software for direct geometry spectrometers, we recommend you familiarize yourself in advance with DAVE and in particular its mslice application at http://www.ncnr.nist.gov/dave/documentation/dcs_mslice.pdf.
For users that require greater sophistication for their analysis, we recommend you familiarize yourself with Horace at http://horace.isis.rl.ac.uk/Main_Page .

iii. If you have an XCAMS account, you should also have an account on the analysis cluster. Go to https://analysis.sns.gov/ and inside the 'connection options' box you will see a variety of ways you can open terminals or move data to your

personal computers.



iv. From https://analysis.sns.gov/, click the 'launch session' button to begin a session on the Analysis Cluster, which uses Linux. It is using a web-based version of the ThinLinc client found in the 'connection options' box.

v. Confirming your IPTS directory is ready (*not yet prior to first run*) involves launching a session as described above, opening a terminal, and attempting to move to the following directory from a terminal using the following command:

cd ~/data/SNS/HYS/IPTS-<#>

Where <#> corresponds to the number for the experiment about to begin. If this doesn't work please contact your Local Contact.

vi. Sometimes this directory isn't yet available

~/data/SNS/HYS/IPTS-<your IPTS #>/

but you can access:

```
/SNS/HYS/IPTS-<your IPTS #>/
```

then type in the following either from the HYSPEC analysis machine or the ANALYSIS cluster:

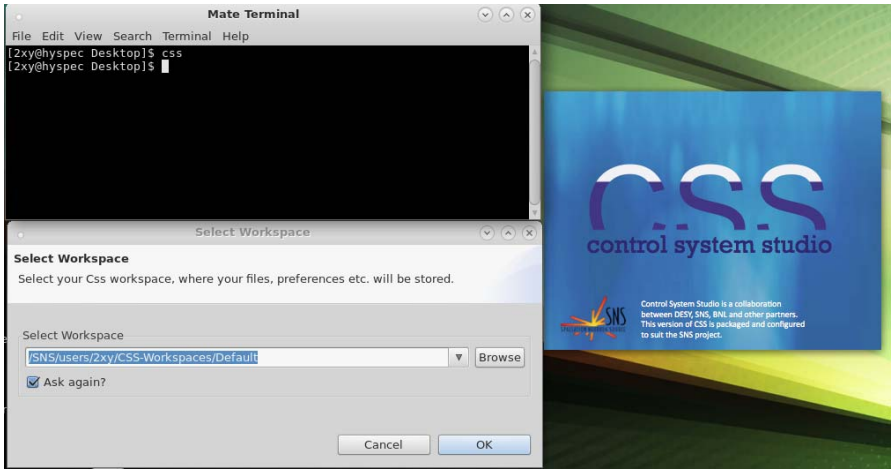
```
/usr/local/sbin/create_symlinks
```

3. Navigating Control Systems Studio (CSS)

a. Starting CSS from DASUSER computer

i. From icon

ii. From terminal

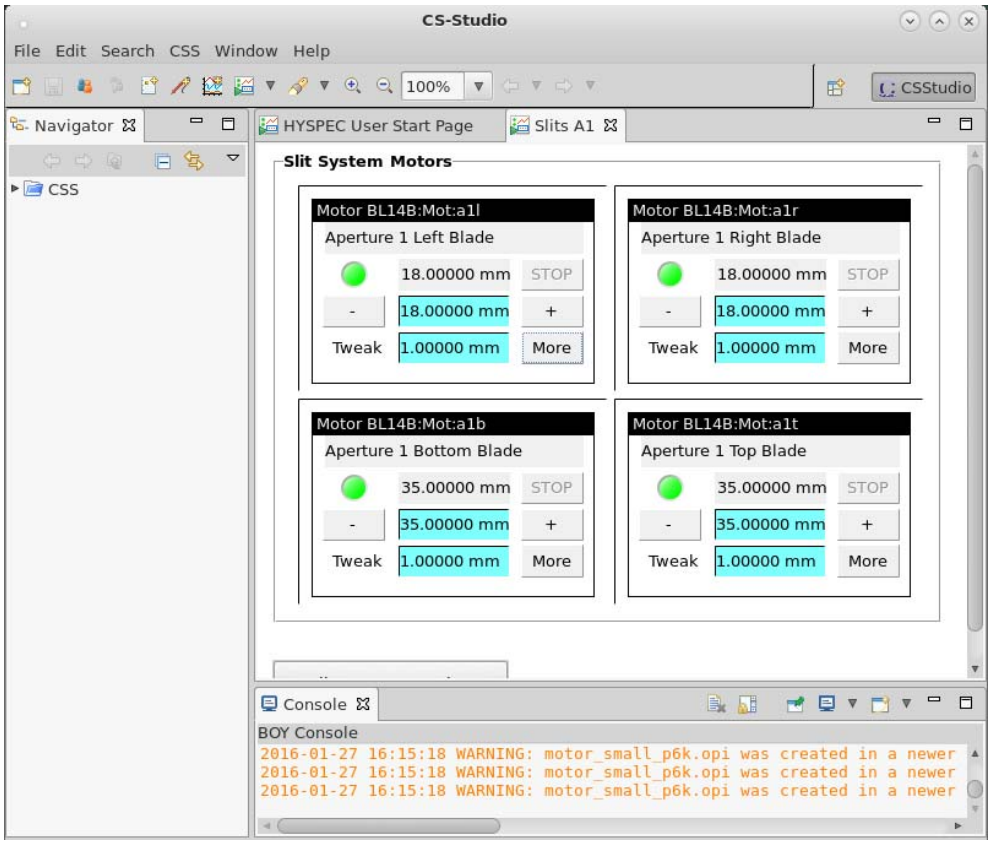


1. Start terminal
2. Type ‘css’ and enter
3. First window ‘Select Workspace’ has a question. Click the ‘OK’ radio button.

iii. Starts in previous configuration

1. You may have some tabs open that you don’t need. Get rid of everything except the HYSPEC user page.

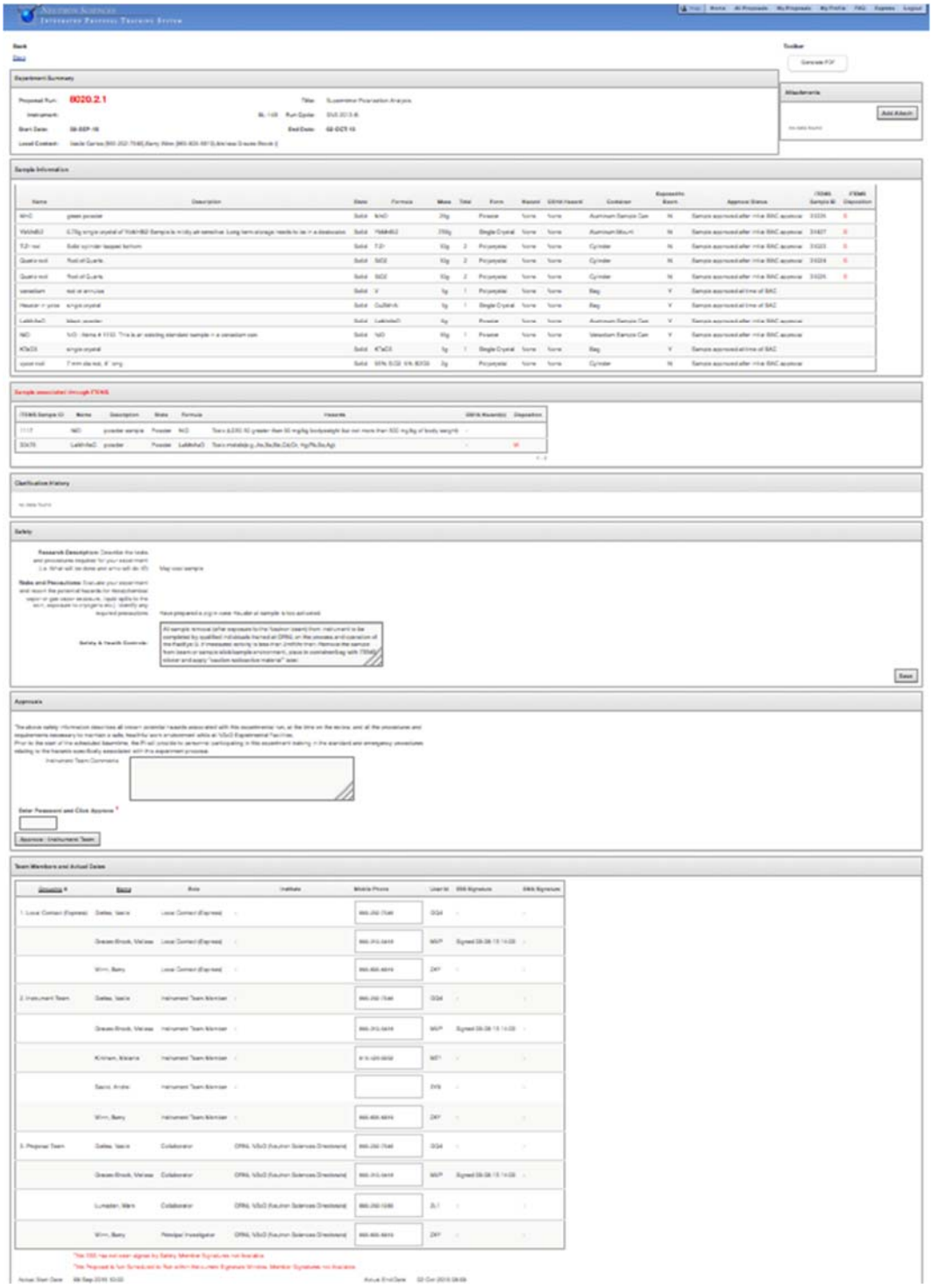
b. ECLIPSE-based Tab'd Graphical User Interface



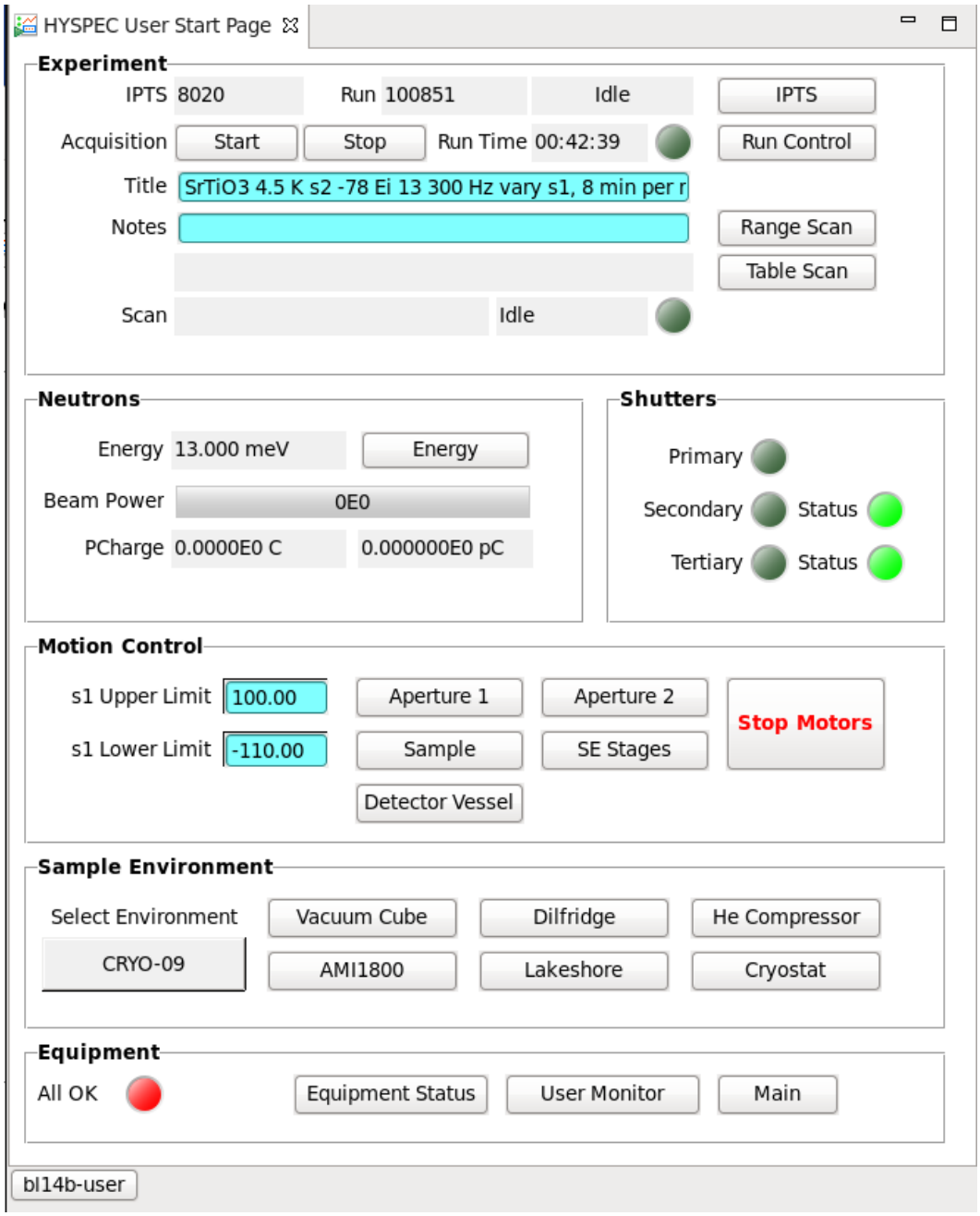
c. Radio buttons
    i. Some drill down to other tab'd GUI's
    ii. Right click allows option to spawn another tab or window
d. Color coded
    i. Grey fields are read-back values: where devices actually are
    ii. Blue fields can be input fields. They are request fields.
        1. No 'Enter', no request!
        2. Compared to Advanced Photon Source, blue field doesn't turn yellow when editing field
    iii. Right click on field to
        1. Copy the PV name, useful for some scans
e. Colon anatomy: understanding the syntax of EPICS variables
    i. Not to worry. They are known as process variables (PV's)
    ii. Master prefix BL14B refers to the HYSPEC instrument (beamline 14-B)
    iii. Next field refers to type of PV: MOT for motors, SE for sample environment, etc.
    iv. Final fields are abbreviations that (at least for motors) follow the HFIR TAX naming standards.
    v. Needed for automated scans.

4. First day at HYSPEC: general setup

a. Reading, understanding, acknowledging and signing off on the Experimental Safety Summary



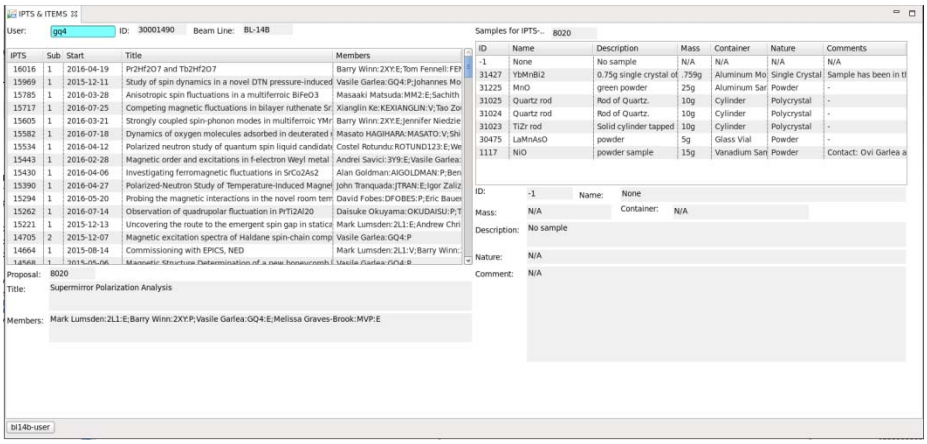
b. CSS User page



c. Assigning the experiment and sample

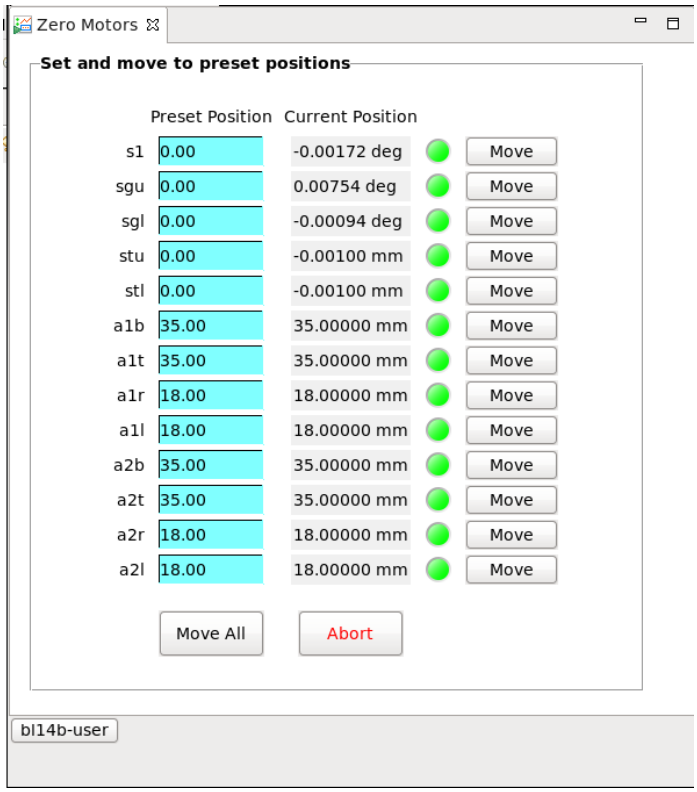
   i. Why bother? Because only the instrument team tied to the assigned IPTS (and the local contacts) can view the data. It would be a shame to generate data without being able to access it!

ii. CSS IPTS page



d. Fresh slate

i. CSS Zero motors page



e. Changing sample environments

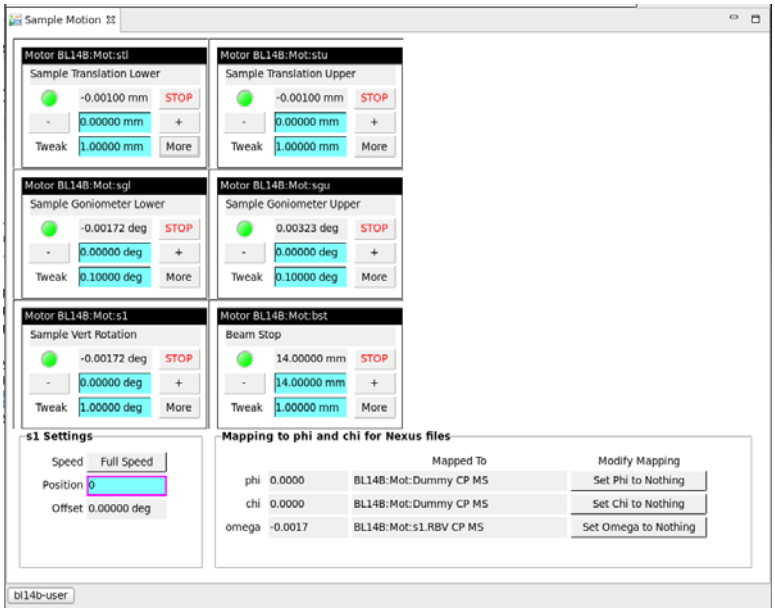
i. Local Contact to restart the associated software driver package

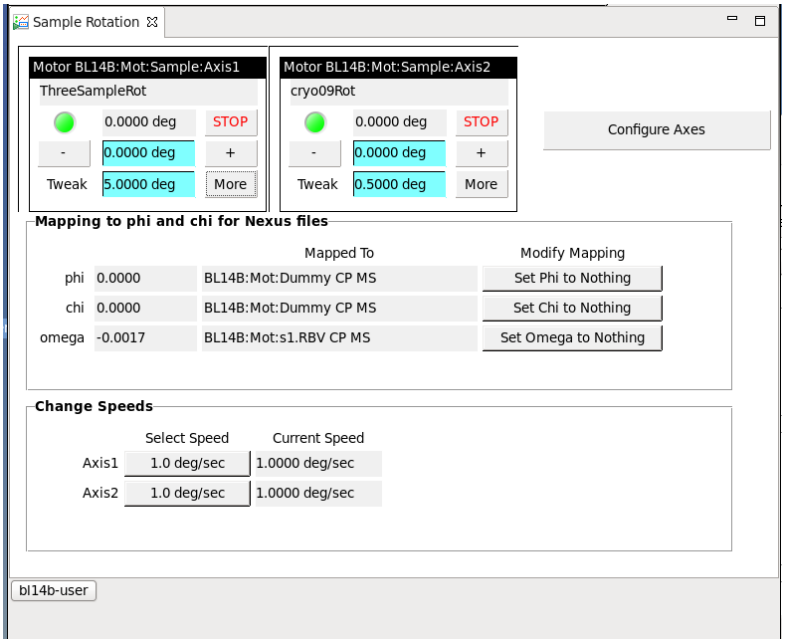
ii. Local Contact to reconfigure software for any changes to rotation stages

f. Setting global's

i. General

ii. What's rotating?



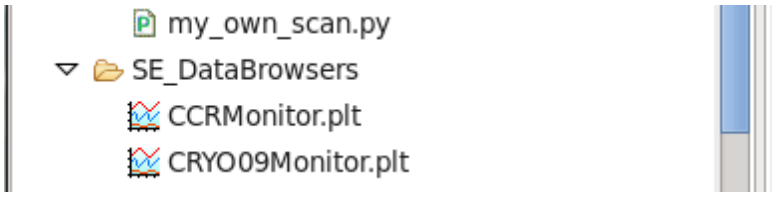


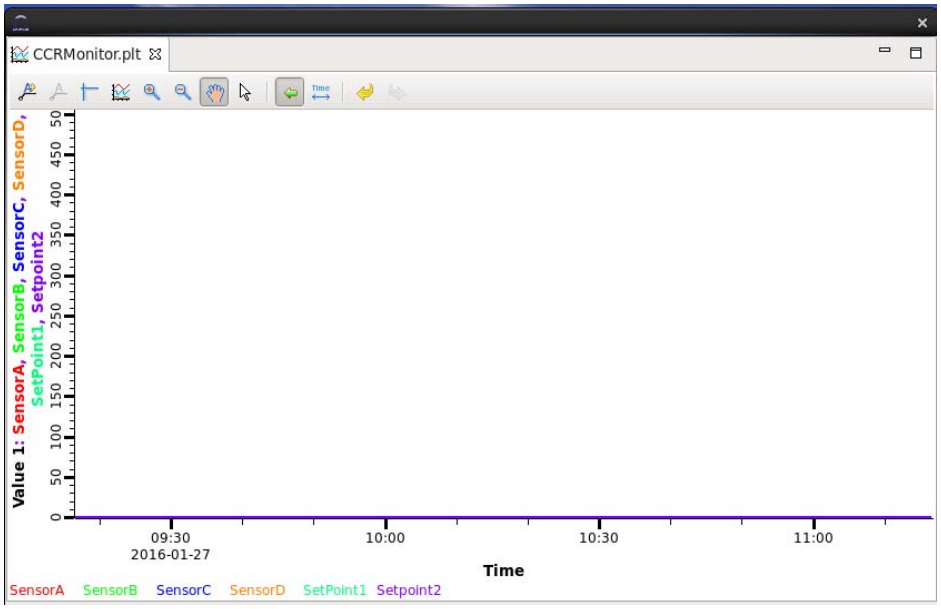
iii. Which sample environment to track? CSS _ page

iv. How do I alarm the right sample environment? For now, go to the main page for a given sample environment. You will find a high-level radio button there to toggle between an alarm-sensitive state or not. This is important for enabling Instrument Hall Coordinators to be alerted to any bad situation.

g. Useful charts

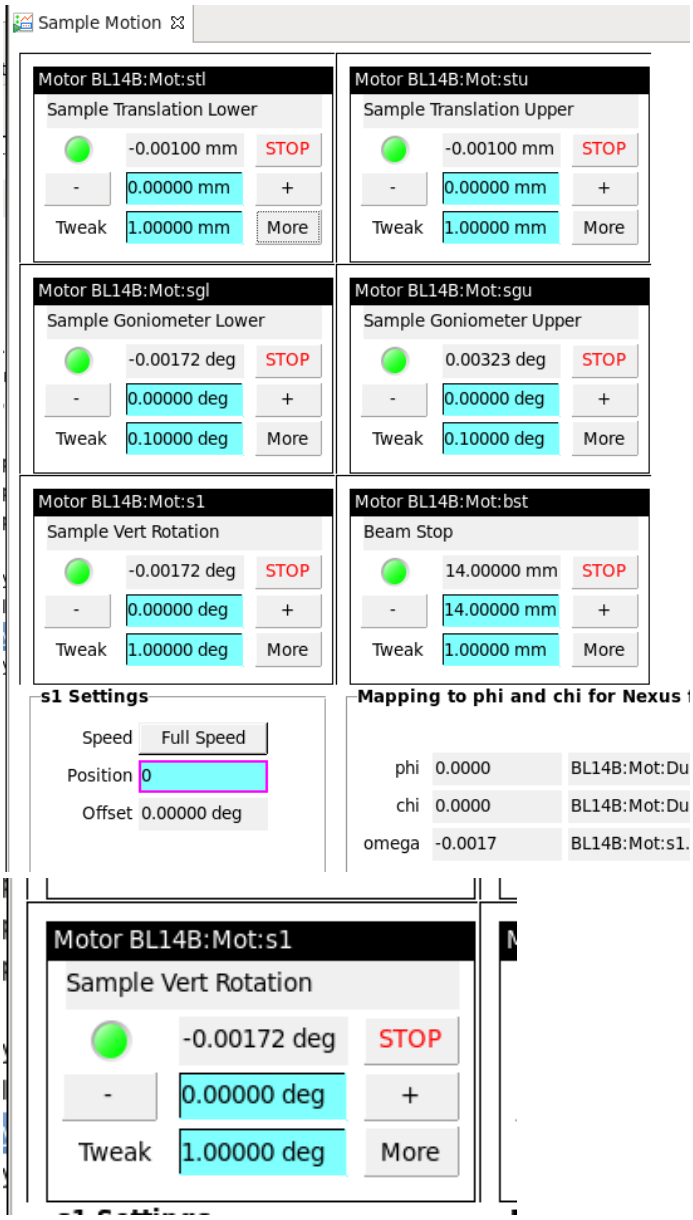
i. Choose depending on sample environment



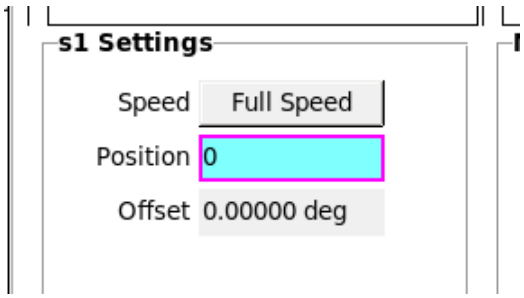


5. Aligning a single crystal

a. Have a powder instead? See section 7.f. for preliminary planning, and then go straight to section 6. You may ignore the rest of this section.
b. Starting with a good guess
    i. Choose two symmetry directions in desired scatter plane
    ii. Line up first direction with incident beam
    iii. If the cyan tilt and translation stages beneath the sample environment don't look roughly square, you forgot to do step 5.c.
c. Spaghetti in the way?
    i. In the field, carefully determine the range of your rotator in advance. The range may be restricted by vacuum lines, compressor lines, cryogen lines, or other cables connecting to the sample environment. Although now rare, if you are rotating the 's1' stage it is also a good idea to look down at the rotation stages to ensure the motor cables are not catching on anything.



d. Slowing down your rotator



e. What am I looking for?

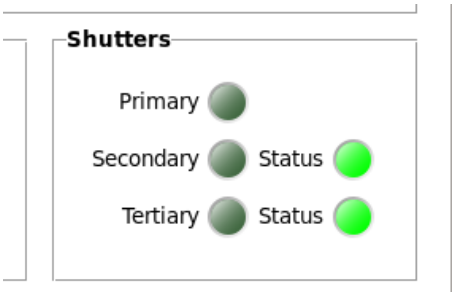
   i. Determining Bragg peak scatter angle and guess of sample angle

      1. Use either the python planning tools (section 7.g.) and/or ICSD (section 2.a.i.) in order to determine scatter and sample angles. ICSD will also

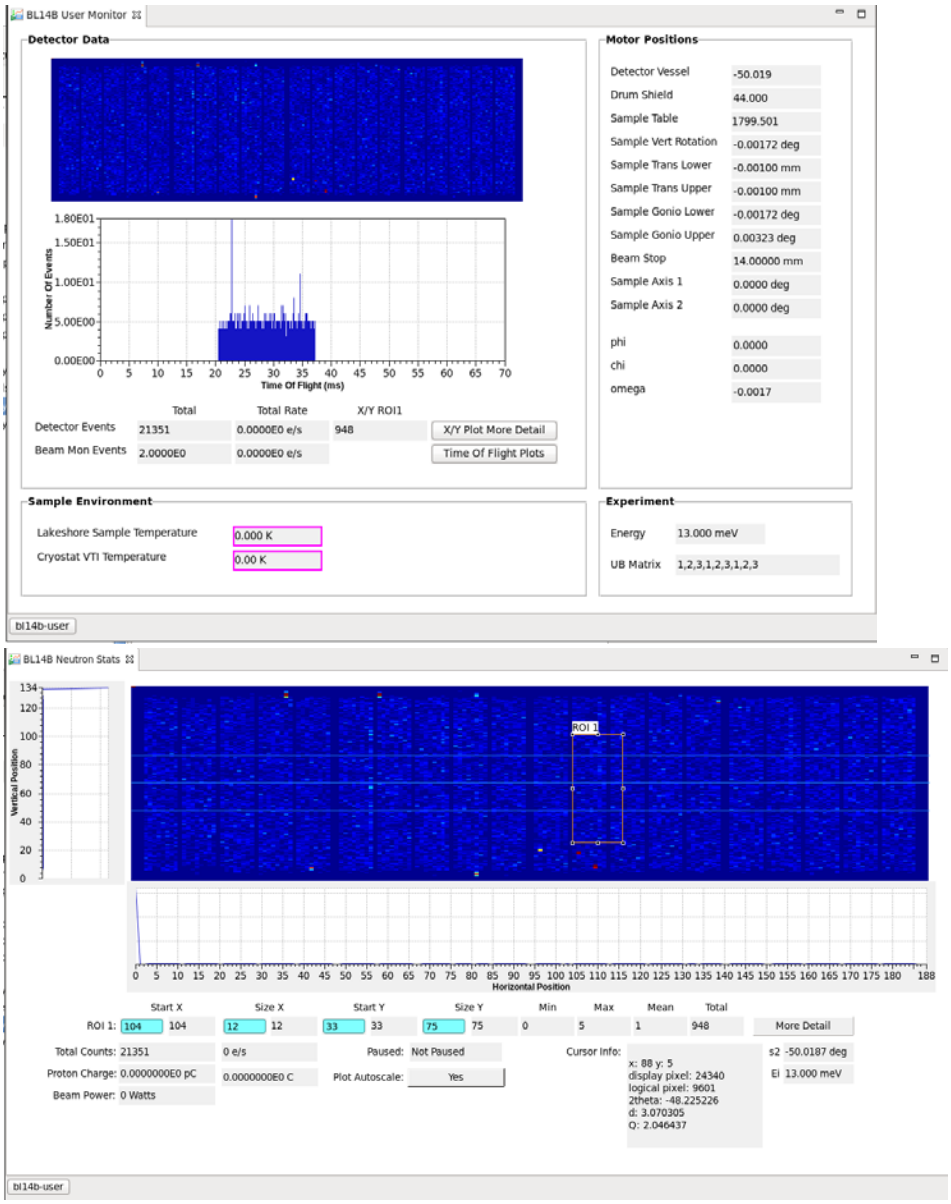
provide relative intensity information useful to choose a good Bragg peak to search for.

2. General recommendation: low Ei's mean fewer and more obvious Bragg peaks
3. May need to modify instrument configuration (see section 8)

ii. Confirming shutters are truly open

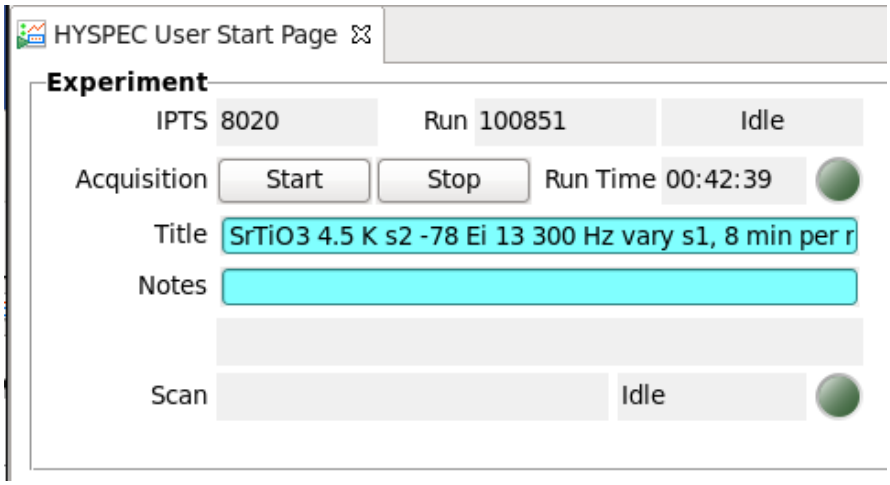


iii. CSS Monitor screen and/or xy view screen



iv. Where will the scatter be? The cursor has a hover feature that tells you all about where the cursor is in angle, elastic d and elastic Q. Note that due to vertical focusing the Bragg peaks are usually extended

f. Keeping an eye out for your first Bragg peak!

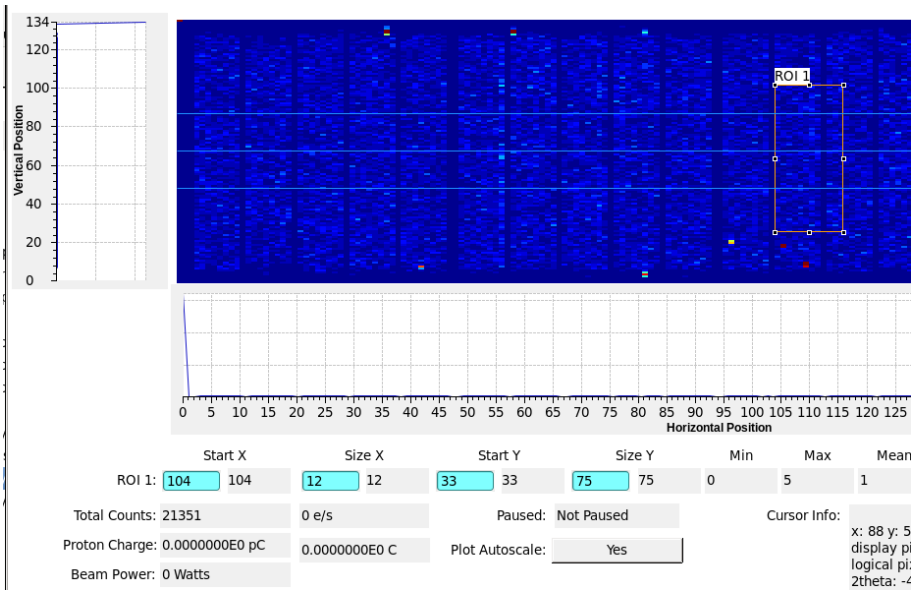


   i. Starting acquisition from HYSPEC User screen
   ii. Start moving your rotation motor slowly by entering a desired destination value in the blue field.
   iii. Hitting motor stop button once you've seen your peak

g. Oh no! I cannot find the peak!
   i. Be patient. Breathe.
   ii. Be willing to go 180 deg
   iii. You may be seriously tilted, beyond about 7 degrees of misaligned tilt the Bragg peaks are no longer visible (they move above or below the position sensitive detectors)
   iv. Contact Local Contact. You two probably have a long night ahead of you.

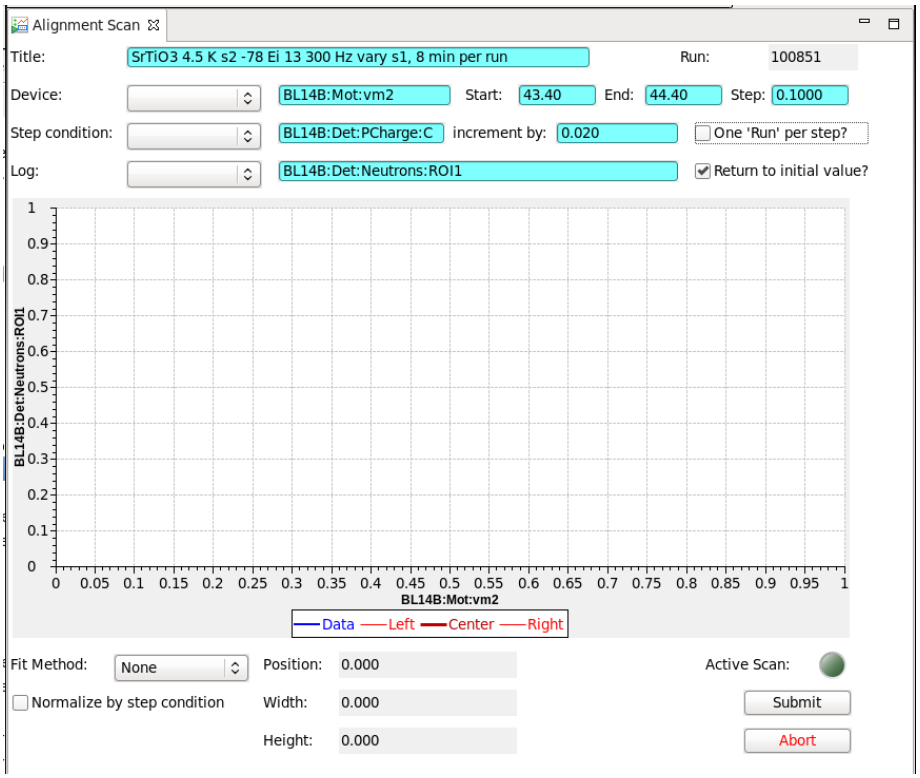
h. Alignment scan, main rotation stage
   i. Fine tuning the location of the Bragg peak
      1. 0.5 to 1 deg steps are OK for the initial check
      2. 0.2 deg steps preferred for fine check.

ii. Choosing your Region of Interest (ROI)



1. CSS Instrument View Screen.

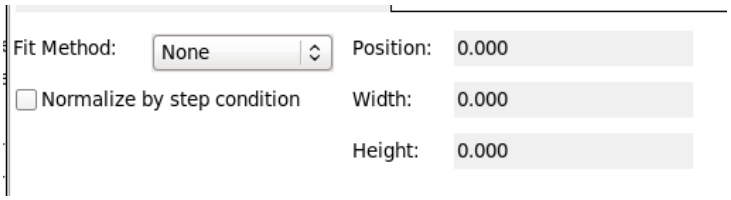
iii. CSS alignment scan screen



1. Pull-down makes choice of what's scanned fairly easy
2. Defaults
    a. Return to original value when scan is done (beware because an abort doesn't cause a return)
    b. One NeXus run for the whole scan
3. Recommend you have scanned variable's page in separate window

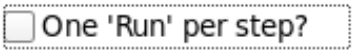
a. Otherwise no clear way to confirm it's moving or have a good idea of desired range
b. A strategy to view the as-stepped value on the alignment screen was proposed and rejected for now…

4. Fitting option selected PRIOR to scan

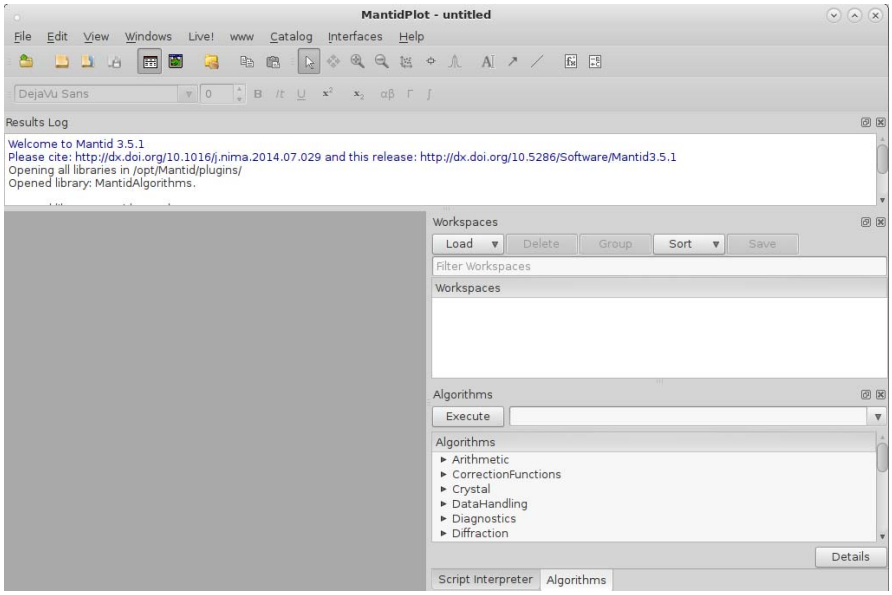


5. Plotting. Right click on the plot field to generate a paper plot of a given alignment scan. Plot before changing scan parameters for the next scan, because the plot axis changes before the data does.

i. If you must work with error bars…
   i. Although CSS is a state-of-the-art system using sophisticated code, it has yet to be able to estimate or to plot statistical errors, so MantidPlot provides an alternative.
   ii. On the CSS alignment scan page, be sure that all steps are in the same run-file.

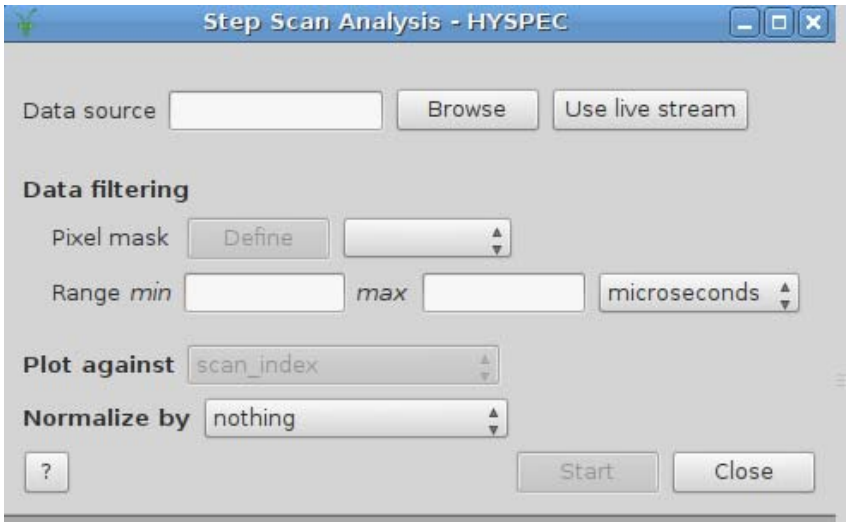


   iii. Open MantidPlot from an analysis session (either HYSPEC or Analysis cluster).



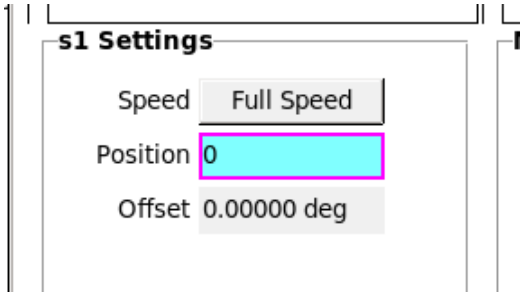
   iv. On 'Interfaces' pull-down menu, open under 'General' subsection the 'Step Scan Analysis' feature. Fill in features as needed and either use Live Stream or a

saved file.



v. Until we have a way to communicate region of interest used on CSS to Mantid, you will need to independently choose your region of interest.

j. Shifting the rotation stage value



k. Complimentary Bragg Peak
   i. Typically parallel to the other symmetry direction
   ii. Usually OK to go directly to nominal rotation stage value and confirm peak is present
   iii. Why bother? In case you have a crazy tilt that wasn't clear at the first Bragg peak

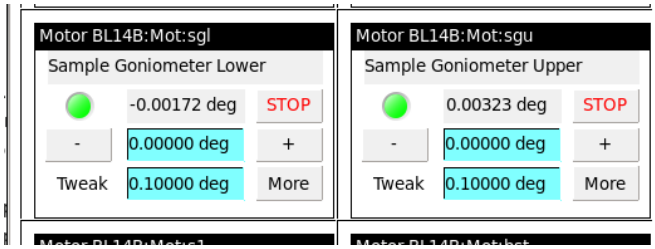
l. How much is too much?
   i. To avoid saturation, peak count-rate needs to be ~100-300 cps. Otherwise saturation will cause non-linear response (counts are no longer proportional to scattered neutron number messing up aperture width selection and rocking scans).
   ii. Attenuation strategy #1: Attenuate via a borated aluminum sheet
   iii. Attenuation strategy #2: Change the Fermi Frequency (see section 8.a.)

m. Getting peaks on the level
   i. Most sample environments are mounted on a tilt and translation stage, and are rotated using the s1 stage. In this case it is fairly trivial to adjust the sample tilt by tilting the entire sample environment. If tilting when using a stick-rotation

mode, we're either unable or not yet ready to implement (tilt would change as a function of rotation angle).

ii. When are they level? When the tall Bragg peaks are centered vertically in the instrument view! There are guides to the eye for normal focusing conditions, and if you're inside them you are probably just fine.

iii. SGU and SGL motors and screen



iv. A perk to a good guess (6.a.) is that the tilt stages are roughly aligned with the symmetry directions.

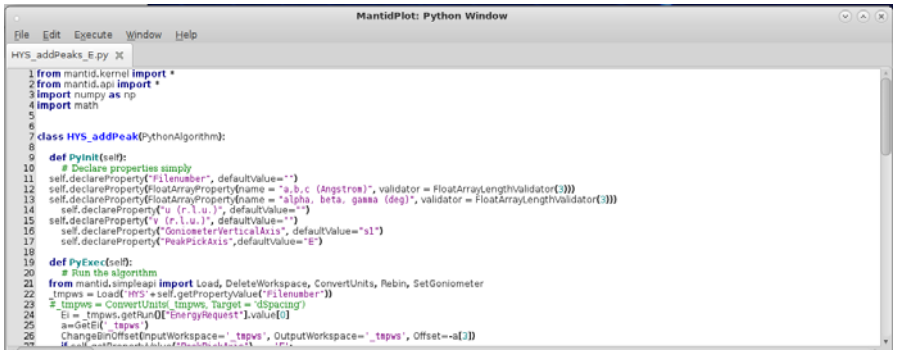
1. If they are not aligned, there is significant cross-talk between tilt stages when optimizing tilts.
2. If your guess was more than, say, 15 degrees off, it's worth your while to physically reorient the sample with respect to the tilt stages

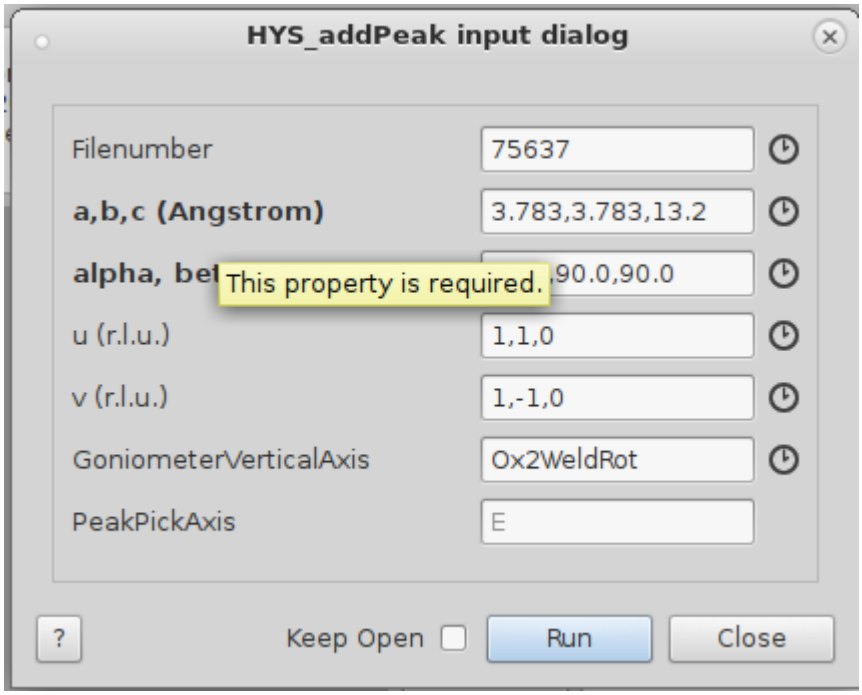
v. Although some prefer an alignment scan (~1 deg steps), we generally find that visual inspection of monitor screen is sufficient. If you do an alignment scan please remember to adjust the Region of Interest to be more or less in the center of the detector array vertically, and about the height of the lines that are guides to the eye.

vi. If you must, we can change to no vertical focusing and you can check again. Most users don't bother.

n. I cannot get my peaks on the level and don't intend to re-align

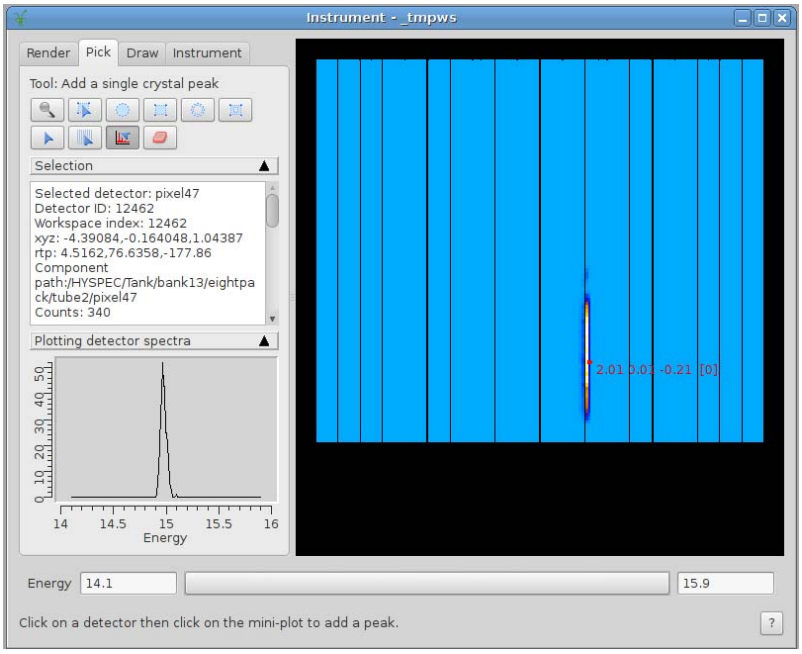
i. In this case you'll need to account for misalignment on the analysis side. Will need UB matrix formalism and 3D U and V vectors for different analysis software.





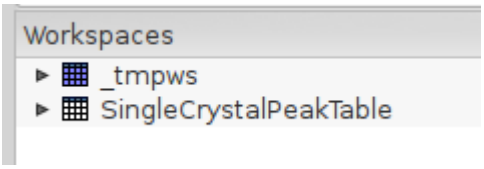
Click on the instrument-view screen, then cleak on the peak position, to set the

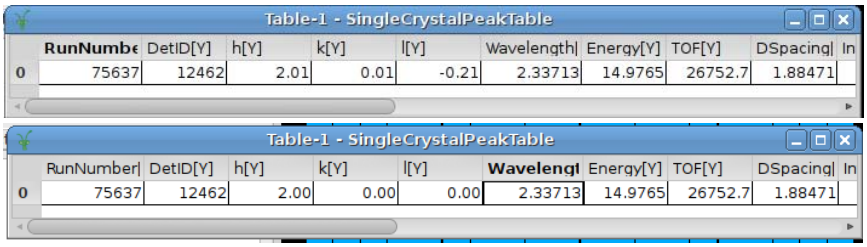
peak and create the SingleCrystalPeakTable.



ii. If you have more files with more peaks to tab, re-run HYS_addPeak with the new run number.

iii. When you are finished locating peaks, right-click on SingleCrystalPeakTable and edit the h, k and l fields as needed to make them integers you expect.

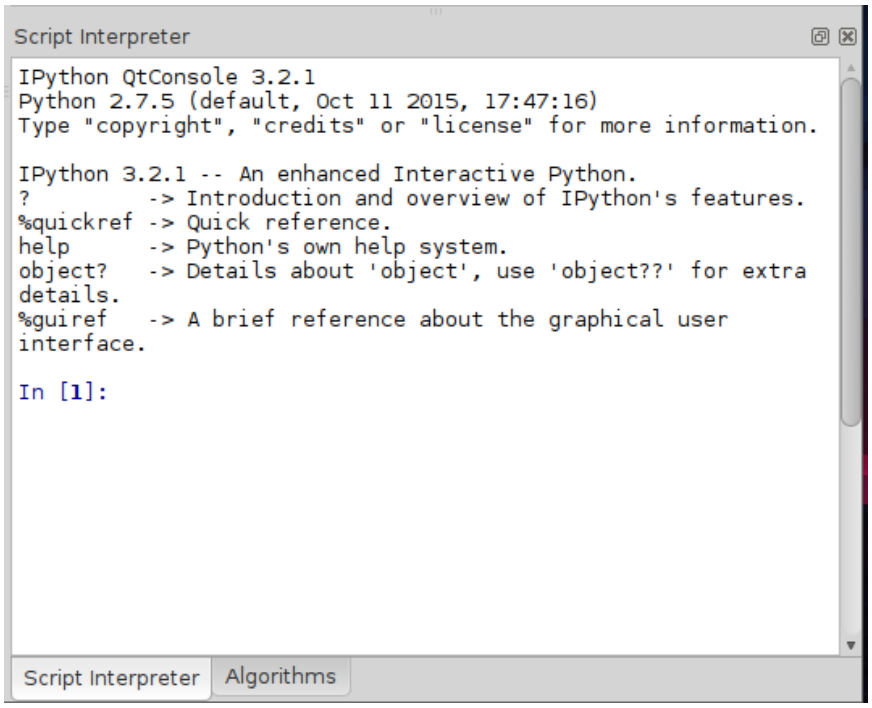




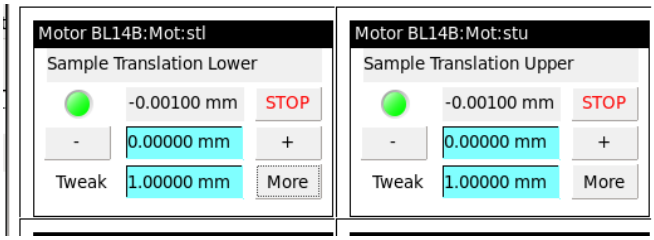
iv. You will then use the CalculateUMatrix Algorithm, with SingleCrystalPeakTable as input whose result will refine the _tmpws workspace U matrix (I think) and will change the index values shown on the instrument view for _tmpws

v. If you then get a handle on the SingleCrystalPeakTable workspace in MantidPlot's screen interpreter screen by typing:
handle=mtd[<SingleCrystalPeakTable>]
you can then get the UB matrix by:
handle.sample().getOrientedLattice().getUB()
and the u or v vectors respectively by:

print handle.sample().getOrientedLattice().getuVector()
or
print handle.sample().getOrientedLattice().getvVector()
and of course the u and v vectors can be input into MSLICE. Finally, you can copy all UB matrix, u vector, v vector, etc over to an arbitrary SPE workspace using:
CopySample(InputWorkspace=<SingleCrystalPeakTable>, OutputWorkspace=<_tmpws>, CopyName=False, CopyMaterial=False, CopyEnvironment=False, CopyShape=False)



o. Is my sample centered on the beam?
    i. Has the potential to increase scattered intensity
    ii. STU and STL, recommended step 2-5 mm.



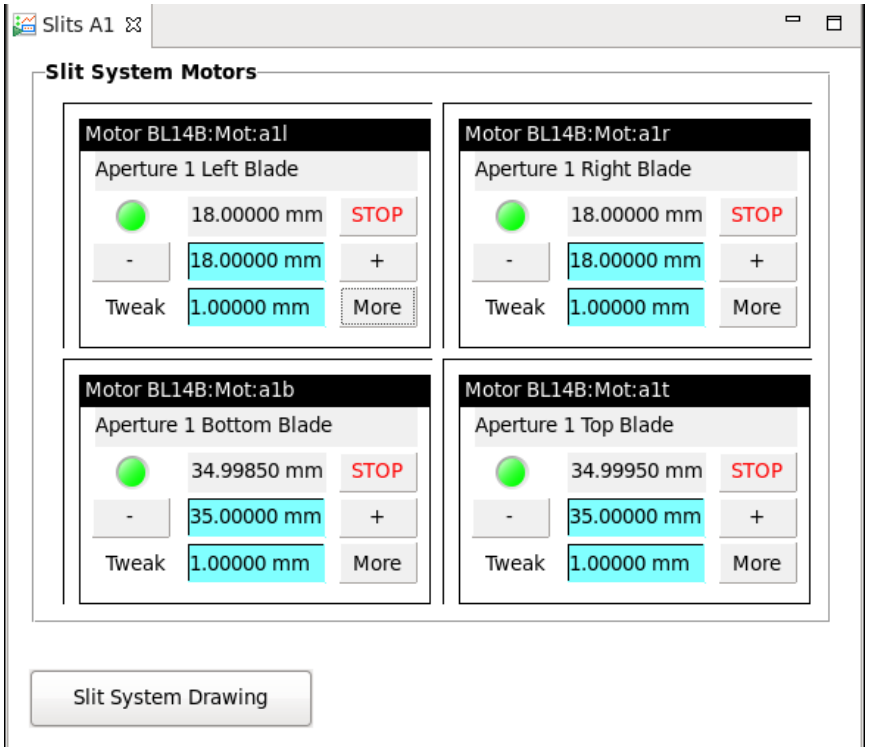
    iii. Recommend that you scan the same translation stage as you did the goniometer stage (STU & SGU on same Bragg peak, for example)
    iv. Rule of thumb: don't go much further than 5 mm in either direction
    v. Needs to be done prior to aperture scans
p. Quirk of symmetry used: general crystallographic know-how
    i. If you have a rhombic crystal, it's often easier to visualize and work with it using a hexagonal notation. HOWEVER, the mapping is only MOSTLY correct. Some Bragg peaks you might think are there are in fact not there. We recently had fun looking for a (1,1,4) peak, couldn't find it, and then went to a (-1,-1,4) peak and the Bragg peak 'appeared'. Since the system was rhombic, there was in fact no (1,1,4) peak to look for. So, word to the wise, if you're in a 'hexagonal' system, and you cannot find your bragg peak in one location, it might be wise to hunt for the other 'equivalent' peaks!

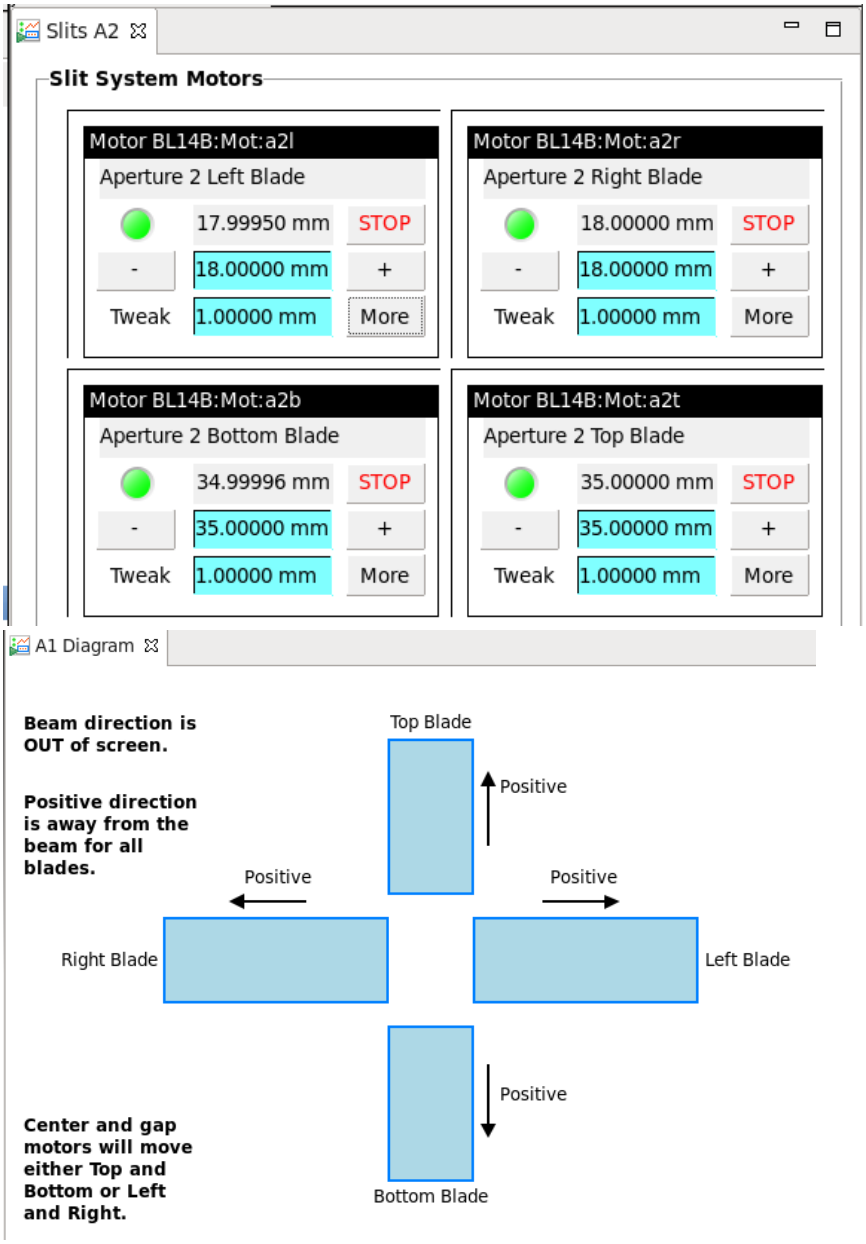
6. Remaining instrument setup tasks

a. Aperture width selection

i. For polarization analysis and with strong cryo-magnets, we generally use manual apertures and have removed the motorized ones

ii. CSS Aperture 1 and Aperture 2 pages





iii. Alignment scan parameters recommended

1. A1T, A1B, A2T, A2B: range(35,-1,-5)
2. A1L, A1R, A2L, A2R: range(18,-1,-3)

b. <u>REMOVE ANY BORATED ALUMINUM ATTENUATORS.</u> Too many users have stories of forgetting to remove the attenuator until the next morning. As an inelastic instrument, we need every neutron we can get.

c. Improving horizontal divergence?

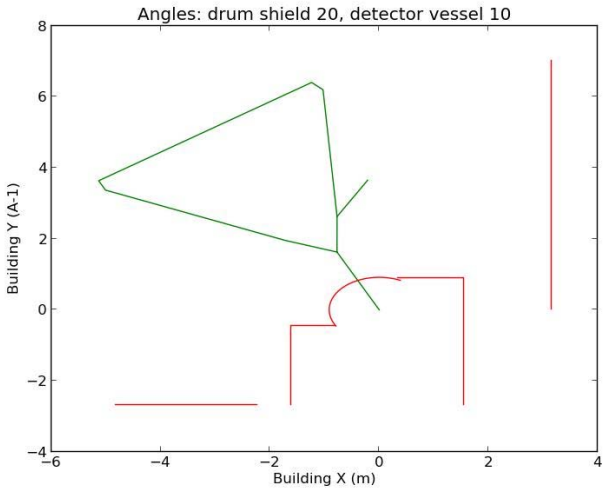
i. Most users DON'T do this.

ii. Soeller collimators manually put in

7. Deciding on instrument configuration

a. Don't hit the wall!

```
#Real_space_plot(M2_deg_try, S2_deg_try, MSD_m_try=1.8,
SafetyRadius_m=0.25, FillStation3He=0 )
```




```
Real_space_plot(20,10)

Is_Position_Safe(15,15)
#Is_Position_Safe(M2_deg_try, S2_deg_try, MSD_m_try=1.8,
SafetyRadius_m=0.25, FillStation3He=0 )
```

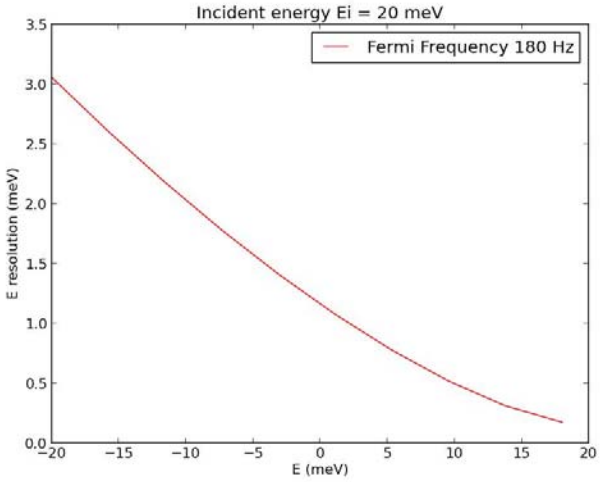
b. HYSPEC's incident energy restrictions

```
#IsEiOverPromptPulse(Ei)
IsEiOverPromptPulse(20)
output:  good Ei
```

a. Energy resolution tools

```
#Resolution_Calc_single(Ei,Ef,msd=1.8,FermiFreq=180.0)
Resolution_Calc_single(20,20)
output:  energy resolution in FWHM is 1.16 meV

#Plot_Resolution_vs_E(Ei,EMin,EMax,nE,msd=1.8,FermiFreq=[18
0.0])
```




```
Plot_Resolution_vs_E(20,-20,18,10)
```

b. Momentum resolution tools

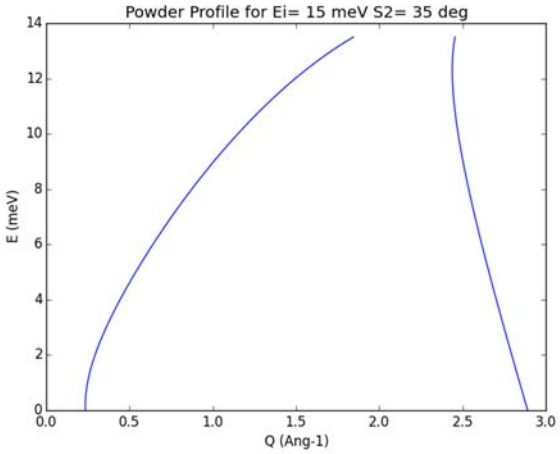
(development state. Not yet ready for prime time)

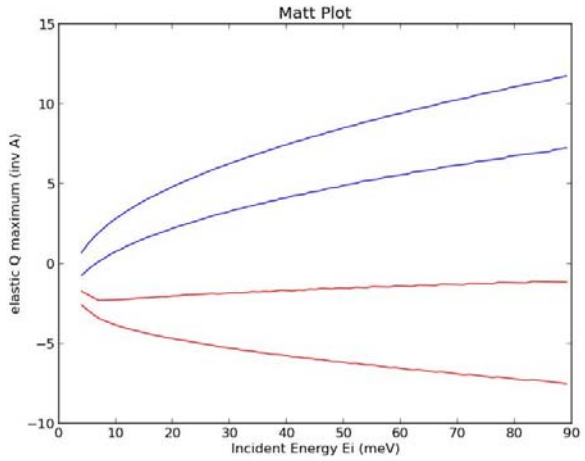
c. Flux tradeoff tools

```
#relative_flux(Ei1_meV,Fermi1_Hz,Ei2_meV,Fermi2_Hz)
relative_flux(20,180,20,420)
output: relative flux ratio is 2.3
```

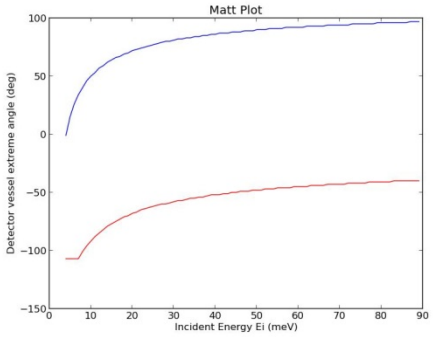
d. Powder planning tools
   i. Typically users know the desired momentum transfer Q and desired energy transfer E.
   ii. Planning tool functions

Plot_PowderRange(Ei, S2)






```
PlotExtremeQ()
```




```
PlotExtremeQ(S2instead=True)
```

c. Single crystal planning tools

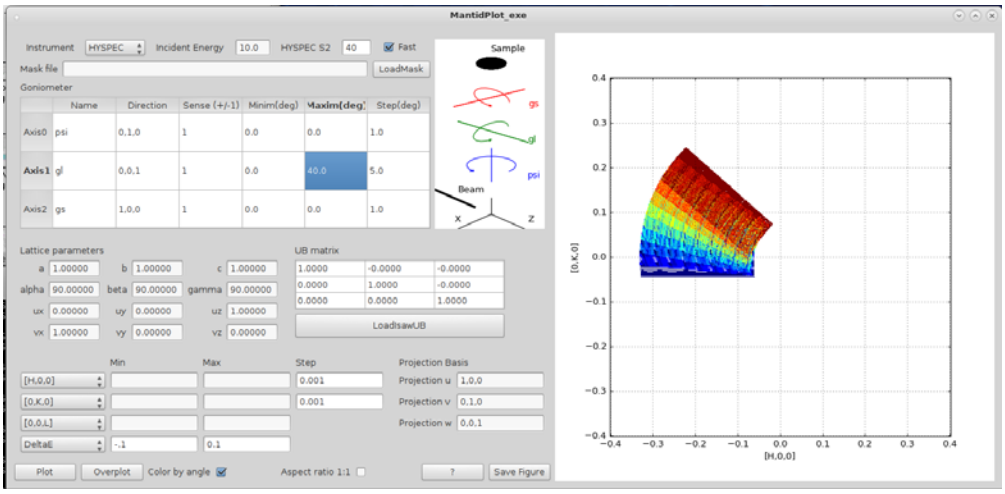
```
CubicCrystal=Crystal((4,4,4),(1,0,0),(0,1,0))

hexCrystal =
Crystal((4,4,4),(1,0,0),(0,1,0),alphabetagamma=(90.0,90.0,1
20.0))

CubicCrystal.WhereIsBragg((1,0,0),25)
CubicCrystal.WhereIsBragg((1,0,0),25,left=True)

Crystal.WhereIsBragg(hkl,Ei_meV,E_meV=0.0,left=False,
S1offset=0.0)
```

e. MANTID experiment planning GUI



f. HORACE planning GUI

   i. Generating the PAR file

g. The final quick easy check

   i. Simulate via very short runs with a larger rotation step size in the desired experiment configuration

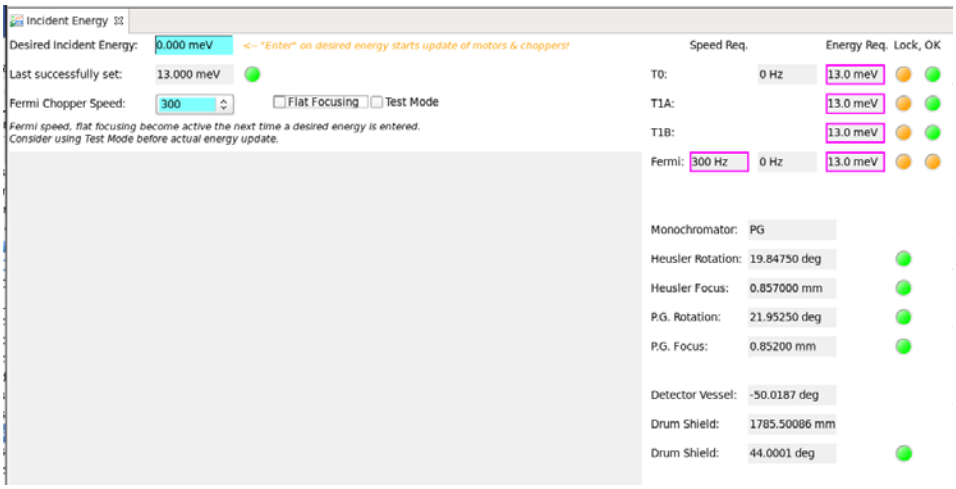
   ii. View using DAVE MSLICE. Is this what you really want?

h. Other strange considerations

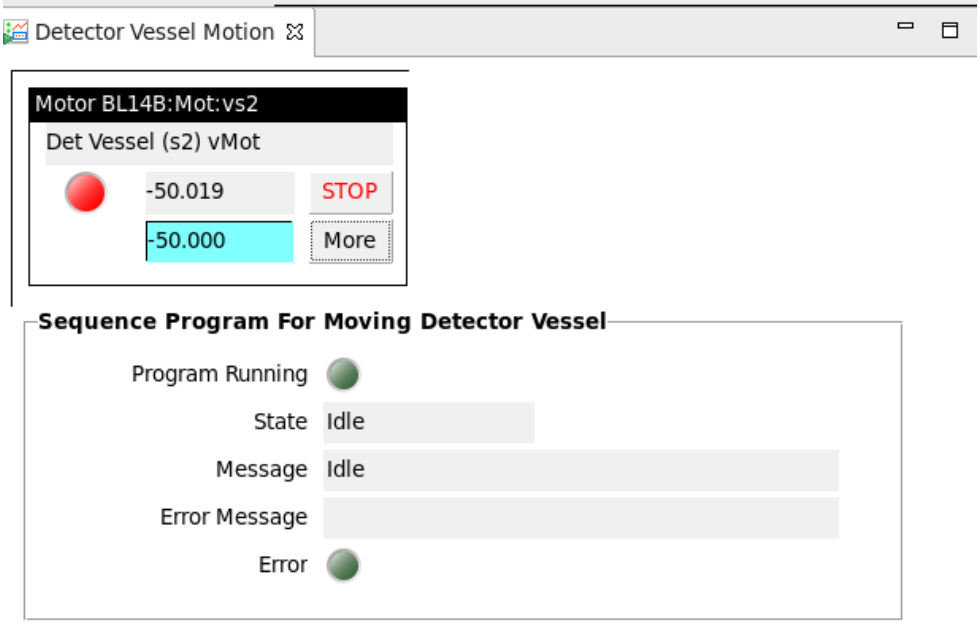
   i. When using a copper mount, common for DF inserts because copper doesn't go superconducting like Aluminum does at about 1 K, you can expect major multiple scattering background and major powder rings from the copper. However, if you use an Ei of 6 meV or less, all that disappears. It's because Cu is cubic with lattice spacing a=b=c=3.615 Angstrom, so above 6.26 meV the scatter can be painful. An easy check of this is to look for powder rings on ICSD for copper at the appropriate energy or wavelength.

8. Moving to desired instrument configuration

a. CSS Ei page



b. CSS User Detector Vessel Page



i. Why is my detector vessel not moving?

ii. When you know you're close to the wall…

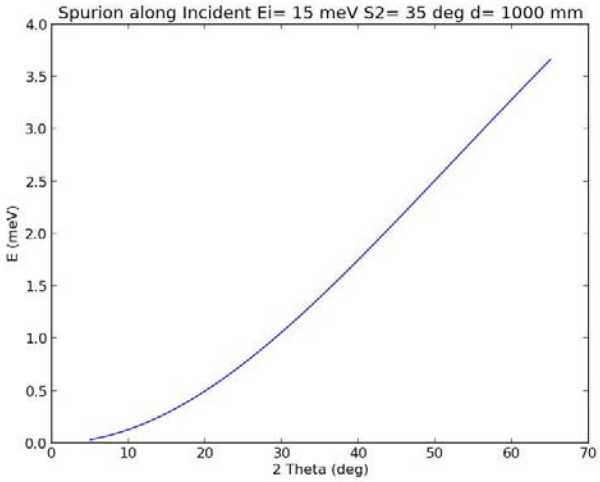
c. If you must avoid vertical focusing…

i. CSS Heusler and PG Pages

9. Locate and minimize spurious scattering

a. If you have a single crystal and have not done step 7.j., go back and get it done.
b. Sit in one position, away from a Bragg peak, and do a 5-10 minute run in a fixed position.
c. Observe the result in a E vs. Q geometry, either from the web interface or using one of the analysis tools.
d. The following spurious planning tools can assist you in diagnosing any unexpected features:
    i. A parabolic energy spurion that may have some aluminum Powder points, arising from scatter upstream or downstream of the sample, somewhere along the monochromatic incident beam. D_along_mm can be positive or negative, causing an energy loss or energy gain feature, respectively

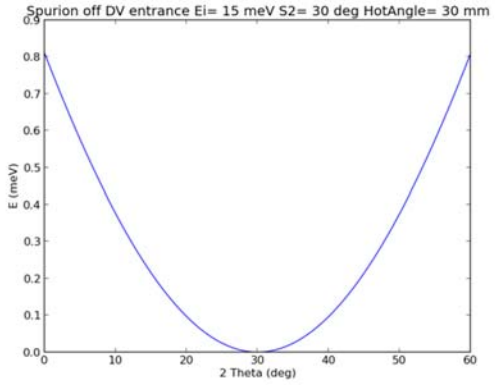
```
Plot_Spurion_along_incident(Ei,S2,d_along_mm)
```




```
Plot_Spurion_along_incident(15,35,1000)
```

    ii. Similarly, an incident beam or strong Bragg peak that hits the entrance window of the detector vessel (at angle 'TwoThetaHot') can also introduce an energy loss dependent background feature.

```
Plot_Spurion_off_DV_Entrance(Ei,S2,TwoThetaHot)
```




```
Plot_Spurion_off_DV_Entrance (15,30,30)
```

iii. Spurion from isotropic scatter from sample position, scattering off of something cylindrically symmetric like our OVC, then back to detectors. Output is flat energy feature in meV.

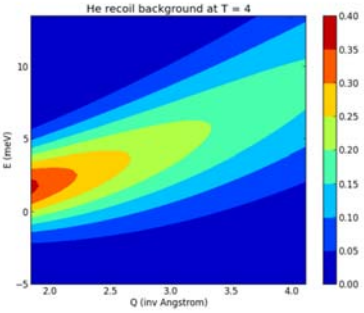
```
Spurion_fromSampleNBackscatter(Ei,r_mm)
Spurion_fromSampleNBackscatter(15,500)
output:  flat energy spurion at 4.95 meV
```

iv. Spurion from isotropic scatter from sample position, scattering directly above or below, then back to detectors. Output is flat energy feature in meV.

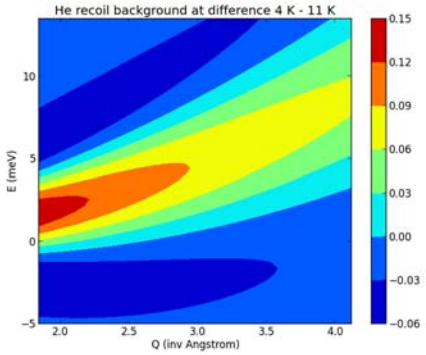
```
Spurion_fromVerticalOffscatter(Ei,r_mm)
Spurion_fromVerticalOffscatter(15,60)
output:  flat energy spurion at 0.39 meV
```

v. Spurion from Helium Recoil

```
RecoilRawContour(Ei,S2,T (temperature in Kelvin))
RecoilRawContour(15,70,4)
```

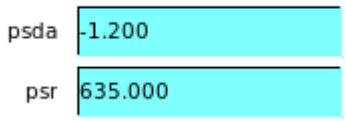


```
RecoilDiffContour(Ei,S2,T_low,T_high)
RecoilDiffContour(15,70,4,11)
```



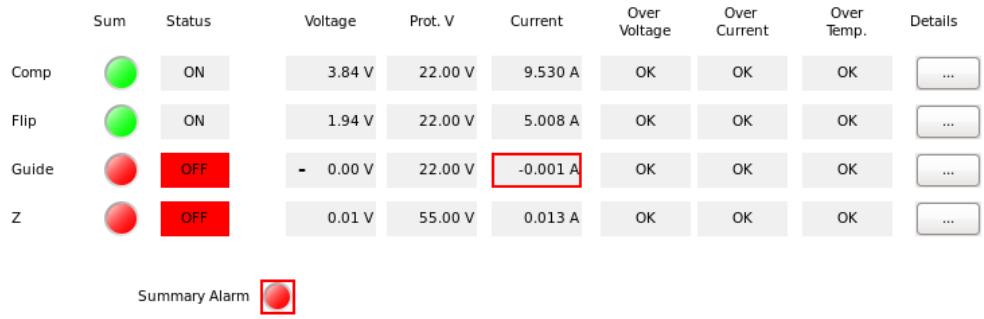
10. Polarization mode

a. Setup

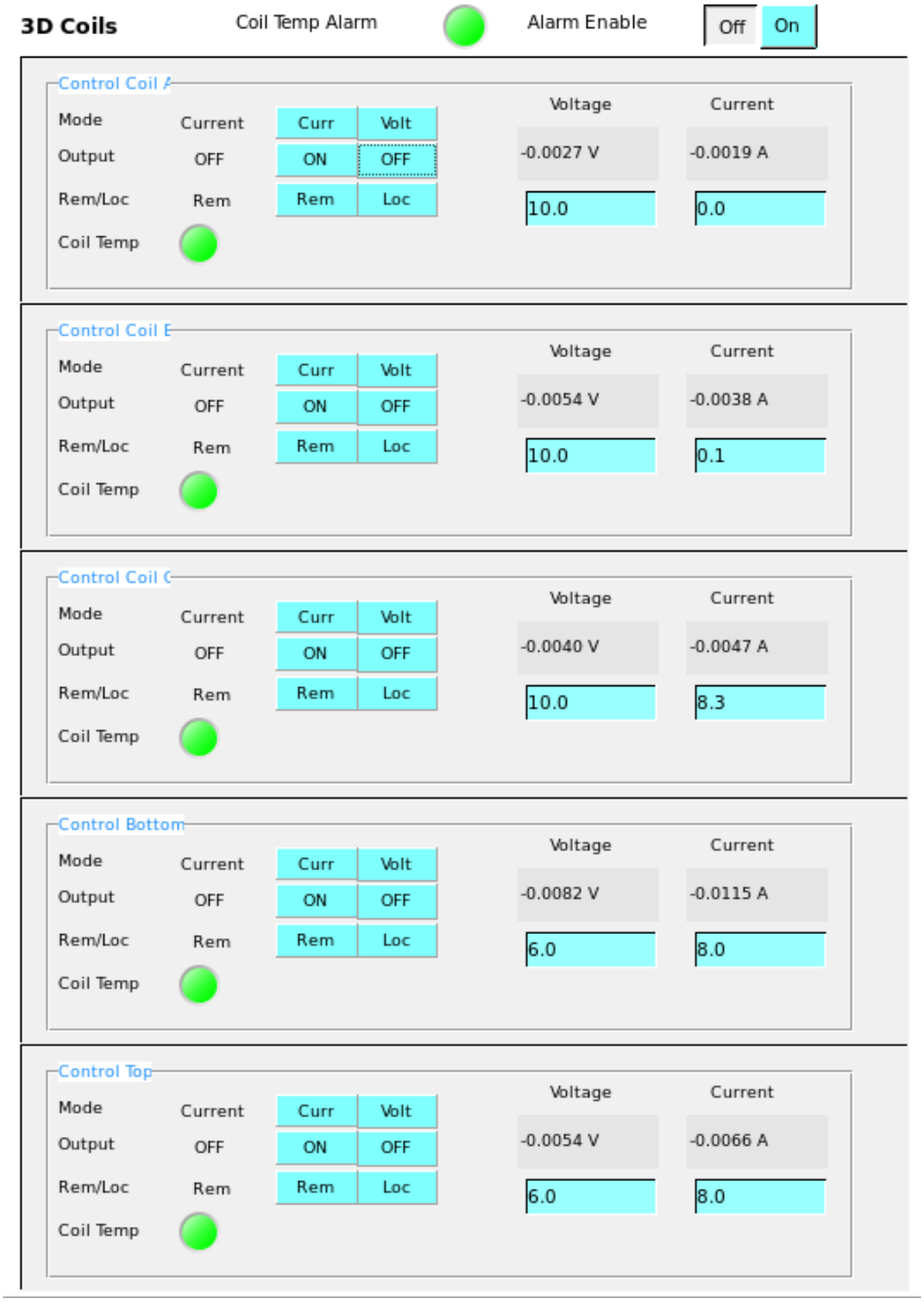


b. Acquisition

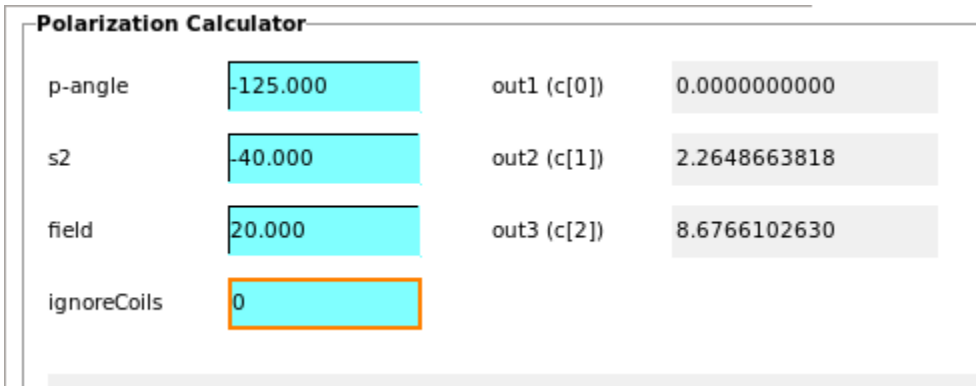
i. CSS Mezei Flipper Page



ii. CSS Sample Coils Page



iii. From direction and magnitude to currents on coils



iv. From HKL-w to currents on coils:

CurrentFromBasics(CrystalClass,Ei,hkl,w_meV,s2,left1=False,Fld=20.0, ignorecurrent=0)

run –i ForCoilOPI.py
CurrentFromBasics(NaCl,15.0,(1,0,0),5.0,-40.0,left1=False,Fld=20.0, ignorecurrent=0)

v. Generate a table scan to track field along desired hkl-E space:
-Edit MyTableGenerator.py, both routines.
(this uses templates that have a static copy in the ForCoilOPI.py file)

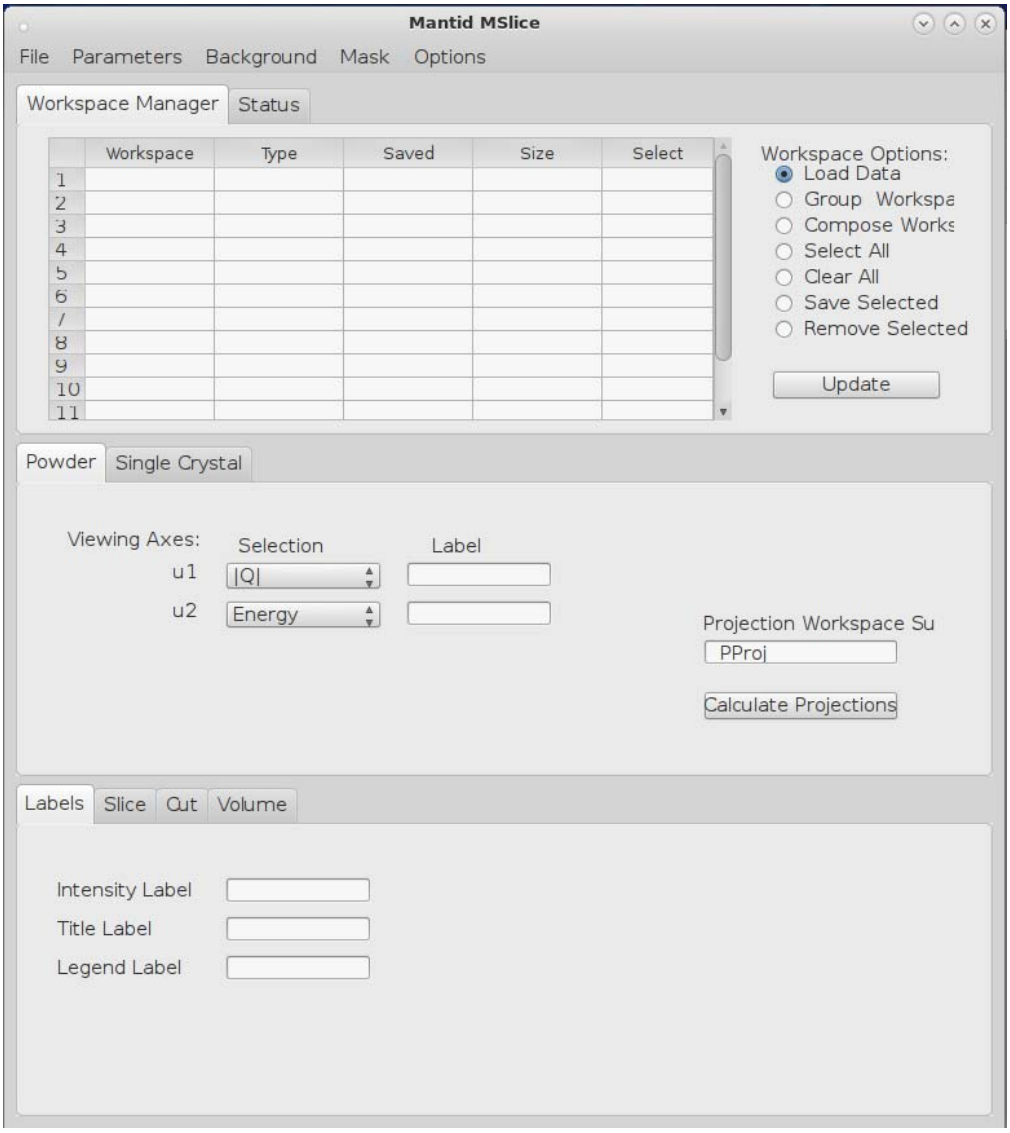
run –i MyTableGenerator.py
MakeCSV_file_mine()

c. Analysis
   i. Done in autoreduction:
      1. TiZr normalization per-tube/pixel intensity normalization
      2. Angle correction
   ii. TiZr flip normalization (not done)
   iii. Done in script after autoreduction:
      1. Ef transmission normalization
      2. Flip ratio normalization
   iv. Sharpf equations: from 3-orthogonal-field with pre-sample flips to magnetic, nuclear coherent, isotope incoherent and spin-incoherent scattering. ONLY GOOD for POWDERS!
   v. Beyond Sharpf: multi-direction corrections (Ehlers et al), possibly useful for out of plane and low Q scattering

11. Visualize your results

a. The HYSPEC Analysis computer

b. Mantid MSLICE



c. Mantid HORACE

d. DAVE M-SLICE

   i. Set up

      1. On analysis cluster, create a terminal window and enter

         dave

      2. On main screen, from the tab row at top, click on:

         a. Data Reduction

            i. NCNR

               1. DGS Reduction (Mslice)

2. Choose *.nxspe format

3. On Mslice screen
    a. Sample type:
        i. Single Crystal
            1. Diffuse Scattering Multiple E
    b. Energy Range
        i. All
    c. Option
        i. View Axis
            1. Allow Extra Viewing Axis
    d. Option
        i. Binning Method
            1. Constant Intervals
                a. Yes

ii. Use: The MSLICE screen is divided into three sections vertically

1. Top: Loading
    a. Use files from the following directory:

    `/SNS/HYS/IPTS-<your IPTS #>/shared/autoreduce/`

    You have the option of either using '4pixel' data or 'msk_tube' autoreduced data. The former bins pixels from each detector tube from 128 pixels into 32 groups, and masks the top and bottom 8 pixels. The latter bins the middle third of the (vertical) detector tube, roughly matching the vertical spread of the vertically focused Bragg peaks at 1.8 m focus element to sample distance. All these files ought to have the suffix *.nxspe. If you prefer another format we can rereduce or modify our reduction script for autoreduction.

2. Middle: Calculating trajectories
    a. Lattice parameters a,b,c in Angstroms; alpha,beta,gamma in degrees
    b. U and V vectors are vectors in the scatter plane in r.l.u.
    They are most likely the vectors you used to initialize the Crystal class, unless you were not able to align in the plane. Then, you may need to use Mantid to determine these vectors. Their length is arbitrary (you don't have to normalize); only their direction matters.
    c. Starting angle: the nominal starting angle for the first file of the set read in. If an offset angle was established during alignment, then you have to either add or subtract that offset angle (?).

3. Bottom: viewing
    a. Volume view is most flexible, allowing for slices and 1D's

iii. Using MSLICE to plan and get trajectories
    1. Top section
        a. Load at least one file for those you want to explore
        b. Clear Data
    2. Middle section: Calculate projections
        a. It asks if Ei is correct: hit OK
        b. It then asks for the desired S1 angle range
    3. Bottom section: Detector trajectory tab

e. Using Horace in MatLab
    i. Open a terminal (either via menu or alt-f2 and type "gnome-terminal")
    ii. Execute /SNS/software/bin/setup_isis_matlab
    iii. Use Matlab-Horace link from the Analysis menu
    iv. This will cause a file ~/startup.m to be created in the user home directory, which means that all versions of Matlab should then try and use Horace. I don't know why the Matlab-Horace link points to r2011b, but I confirmed earlier that 2014a will run and says that it is using Horace.
    v. You will need a *.par file for each detector vessel geometry you use. For this, start MantidPlot, open up any raw data file that has the desired detector vessel geometry, and execute the algorithm SavePAR.

f. Using TobyFit (????)

12. Autoreduction and Re-Reduction

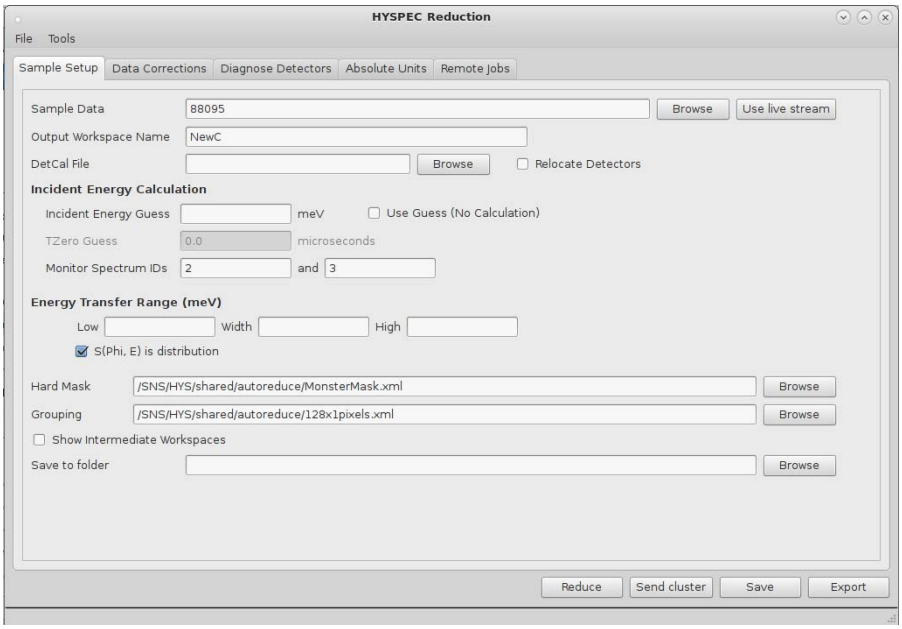
a. Autoreduction: what you're getting

b. Also look for the following csv file that can be read by most spreadsheet programs:

```
/SNS/HYS/IPTS-<your IPTS #>/shared/autoreduce/experiment_log.csv
```

c. Re-Reduction: in case you want to get something different

d. Brute force GUI (almost never used but if you're curious…)

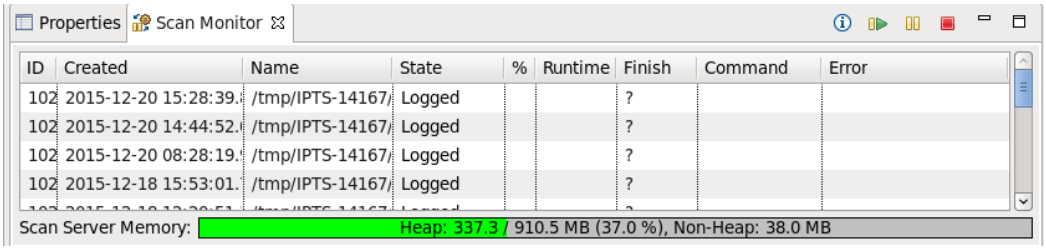


13. Automating your experiment acquisition

a. General comments

   i. Typically users set up scans to last ~20 to 24 hours, so they can come in the next day, look at analyzed data, and determine what the next step in the experiment needs to be

b. CSS Scan Server Interface



   i. If you have used the CSS Alignment Scan window, you have already used this software.

   ii. Note that when the scan server is active, some functions (buttons and blue fields) are frozen out for general users.

   iii. Bringing up Scan Server window from CSS

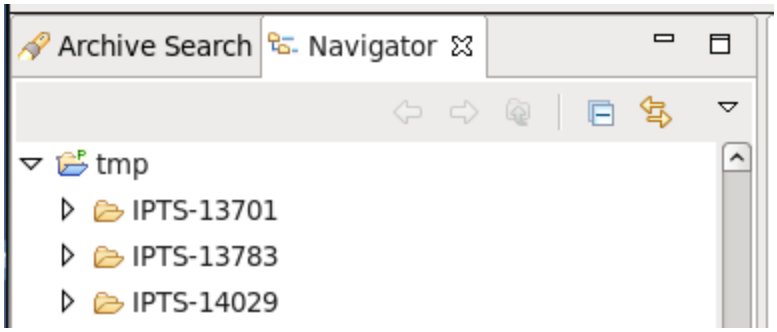
   iv. Stop Scan Server from CSS HYSPEC User page

   v. Stop / Pause / Resume Scan Server from CSS Server Window

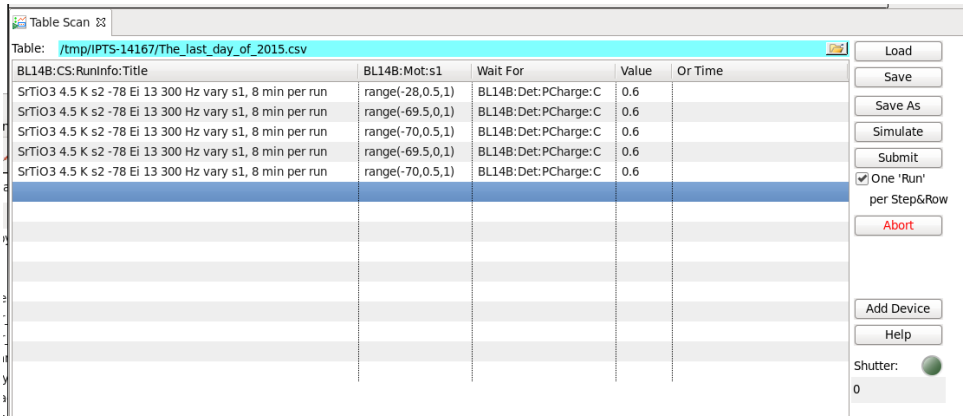
   vi. Show Scan status table. Right click on active scan.

c. CSS Table Scans

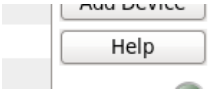
   i. Generate your IPTS subdirectory



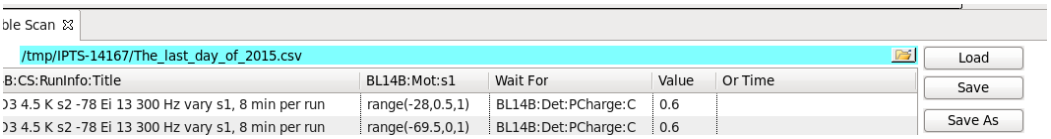
ii. CSS Table page



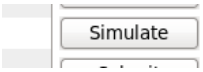
iii. Useful how-to radio button



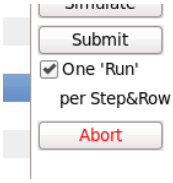
iv. Please be sure to save your scan so the Local Contact can view the same information via remote access



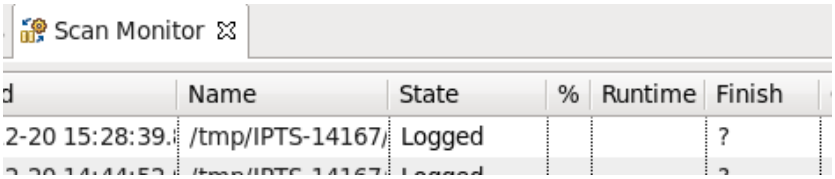
v. Reality check before submitting the scan



vi. Starting the scan

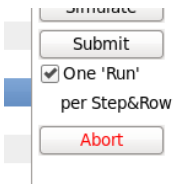


vii. Estimate when a scan will be completed



viii. Defaults

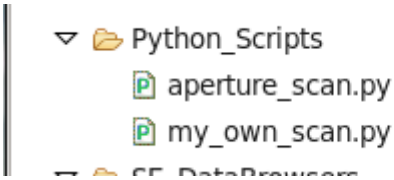
1. One NeXus run for the whole scan



ix. List / table of typical PV's scanned for motors and sample environments <really need this table!>

x. Template subdirectory

d. CSS Script Scans



e. Monitoring your experiment
    i. At CSS
        1. CSS Monitor page
        2. CSS Scan Monitor functions
            a. Scan status
    ii. On the Web

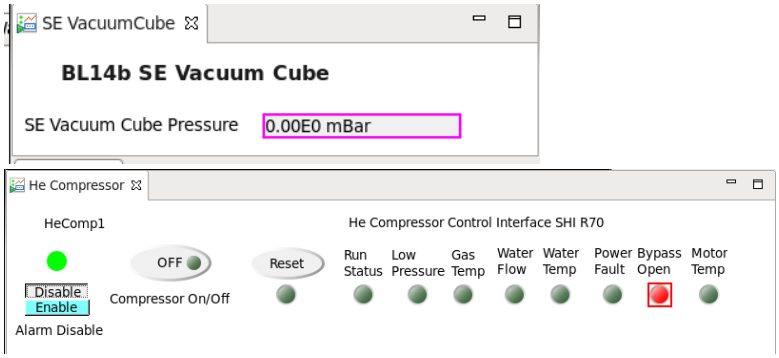
14. What to do when you get home after your experiment is done

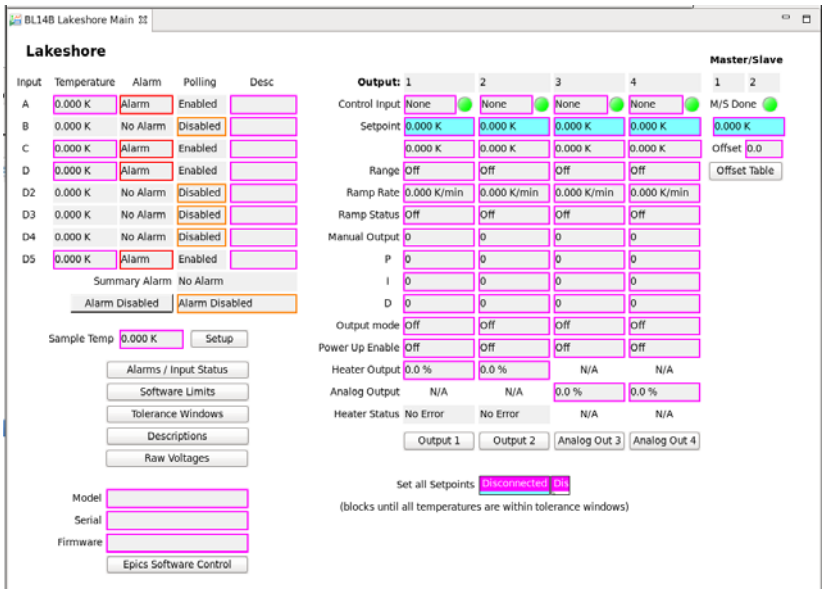
a. Accessing the Analysis Cluster
b. Obtaining your data
c. Preparing figures or movies
d. Giving fantastic talks
e. Presenting provocative posters
f. Publishing results
g. Letting us know

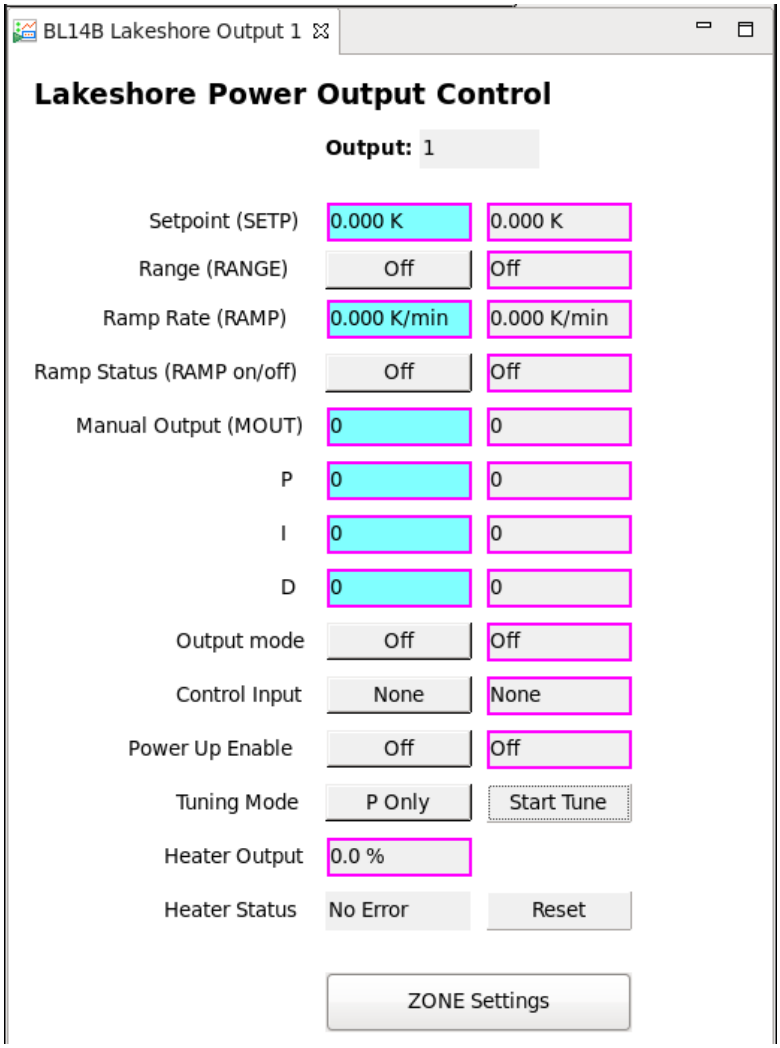
15. Software for data acquisition, under the hood

a. EPICS
   i. EPICS communication protocol
   ii. EPICS database
   iii. EPICS records
   iv. EPICS alarming
   v. EPICS equipment control (IOC software drivers)

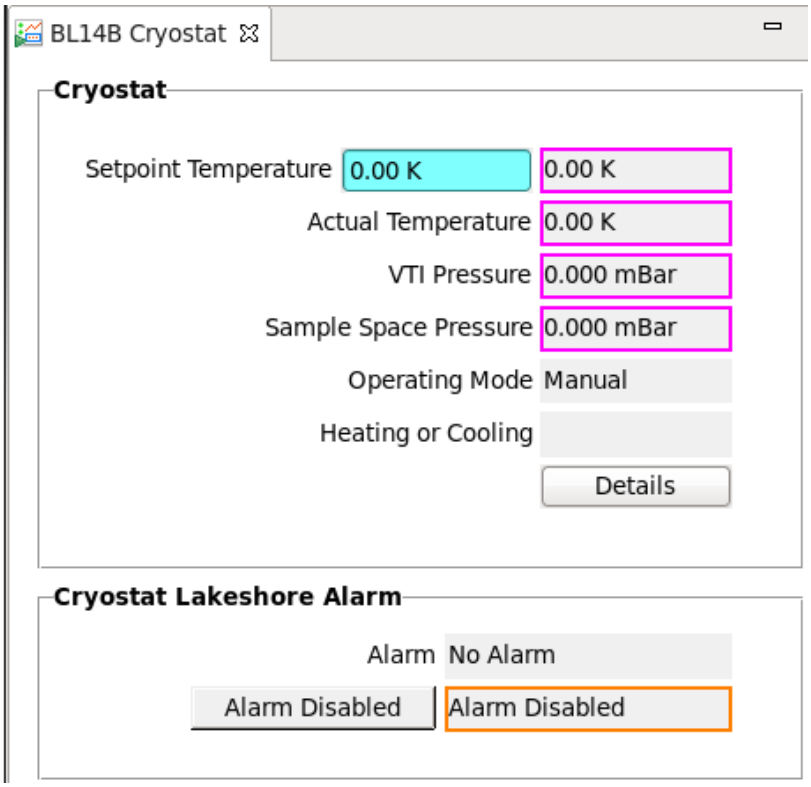
b. CSS
   i. CSS Main Page
   ii. CSS important mouse tricks
      1. For tablet and touchpad users: A mouse is moved over a surface (table or foam pad) to move a cursor around a screen. It also has one or more buttons and possibly a wheel at the finger positions, used to select various functions on various windows and regions of applications.
      2. For Mac users: Mice we use have two buttons. The left button usually makes a field active or enables the start of an application. The right button usually opens a pull-down menu from which to choose options with the left button.
   iii. CSS plotting archived data
   iv. CSS Chopper Pages
   v. CSS Sample Environment Pages
      1. CCR-19 & CCR-10

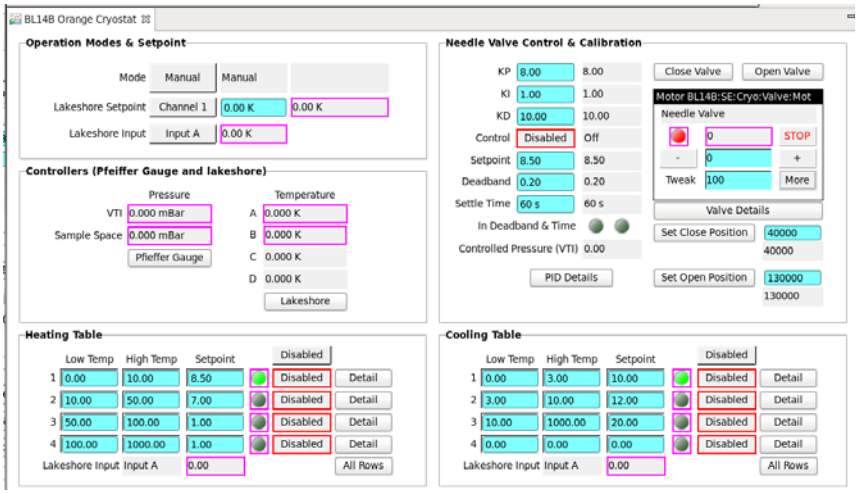


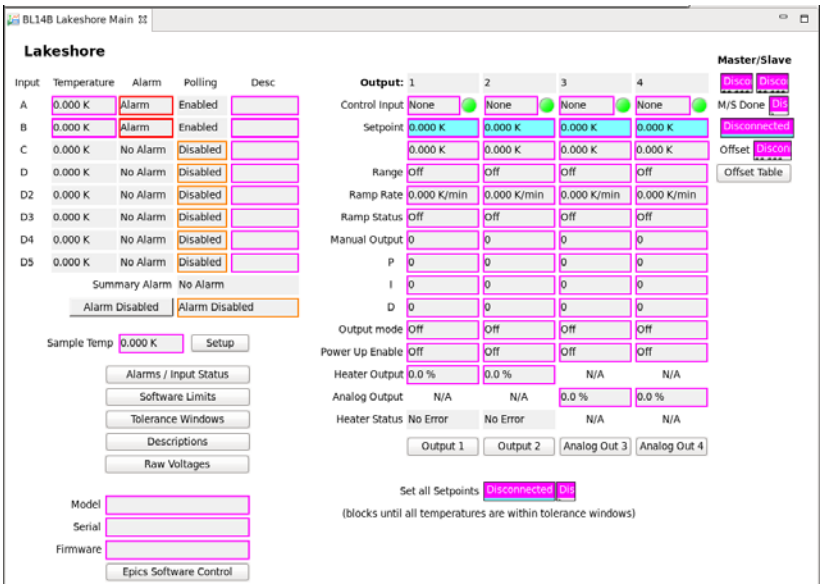

BL14B Lakeshore Main
Lakeshore
Input Temperature Alarm Polling Desc
A 0.000 K Alarm Enabled
B 0.000 K No Alarm Disabled
C 0.000 K Alarm Enabled
D 0.000 K Alarm Enabled
D2 0.000 K No Alarm Disabled
D3 0.000 K No Alarm Disabled
D4 0.000 K No Alarm Disabled
D5 0.000 K Alarm Enabled
Summary Alarm No Alarm
Alarm Disabled Alarm Disabled
Sample Temp 0.000 K Setup
Alarms / Input Status
Software Limits
Tolerance Windows
Descriptions
Raw Voltages
Model
Serial
Firmware
Epics Software Control
Output: 1 2 3 4
Control Input None None None None
Setpoint 0.000 K 0.000 K 0.000 K 0.000 K
0.000 K 0.000 K 0.000 K 0.000 K
Range Off Off Off Off
Ramp Rate 0.000 K/min 0.000 K/min 0.000 K/min 0.000 K/min
Ramp Status Off Off Off Off
Manual Output 0 0 0 0
P 0 0 0 0
I 0 0 0 0
D 0 0 0 0
Output mode Off Off Off Off
Power Up Enable Off Off Off Off
Heater Output 0.0 % 0.0 % N/A N/A
Analog Output N/A N/A 0.0 % 0.0 %
Heater Status No Error No Error N/A N/A
Output 1 Output 2 Analog Out 3 Analog Out 4
Master/Slave
1 2
M/S Done
0.000 K
Offset 0.0
Offset Table
Set all Setpoints Disconnected Dis
(blocks until all temperatures are within tolerance windows)


BL14B Lakeshore Output 1
Lakeshore Power Output Control
Output: 1
Setpoint (SETP) 0.000 K 0.000 K
Range (RANGE) Off Off
Ramp Rate (RAMP) 0.000 K/min 0.000 K/min
Ramp Status (RAMP on/off) Off Off
Manual Output (MOUT) 0 0
P 0 0
I 0 0
D 0 0
Output mode Off Off
Control Input None None
Power Up Enable Off Off
Tuning Mode P Only Start Tune
Heater Output 0.0 %
Heater Status No Error Reset
ZONE Settings

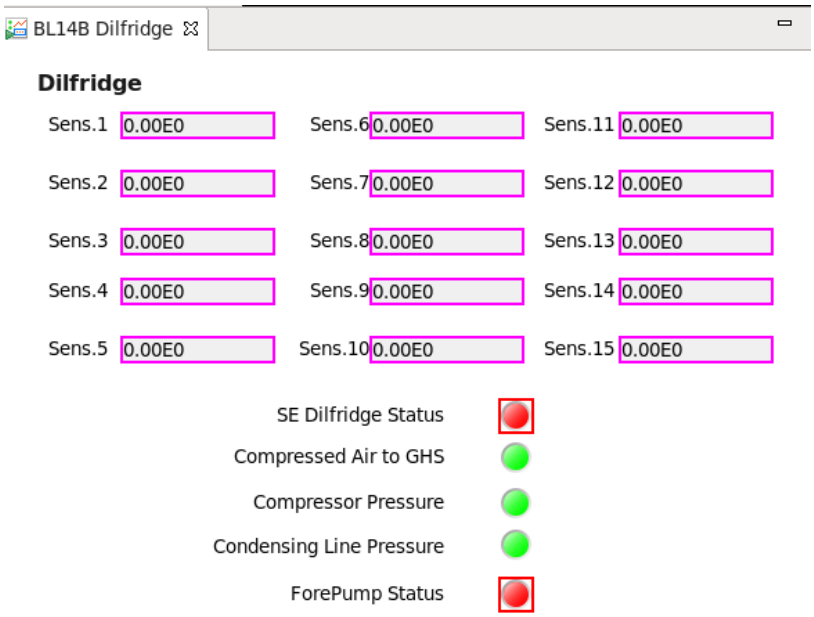
2. CRYO-09


BL14B Cryostat
Cryostat
Setpoint Temperature
0.00 K
0.00 K
Actual Temperature
0.00 K
VTI Pressure
0.000 mBar
Sample Space Pressure
0.000 mBar
Operating Mode
Manual
Heating or Cooling
Details
Cryostat Lakeshore Alarm
Alarm
No Alarm
Alarm Disabled
Alarm Disabled


BL14B Orange Cryostat
Operation Modes & Setpoint
Mode
Manual
Lakeshore Setpoint
Channel 1
0.00 K
Lakeshore Input
Input A
Controllers (Pfeiffer Gauge and lakeshore)
Pressure
Temperature
VTI
Sample Space
Pfieffer Gauge
Lakeshore
Needle Valve Control & Calibration
KP
KI
KD
Control
Setpoint
Deadband
Settle Time
In Deadband & Time
Controlled Pressure (VTI)
PID Details
Close Valve
Open Valve
Motor BL14B:SE:Cryo:Valve:Mot
Needle Valve
STOP
Tweak
More
Valve Details
Set Close Position
Set Open Position
Heating Table
Cooling Table
Low Temp
High Temp
Setpoint
Disabled
Detail
All Rows


BL14B Lakeshore Main
Lakeshore
Master/Slave
Input
Temperature
Alarm
Polling
Desc
Summary Alarm
Alarm Disabled
Sample Temp
Setup
Alarms / Input Status
Software Limits
Tolerance Windows
Descriptions
Raw Voltages
Model
Serial
Firmware
Epics Software Control
Output:
Control Input
Setpoint
Range
Ramp Rate
Ramp Status
Manual Output
P
I
D
Output mode
Power Up Enable
Heater Output
Analog Output
Heater Status
Output 1
Output 2
Analog Out 3
Analog Out 4
M/S Done
Disconnected
Offset
Offset Table
Set all Setpoints
(blocks until all temperatures are within tolerance windows)

3. CRYO-09 with DF



4. CRYO-09 with 3He: Using the Lakeshore shown in section 1 but with a different Lakeshore (350 instead of 336).
5. SLIM-SAM

vi. Least User Privileges

1. Your local contact can become a 'super user' that can do things you cannot, including
    a. Modifying things while a scan is running
    b. Change sample environments
    c. Stop and restart software drivers associated with different instrument functions.

c. ADARA

i. Adding PV's to the NeXus file and for the HYS.MONITOR.GOV webpage remote monitoring:

1. On the OPI machine, even under the user account, edit the /home/controls/bl14b/beamline.xml file
(not for the squeamish)

d. NEXUS

e. MANTID

i. Mantid algorithms verified (?)
ii. Live Viewing with Mantid
iii. DGS Reduction Interface

f. Planning tools in Python

i. Starting on Analysis Cluster or HYSPEC Analysis PC

```
cd /SNS/users/inelastic/HYSPEC
```

ipython
run -i rotations.py
run -i ubmatrix_out.py
run -i userlib_hys_out.py

ii. Starting on OPI

./mountHYS…
cd /SNS/PLAN
ipython
run -i rotations.py
run -i ubmatrix_out.py
run -i userlib_hys_out.py

iii. List of commands in alphabetical order, and section to go to for learning about them.

16. How HYSPEC is calibrated

a. Assumptions at the start of calibration
    i. Engineered drawings locate choppers, sample and detector 8-packs
    ii. Position and time-delay profile of moderated pulse
        i. From neutronics group (?)
        ii. Same functional form used for chopper phase setting and Mantid autoreduction
b. Functional form for Fermi chopper phase as a function of energy
    i. Speed as a function of neutron kinetic energy
    ii. Incorporate time delay profile of moderated pulse
    iii. Chopper speed related phase offset when Top Dead Center (TDC) sensor is not exactly at chopper opening
    iv. Confirm chopper direction and TDC sensing mode prior to calibration
    v. Very slight empirical adjustment to fit to vanadium elastic line
        i. First round, middle of each of 4 panels
        ii. Plot, TOF vs detector tube
        iii. Plot, converted to E vs detector tube
        iv. Energy resolution FWHM for V is same as for predicted energy resolution
c. Verifying that low-resolution choppers are centered
    We can and should measure against neutron monitor 2 for this, to avoid any complications concerning possible misalignment downstream. All three choppers when scanning against phase have very broad plateaus due to the wide acceptance angles of these choppers.
    i. T0
    ii. T1A
    iii. T1B
        i. Temporary offset due to leak in Fermi chopper
d. Focus array and drum shield calibration
    i. Note the MTHU and MGHU motors are constrained as described in (), so we have set their positions, turned off their drives, and don't intend to run them again unless we observe some real problems.
    ii. Ensure that sample is centered by confirming same count-rate at a variety of angles. Adjust STL and STU as needed to center.
e. Scatter angles from powder samples: detector vessel calibration
    i. Preferred material: alumina powder
    ii. Either multiple S2 angles or verifying that ring is mostly on a single 8-pack ensures good coverage of a Powder ring
    iii. Location in 2theta of powder ring on both sides determines nominal S2 offset
    iv. Indirect measure of energy via 2theta angle
f. Maintaining calibration
    i. Periodic visual checks of calibration

ii. Motorized stage position verification
    i. S2 absolute encoder
    ii. Msd stop
    iii. M2 multiple encoders
    iv. Focus array encoders

g. Next round: possible multi-energy calibration using flat energy loss modes
    i. Gamma picoline? Can be purchased easily.
    ii. Para-hydrogen? Need gas handling sample environment with T < 14 K. See flat excitation at 14.7 meV.
    iii. Acetomenaphrin?
    iv. Other?

17. Modeling excitations to compare against measurements

a. Back of Envelope
b. Density Functional Theory
    i. CASTEP
    ii. VASP
c. Spin Waves
    i. Spin Genie
    ii. Spin W
d. Crystal Field Excitations
    i. McPhase
e. Scattering kernel, monte carlo
    i. McVine
f. Phonons brute force
    i.
g. Accelerys Materials Studio

18. Accounting for corrections

a. From model to measurement: sample & instrument simulation
    a. Instrument simulation using McStas
    b. Sample simulation using McVine
b. From measurement backwards
    a. Resolution function
        i. Estimating using python functions
        ii. Estimating using McStas
        iii. Estimating using TobyPlot
        iv. Deconvolution using TobyPlot
        v. Mantid not there yet…
    b. Multiple scattering correction
    c. MultiPhonon scattering correction

19. Remote access

a. When you're on the HYS-OPI or any analysis PC and need access to the FireFox browser for cameras or other useful things: from a command line in a terminal, type **fix-firefox-settings**, hit enter, and the browser on your other account on another machine will end so you can start afresh!

20. Camera views

Hyspececam.ornl.gov
hyspecwcam.ornl.gov
hyspecmezcam.ornl.gov