Single Crystal Instrument Calibration Using Mantid and ISAW

Arthur J. Schultz, Leighton Coates

This demonstration is based on data from a natrolite crystal measured on the MaNDi instrument. Before running the calibration, an indexed peaks file needs to be obtained from an analysis of the Nexus event files. Copy the files in `/SNS/MANDI/shared/SCDcalib_demo` to a working directory in your account. You will need to edit the `ReduceSCD.config` file with the links to your working directory here:

`calibration_file_1`
`/SNS/users/`**`your_userid/your_directory`**`/MANDI_2015-09-17.DetCal`

and here:

`output_directory  /SNS/users/`**`your_userid/your_directory`**

Then type the command:

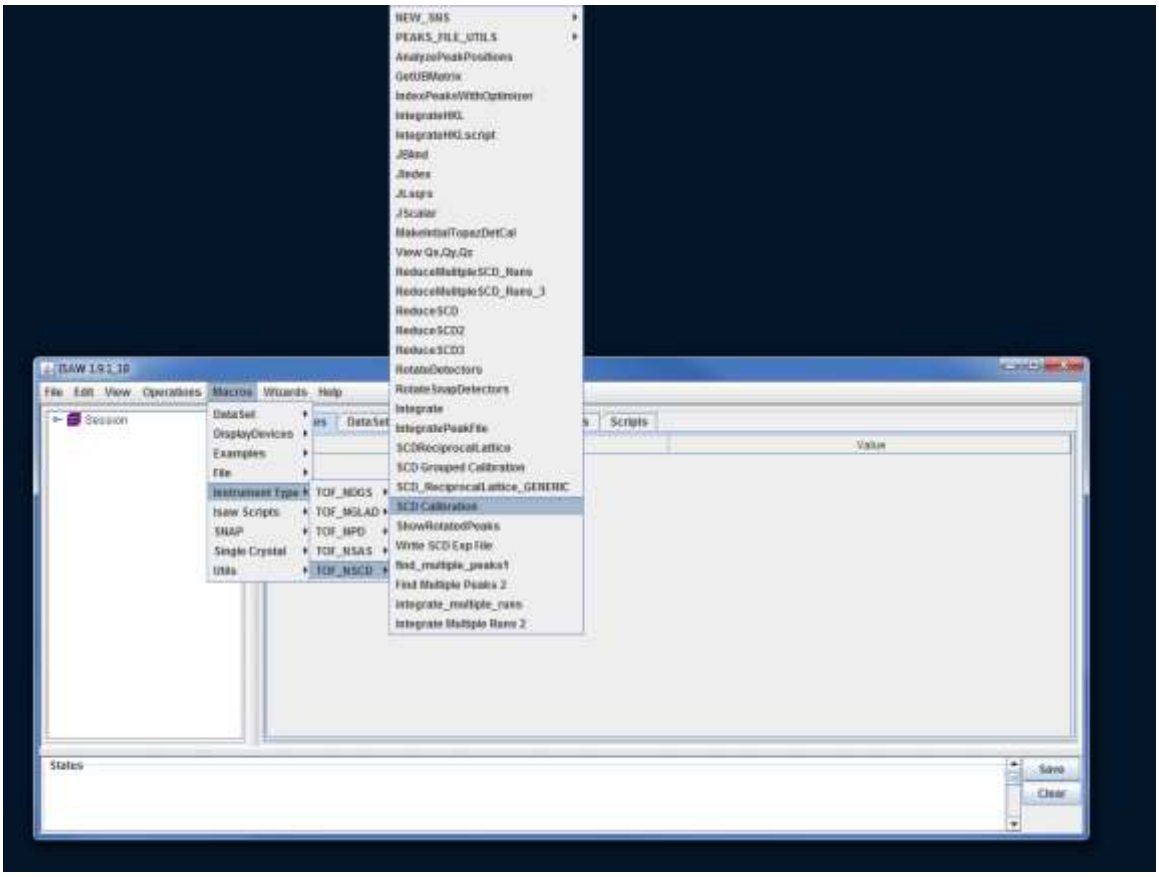
```
$ python ReduceSCD_OneRun.py ReduceSCD.config 4362
```

where 4362 is the run number. If this is successful, files `natrolite_Niggli.integrate` and `natrolite_Niggli.mat` will appear in your working directory. Then run ReduceSCD_Parallel.py with the command:

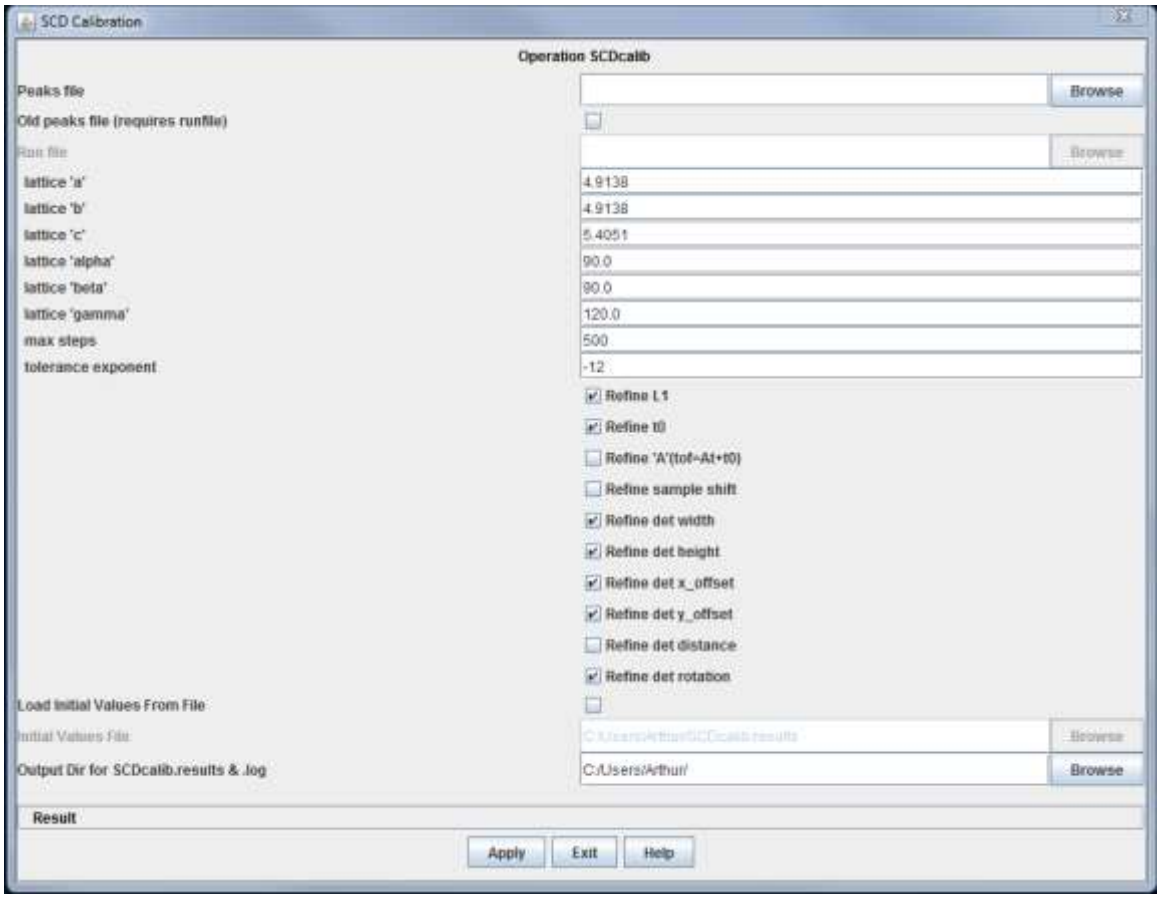
```
$ python ReduceSCD_Parallel.py ReduceSCD.config
```

This will analyze 15 MaNDi runs on 15 processors in parallel with run numbers 4362 to 4376. Be patient. After analyzing all 15 runs and creating 15 ISAW integrate files, the script will combine and re- index all the peaks with the same UB matrix. Loading an ISAW peaks or integrate file into Mantid can currently take several minutes, so the script can easily run for tens of minutes. The config file is set up to bypass the integrate of the peaks, so I renamed the `natrolite_Niggli.integrate` file to `natrolite_Niggli.peaks`.

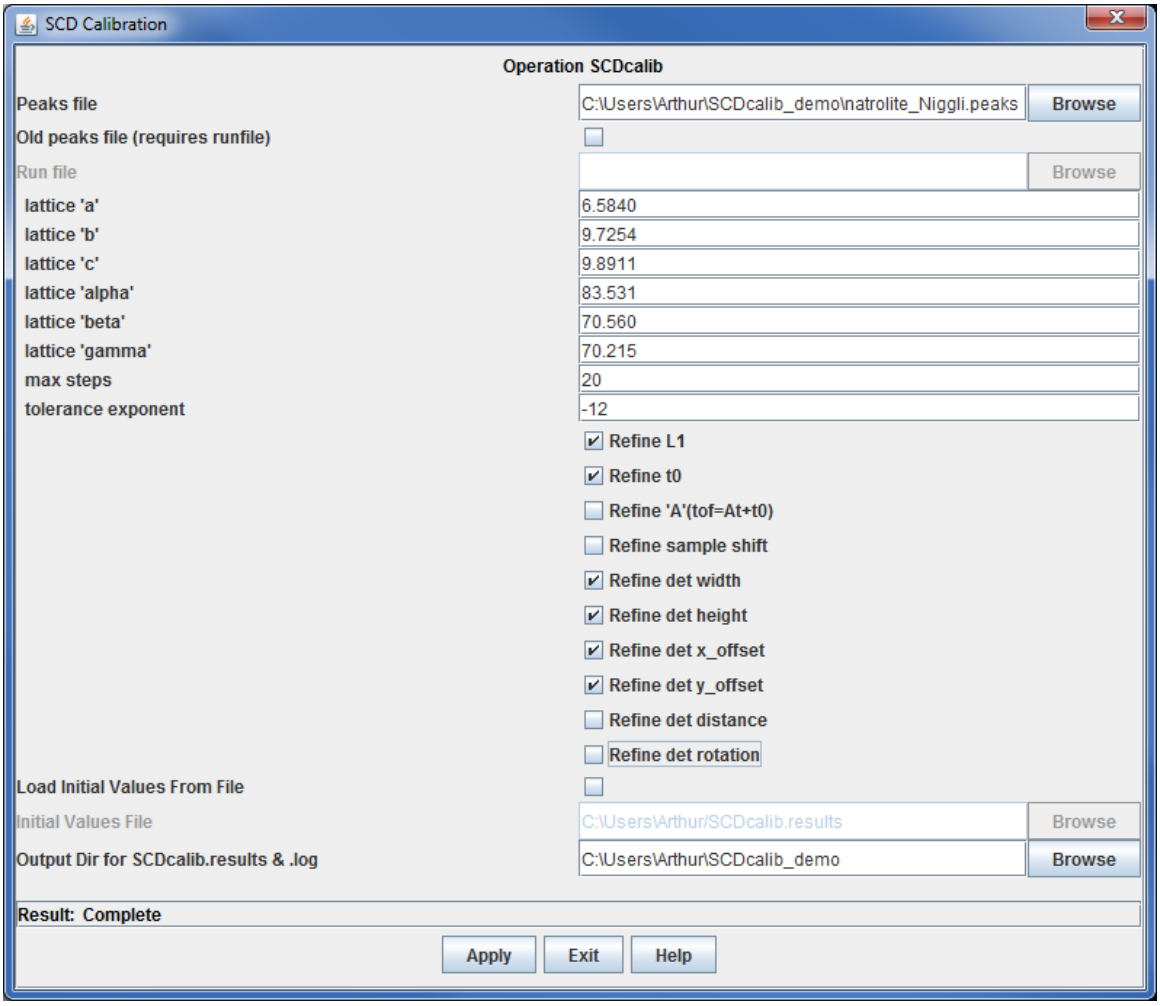
Then launch ISAW on one of the SNS Linux computers or on a Windows PC and launch Macro > Instrument Type > TOF_NSCD > SCD Calibration.



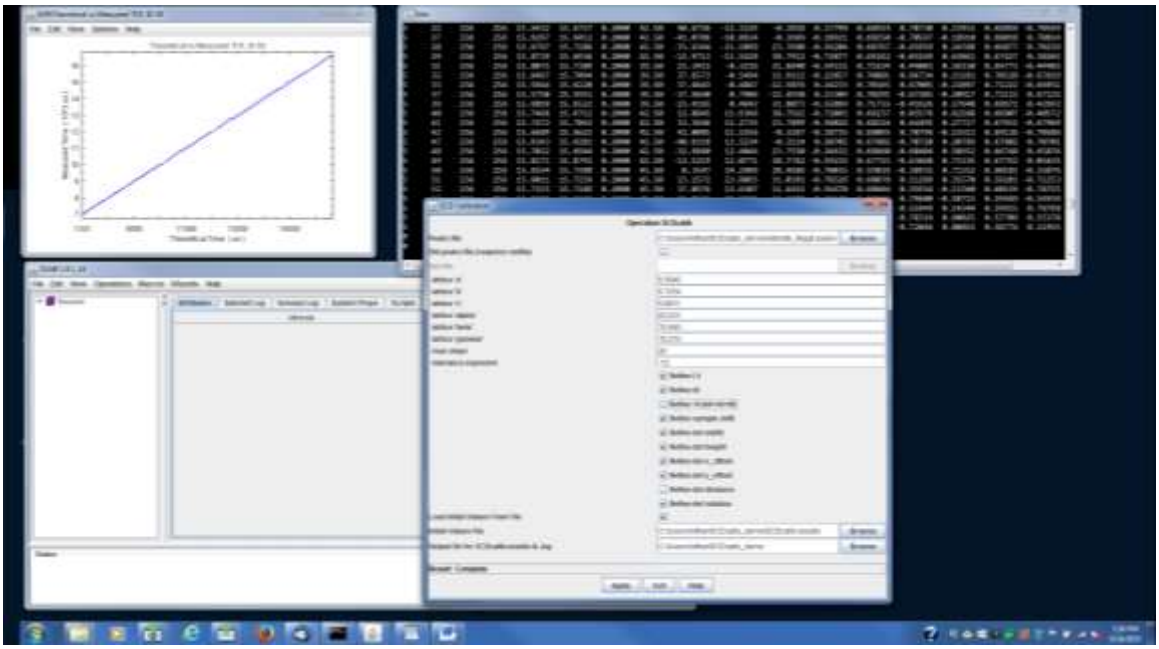
The SCDcalib panel opens with sapphire lattice constants by default.



On my Windows 7 PC, I created a directory `C:\Users\Arthur\SCDcalib_demo` into which the natrolite ISAW peaks file `natrolite_Niggli.peaks` was copied from the `analysis.sns.gov` computer. For "Peaks file" browse to the file. The data were obtained from a natrolite crystal which has an F-centered orthorhombic lattice with approximate lattice constants of 18.3 x 18.6 x 6.6. In order to have similar delta-hkl resolution along each axis, the **primitive reduced lattice constants** were input as shown below. Change "max steps" to 20. In my experience, the refinements do not automatically converge and stop, and 20 steps is more than sufficient. Also, uncheck "Refine det rotation" and browse to select the output directory. It is not possible to refine the detector distance and the detector widths and heights simultaneously since they are correlated. Then click "Apply".

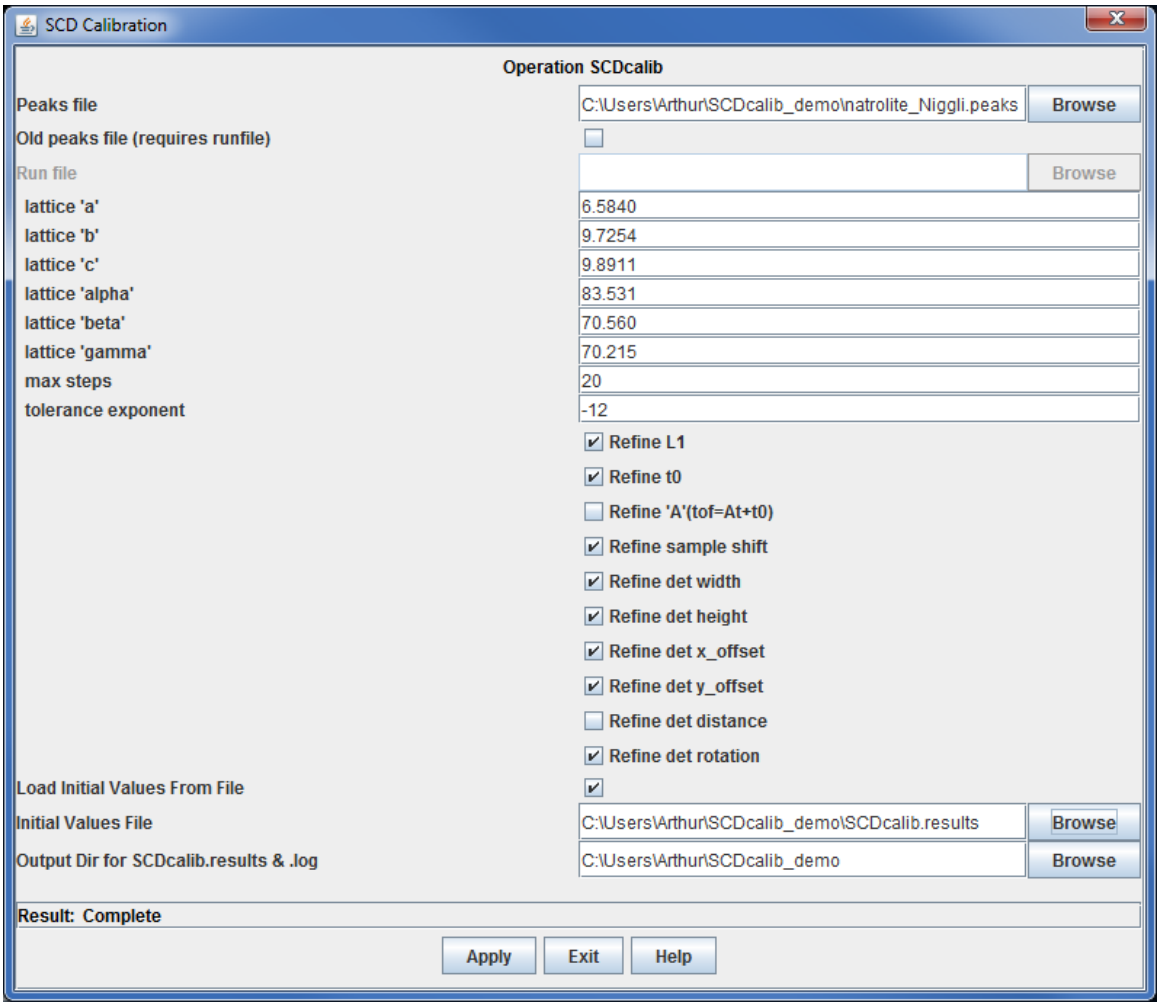


ISAW produces three plots for each detector. They are plots of observed and calculated column, row and time-of-flight channels. You will need to close each plot window by clicking on it. For 50 detectors, this means closing 150 windows.



The script will also produce two files in the output directory: `SCDcalib.log` and `SCDcalib.results`.

For the next refinement cycles, “Refine sample shift” and “Refine det rotation” are turned on. Also, to use the calibrated parameters that were just obtained, check “Load Initial Values from File” and browse to the `SCDcalib.results` file in the output directory. Then click “Apply” again. You will need to close all the plot windows again.



At this point you should examine the `SCDcalib.results` file with a simple text editor. The beginning of the file has this information:

```
#
# ALL POSSIBLE CALIBRATION PARAMETERS (IPNS Coordinates)
# Thu Sep 24 13:37:08 CDT 2015
# Lengths in meters
# Times in microseconds
# Angles in degrees
#
L1:               30.05298417527868
T0:              -0.904231914564205
A(tof=A*t+T0):    1.0
SX:              -8.726470316865504E-4
SY:              -1.2808554212447116E-4
SZ:               7.004384343948619E-5
Det 1    Width:   0.1589086554596202
Det 1   Height:   0.15832040567953773
Det 1 x_offset:   1.961378765124681E-5
Det 1 y_offset:  -7.329240300750523E-4
Det 1 distance:   0.4091944535270632
Det 1      phi:  -0.141479254789618
Det 1      chi:  -0.04870839793720535
Det 1    omega:  -0.14149038246463574
```

Note the crystal offset `SX` is close to a millimeter, which is a bit large. Later in the file is the line:

```
One standard dev error distance in Q = 0.026748242021746436
```

This is a metric indicating the quality of the overall fit. At the end of the file there are these lines beginning with the pound character:

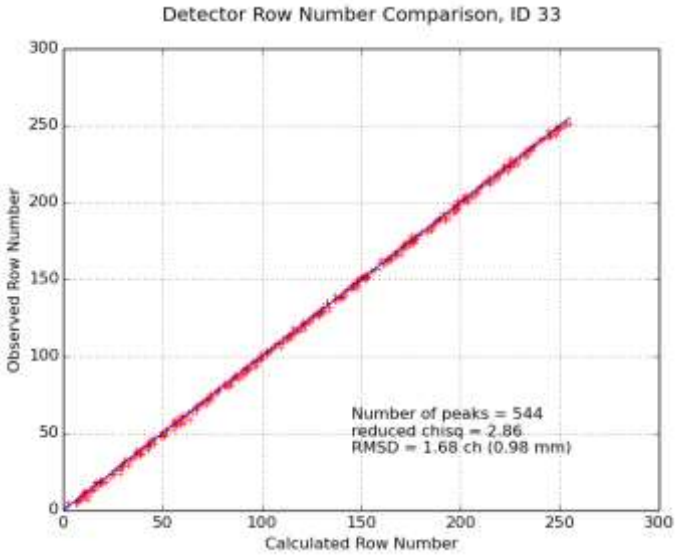
```
#
# NEW CALIBRATION FILE FORMAT (in NeXus/SNS coordinates):
# Lengths are in centimeters.
# Base and up give directions of unit vectors for a local
# x,y coordinate system on the face of the detector.
#
#
# Thu Sep 24 13:37:08 CDT 2015
```

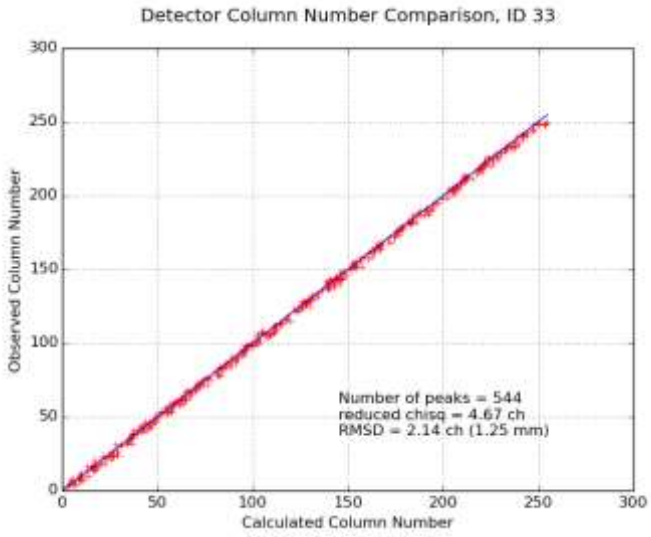
Copy the lines from these lines to the end of the file, and then paste into a new DetCal file, such as `MaNDi_`**`current_date`**`.DetCal`.

The `SCDcalib.log` file contains some similar information, but mostly it lists the "Theoetical" [*sic*] and "Measured" channel for the row, column and TOF for the observed peaks on each detector. Although SCDcalib plots these data, a better way to is to run the `SCDcalib_plot.py` Python script. On `analysis.sns.gov`, the script can be copied from the `/SNS/MANDI/shared/PythonPrograms` or the `/SNS/MANDI/shared/SCDcalib_demo` directory. Alternatively, if you have created a Mantid script repository in your own account (see http://www.mantidproject.org/ScriptRepository), the script should be in the "SingleCrystal" folder. Either way, copy the script to your calibration output directory and run it in a command window:

```
> python SCDcalib_plot.py
```

The script will create a subdirectory `./plots` containing row and channel plots for each detector:





The script also produces the file `SCDcalib_plot.log` containing RMSD values for each detector. Most detector modules are expected to have RMSDs clustered around 1mm (~one pixel) similar values are seen on MaNDi and TOPAZ.

Appendix

Beginning on the next page is a listing of the ReduceSCD.config file that was used to create the peaks file for the calibration. Note that many of the parameters, such as the integration parameters, are not used and are therefore ignored by the script.

```
# Configuration file for ReduceSCD_OneRun.py and ReduceSCD_Parallel.py.
#
# Each line can either start with a comment, indicated by a '#' mark or start
# with a parameter name and value, optionally followed by a comment.  ALL
# parameters used by the script must be specified.  If a required parameter
# is not specified, the script will terminate with a message indicating which
# parameter was missing.
#

#
# _v1: December 3rd 2013. Mads Joergensen
# This version now includes the posibility to use the 1D cylindrical integration method
# and the posibility to load a UB matrix which will be used for integration of the individual
# runs and to index the combined file (Code from Xiapoing).
#

#
# _v2: December 3rd 2013. Mads Joergensen
# Adds the posibility to optimize the loaded UB for each run for a better peak prediction
# It is also possible to find the common UB by using lattice parameters of the first
# run or the loaded matirix instead of the default FFT method
#

# ============================================================================
# Parameters needed by ReduceOneSCD_Run.py, to process ONE run.
# ============================================================================
#
instrument_name   MANDI                        # prefix for run file names

#
# Specify calibration file(s).  SNAP requires two calibration files, one
# for each bank.  If the default detector position is to be used, specify
# None as the calibration file name.
#
calibration_file_1  /SNS/users/ajschultz/MaNDi/natrolite_ipts_8776/MANDI_2015-09-17.DetCal
calibration_file_2  None

#
# Set the data_directory to None to use findnexus to get the run file when
# running this on the SNS systems.  On other systems, all of the input files
# must be copied into one directory and that directory must be specified as
# the data_directory
#
data_directory    None
output_directory  /SNS/users/ajschultz/MaNDi/natrolite_ipts_8776

#
# If use_monitor_counts is True, then the integrated beam monitor
# counts will be used for scaling. If use_monitor_counts is False,
# then the integrated proton charge will be used for scaling. These
# values will be listed under MONCNT in the integrate file.
use_monitor_counts   False

#
# Min & max tof determine the range of events loaded.
# Max Q determines the range of Q values that will be mapped to
# reciprocal space.
# Min & max monitor tof determine the range of tofs integrated
# in the monitor data to get the total monitor counts
#
min_tof           1000
max_tof          16666
max_Q               30
```

```
monitor_index        0
min_monitor_tof   1000
max_monitor_tof  12500

#
# Read the UB matrix from file. This option will be applied to each run and used for
# combined file. This option is especially helpful for 2nd frame TOPAZ data.
read_UB       False
UB_filename  /SNS/TOPAZ/IPTS-9890/shared/test/test.mat

# Use FundUBUsingLatticeParameters to optimize the given UB for each run?
optimize_UB  True

# Use FundUBUsingLatticeParameters to find common UB (instead for FFT)
# This option will find the UB for the fist run and the cell parametes in the
# algorithm, unless a UB has been specified: in this case the values in the specified
# file will be used.
UseFirstLattice  True

#
# Specifiy a conventional cell type and centering.  If these are None, only
# one .mat and .integrate file will be written for this run, and they will
# be in terms of the Niggli reduced cell.  If these specifiy a valid
# cell type and centering, an additional .mat and .integrate file will be
# written for the specified cell_type and centering.  NOTE: If run in
# parallel, the driving script will only read the Niggli version of the
# .integrate file, and will combine, re-index and convert to a conventional
# cell, so these can usually be left as None.
#
# Cell transformation is not applied to cylindrical profiles,
# i.e. use None if cylindrical integration is used!
#
cell_type     None
centering     None
allow_perm    False

#
# Number of peaks to find, per run, both for getting the UB matrix,
# AND to determine how many peaks are integrated, if peak positions are
# NOT predicted.  NOTE: This number must be choosen carefully.  If too
# many peaks are requested, find peaks will take a very long time and
# the returned peaks will probably not even index, since most of them
# will be "noise" peaks.  If too few are requested, then there will be
# few peaks to be integrated, and the UB matrix may not be as accurate
# as it should be for predicting peaks to integrate.
#
num_peaks_to_find 600

#
# min_d, max_d and tolerance control indexing peaks.  max_d is also
# used to specify a threshold for the separation between peaks
# returned by FindPeaksMD, so it should be specified somewhat larger
# than the largest cell edge in the Niggli reduced cell for the
# sample.
#
min_d         8
max_d        20
tolerance  0.12

#
# If predicted peak positions are to be integrated,
# the integrate_predicted_peaks flag should be set to True and the range
# of wavelengths and d-spacings must be specified
```

```
#
integrate_predicted_peaks   False
min_pred_wl                 0.4
max_pred_wl                 3.5
min_pred_dspacing           0.5
max_pred_dspacing           8.5

#
# Select only ONE of the following integration methods, by setting the
# use_*****_integration flag True.
#
use_sphere_integration          False
use_ellipse_integration         False
use_fit_peaks_integration       False
use_cylindrical_integration     False

#
# Specify sphere and ellipse integration control parameters. Check that these
# are correct, if use_sphere_integration, or use_ellipse_integration is True.
# Otherwise the values aren't used.
#
peak_radius             0.075      # for sphere integration only
bkg_inner_radius        0.075      # for sphere or ellipse integration
bkg_outer_radius        0.095     # for sphere or ellipse integration
integrate_if_edge_peak  True       # for sphere integration only

#
# Specify ellispe integration control parameters
#
ellipse_region_radius   0.16
ellipse_size_specified  True

#
# Specify fit peaks integration control parameters.  Check that these are
# correct, if use_fit_peaks_integration = True.  Otherwise the values
# aren't used.
#
rebin_step            -0.004
preserve_events       True
use_ikeda_carpenter   False
n_bad_edge_pixels      0


#
# Specify cylindrical integration control parameters
#
cylinder_radius      0.05
cylinder_length      0.30

# ============================================================================
# Additional Parameters needed by ReduceSCD_Parallel.py, to process
# multiple runs in parallel.
# ============================================================================
#
exp_name               natrolite
reduce_one_run_script  ReduceSCD_OneRun.py

#
# Specify the run numbers that should be reduced.  This can be done on several
# lines.  Each line must start with the parameter name run_nums and be followed
# by a comma separated list of individual run numbers or ranges of run numbers.
# A range of run numbers is specified by listing the first number and last
# number in the range, separated by a colon.
```

```
#
run_nums  4362:4376

#
# Specify the slurm partion, or None to use local processes.  The parameter
# max_processes controls the maximum number of processes that will be run
# simultaneously locally, or that will be simultaneously submitted to slurm.
# The value of max_processes should be choosen carefully with the size of the
# system in mind, to avoid overloading the system.  Since the lower level
# calculations are all multi-threaded, this should be substantially lower than
# the total number of cores available.
# All runs will be processed eventually.  If there are more runs than then
# max_processes, as some processes finish, new ones will be started, until
# all runs have been processed.
#
#slurm_queue_name    topazq
slurm_queue_name    None
max_processes       16
```

Appendix (MaNDi at 40 Detectors ☺)

ID=Detector ID

RMSD in mm units

ID	NumPeaks	Row	Column	Combined
1	339	0.97	1.26	1.12
2	269	1.11	1.36	1.24
3	494	1.21	1.13	1.17
5	615	1.25	1.17	1.21
7	486	1.27	1.11	1.19
8	273	1.36	1.06	1.22
11	130	1.20	1.05	1.13
12	309	1.27	1.14	1.21
13	435	1.36	1.07	1.22
17	440	1.14	1.26	1.20
18	303	1.06	1.24	1.15
19	152	1.01	1.14	1.08
20	50	1.05	0.78	0.93
21	208	1.24	1.03	1.14
22	409	1.28	1.03	1.16
23	529	1.31	1.20	1.26
26	524	1.17	1.15	1.16
27	457	1.03	1.13	1.08
28	244	0.98	1.14	1.06
29	58	1.05	1.00	1.02
31	119	1.03	1.07	1.05
32	336	1.20	0.99	1.10
33	544	1.25	0.98	1.13
37	549	0.99	1.07	1.03
39	119	0.96	1.13	1.04
40	44	1.00	0.94	0.97
41	197	1.15	1.08	1.11
42	420	1.22	1.06	1.14
43	538	1.31	1.11	1.21
46	504	1.14	1.05	1.10
47	414	0.97	1.20	1.09
48	194	1.06	1.21	1.14
49	44	1.42	1.01	1.23
50	22	1.58	1.20	1.40
51	132	0.95	1.52	1.27
52	307	1.22	1.22	1.22
53	415	1.29	1.17	1.23
57	424	1.03	1.22	1.13
58	307	1.08	1.28	1.18
59	152	1.41	1.02	1.23