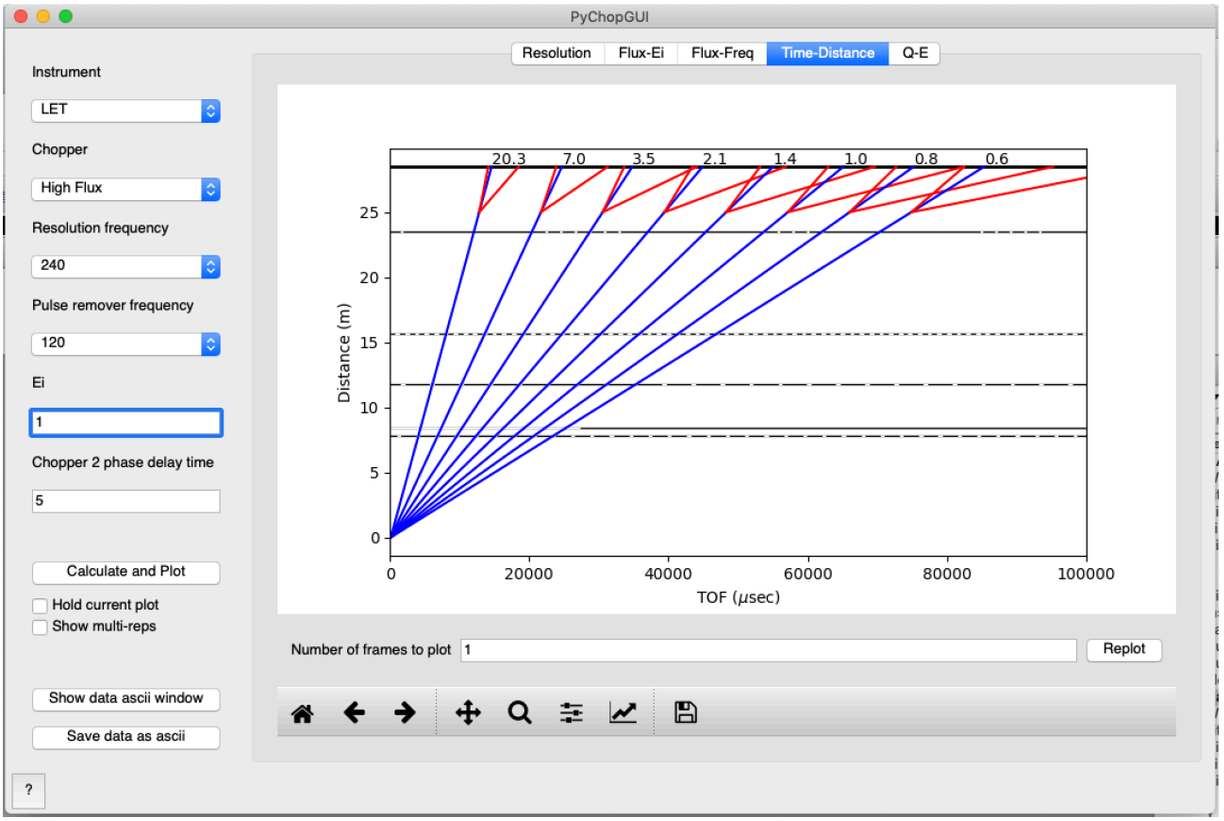
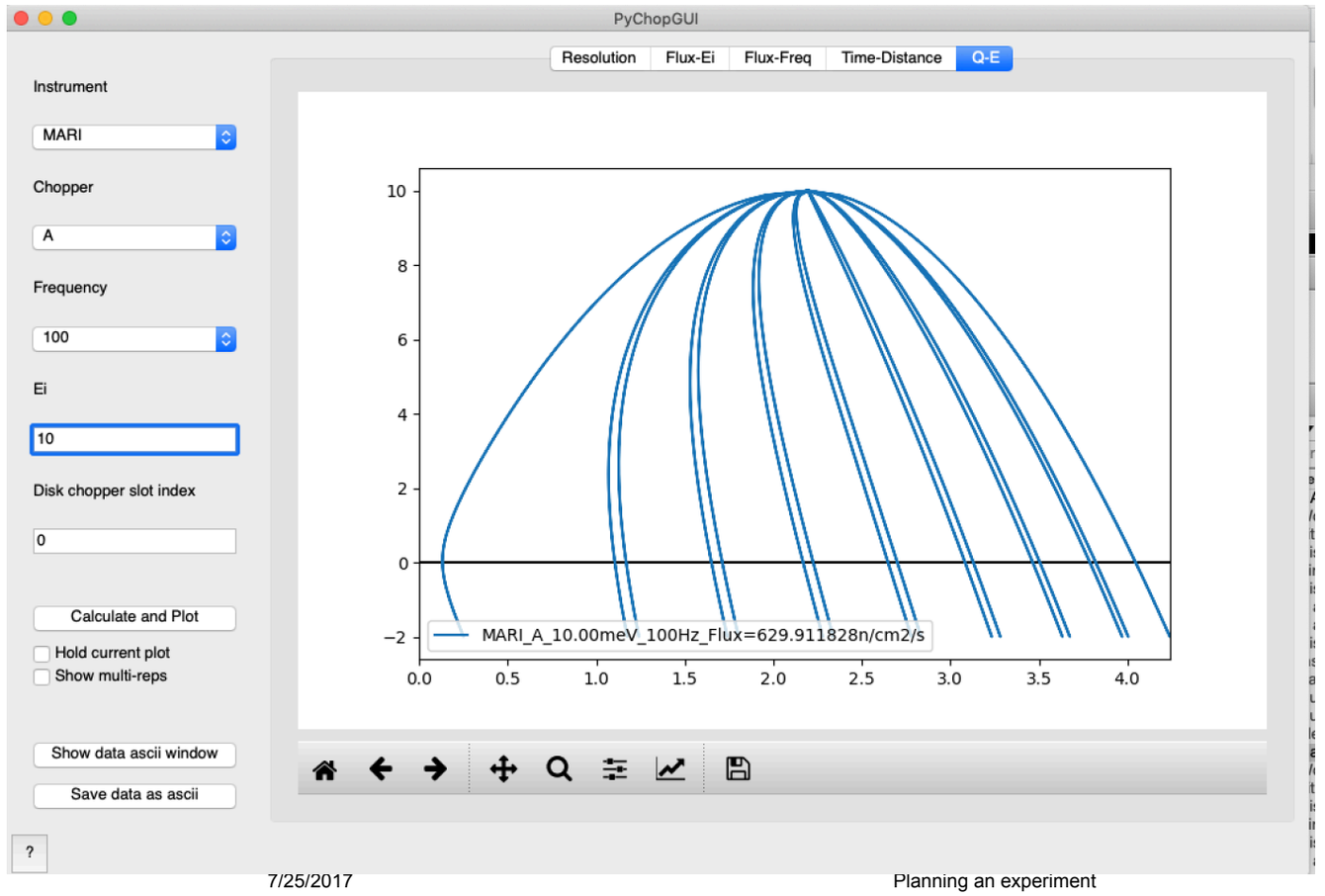
Experiment planning





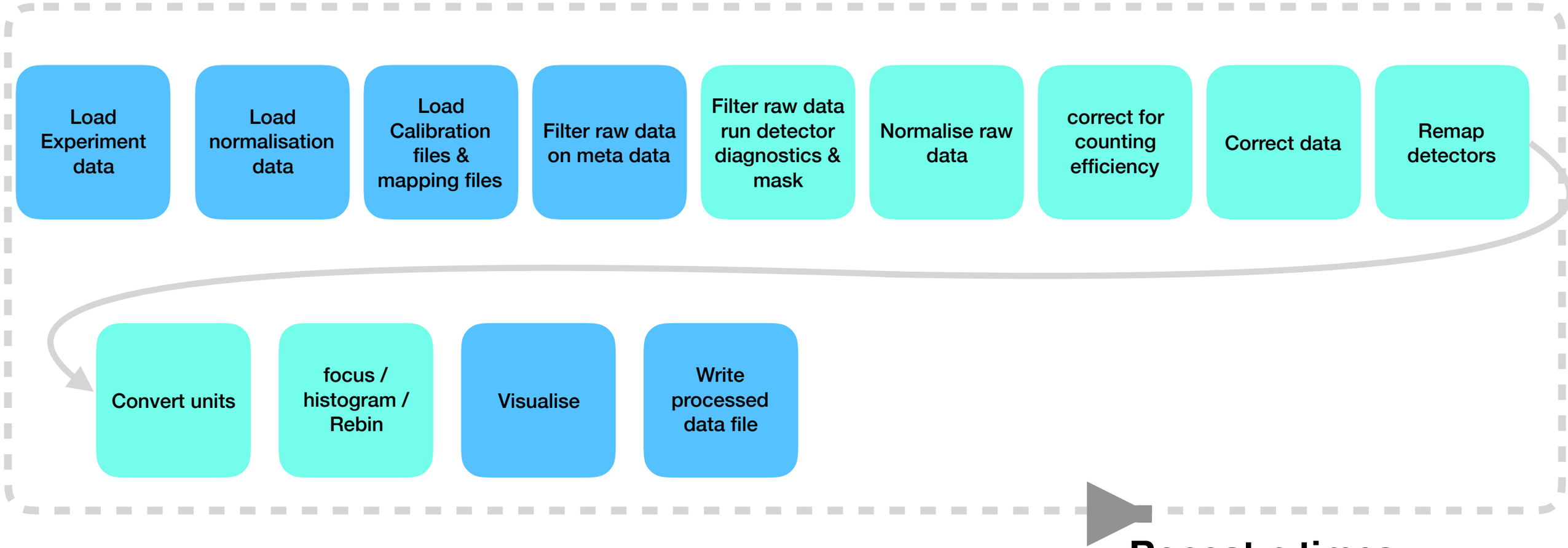
- Flux on sample
- Resolution In Q & E vs Ei and chopper speed
- Detector coverage in Mod Q
- Coverage in QxQy
- Xtal alignment & rotations for 4D
- …

7/25/2017 Planning an experiment

Planning an experiment

```
%============Fake data=====================

en=[0:10:500];
par_file='C:\Russell\Horace_workshop\Matlab\4to1_102.par';
sqw_file='C:\Russell\Horace_workshop\Matlab\my_fake_file.sqw';
efix=550;
psi=[-75:5:75];
emode=1;
alatt=[2.87,2.87,2.87];
angdeg=[90,90,90];
u=[1,0,0]; v=[0,1,0];
omega=0; dpsi=0; gl=0; gs=0;

fake_sqw (en, par_file, sqw_file, efix, emode, alatt, angdeg,...
                    u, v, psi, omega, dpsi, gl, gs);

%Play around with different proj.u and proj.v, always remembering to ensure that
%the two are orthogonal to one another!
proj.u=[-1,-1,1]; proj.v=[0,1,1]; proj.uoffset=[2,0,0,0]; proj.type='rrr';

my_cut=cut_sqw(sqw_file,proj,[-1,0.05,1],[-0.1,0.1],[-0.1,0.1],[0,10,400],'-nopix');


plot(compact(my_cut));

%Notice that the image here is colour coded according to the value of psi
%for detectors from the run that contributed to these data.

%You can also fire up the horace planner interactive gui, for a quick and dirty way of
%planning your experiment
horace_planner
```

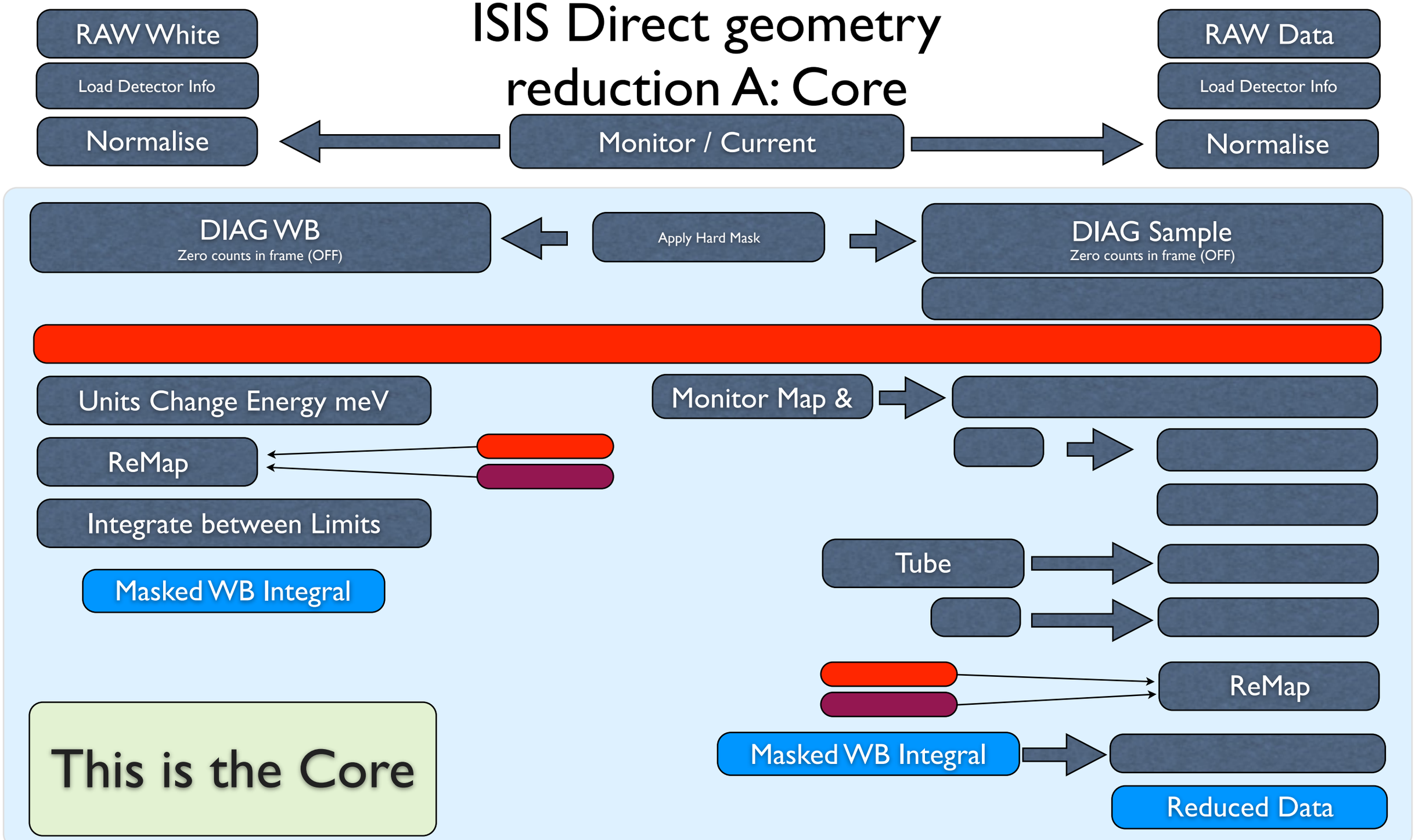
Data Processing / data reduction



Each box requires a myriad of input data or parameters which have a direct effect on the processed data.

Is part of a data reduction workflow

ISIS Direct geometry reduction A: Core



White beam data is the ISIS term for the data set that corrects for counting efficiency of each detector channel

Direct geometry data reduction workflow - Histogram mode

Import required python modules

```
from qtiGenie import *
from PySlice2 import *
```

Define run numbers, Ei guess, rebin, mapfile and other keyword arguments for reduction

```
inst="mari"
iliad_setup(inst)
ext='.raw'
mapfile='mari_res'
#det_cal_file must be specified if the reduction sends out put to a workspace
cal_file='MAR16637.raw'
whitebeamfile="16637"
ei=100
rebin_params='-10,.2,95'
runs=[16654]
```

Execute python line

```
w2=iliad("whitebeamfile","runs",ei,rebin_params,mapfile,det_cal_file=cal_file,norm_method='current')
```

Create instance of reduction class for selected

Load Instrument parameter file

load White beam run

```
LoadRaw(Filename=r'/Users/jon/mprogs/mari_data/RAW/MAR16637.raw',OutputWorkspace='wb_wksp',LoadLogFiles='0')
```

Load Detector

Normalise

Monitor / Current
Monitor Integral

DIAG WB
Zero counts in frame (OFF)
Median Rate in bank --> Reject outside of pre-determined range

Apply Hard Mask

Load sample run

```
LoadRaw(Filename=r'/Users/jon/mprogs/mari_data/RAW/
MAR16652.raw',OutputWorkspace='run_wksp',LoadLogFiles='0')
```

Load Detector Info

Normalise

```
NormaliseByCurrent(InputWorkspace='run_wksp',OutputWorkspace='run_wksp')
```

Find bad spectra for sample run
Zero counts in frame (OFF)
Median Rate in bank --> Reject outside of pre-determined range
Run bleed test

```
FindDetectorsOutsideLimits(InputWorkspace='_wksp.spe-white',OutputWorkspace='white_masks',HighThreshold='10000000000',LowThreshold='1e-10')
MaskDetectors(Workspace='_wksp.spe-white',MaskedWorkspace='white_masks')
MedianDetectorTest(InputWorkspace='_wksp.spe-white',OutputWorkspace='white_masks',SignificanceTest='0')
MaskDetectors(Workspace='_wksp.spe-white',MaskedWorkspace='white_masks')
MaskDetectors(Workspace='_wksp.spe-white',MaskedWorkspace='white_masks')
MaskDetectors(Workspace='background_int',MaskedWorkspace='_wksp.spe-white')
MedianDetectorTest(InputWorkspace='background_int',OutputWorkspace='mask_bkgd',SignificanceTest='3',LowThreshold='0',HighThreshold='2',LowOutlier='0',HighOutlier='1e+100',ExcludeZeroesFromMedian='1')
MaskDetectors(Workspace='_wksp.spe-white',MaskedWorkspace='mask_bkgd')
ExtractMask(InputWorkspace='_wksp.spe-white',OutputWorkspace='diag_mask')
RenameWorkspace(InputWorkspace='diag_mask',OutputWorkspace='masking')
```

Collect Masked Spectra into a workspace called masking

Units Change

```
ConvertUnits(InputWorkspace='_wksp.spe-white',OutputWorkspace='_wksp.spe-white',Target='Energy')
```

ReBin

```
Rebin(InputWorkspace='_wksp.spe-white',OutputWorkspace='_wksp.spe-white',Params='20,160,100')
```

Apply mask to

```
MaskDetectors(Workspace='_wksp.spe-white',MaskedWorkspace='masking')
```

ReMap

```
GroupDetectors(InputWorkspace='_wksp.spe-white',OutputWorkspace='_wksp.spe-white',
MapFile=r'/Users/jon/Work-computing/mantid_test_data/mari/
```

Generate Masked WB Integral workspace

Ei Guess

Calculate Ei

M2&M3 spectrum #s & flightpaths

```
GetEi(InputWorkspace='run_wksp',Monitor1Spec='2',Monitor2Spec='3',EnergyEstimate='100')
```

Move instrument components to define T0 as M2 position

```
ChangeBinOffset(InputWorkspace='run_wksp',OutputWorkspace='_wksp.spe',Offset='-2379.33846378')
MoveInstrumentComponent(Workspace='_wksp.spe',ComponentName='Moderator',Z='-1.4419999999999999',RelativePosition
```

Move detectors to position specified in calibration file

```
LoadDetectorInfo(Workspace='_wksp.spe',DataFilename=r'/Users/jon/mprogs/mari_data/RAW/MAR16637.raw',RelocateDets='
```

Units E trans meV

```
ConvertUnits(InputWorkspace='_wksp.spe',OutputWorkspace='_wksp.spe',Target='DeltaE',EMode='Direct')
```

ReBin

```
Rebin(InputWorkspace='_wksp.spe',OutputWorkspace='_wksp.spe',Params='-10,0.2,95',PreserveEvents='0')
```

Tube

Detector efficiency correction

```
DetectorEfficiencyCor(InputWorkspace='_wksp.spe',OutputWorkspace='_wksp.spe')
```

Ei

```
CorrectKiKf(InputWorkspace='_wksp.spe',OutputWorkspace='_wksp.spe')
```

Apply mask to

```
MaskDetectors(Workspace='_wksp.spe',MaskedWorkspace='masking')
```

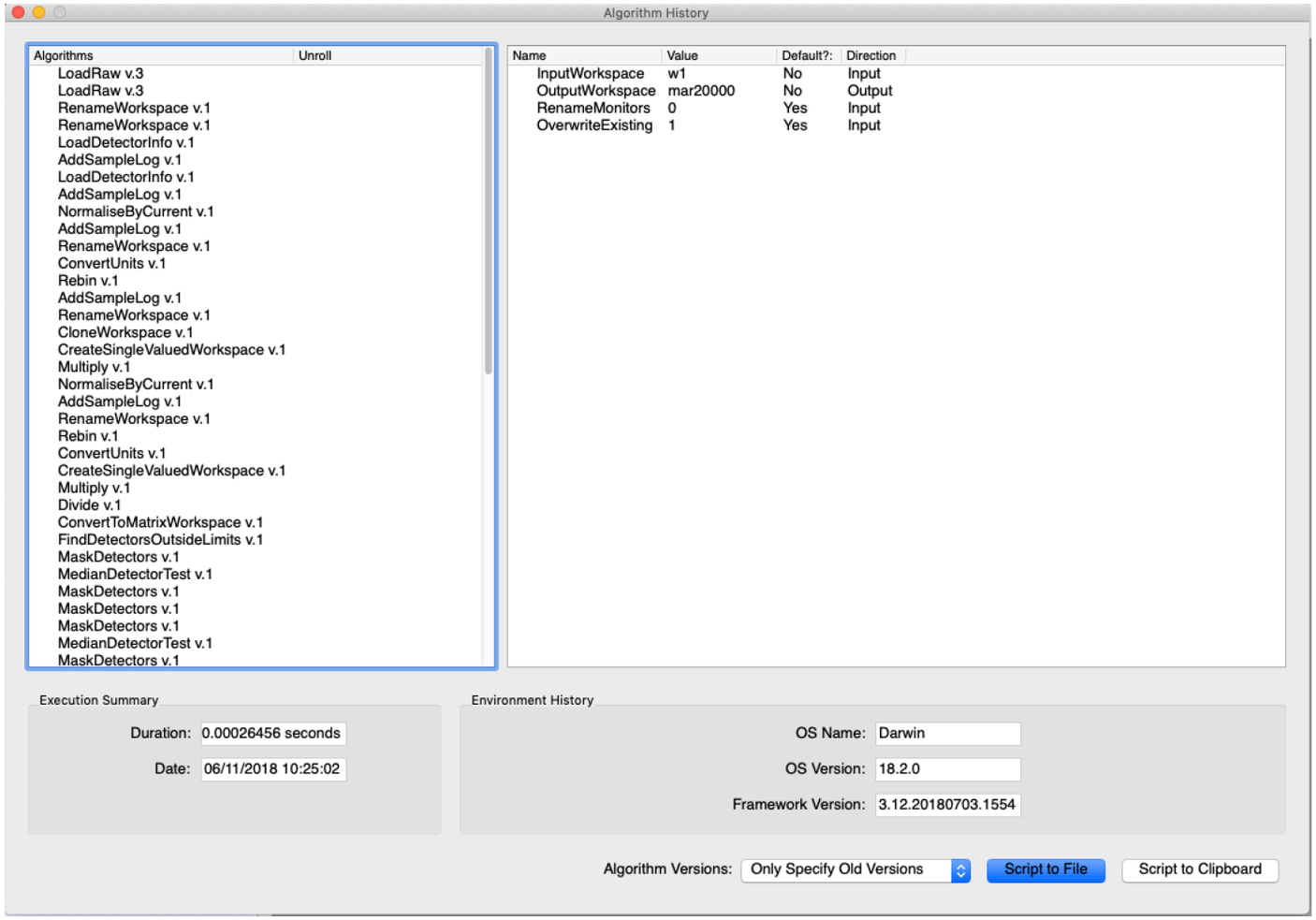
ReMap

```
GroupDetectors(InputWorkspace='_wksp.spe',OutputWorkspace='_wksp.spe',
MapFile=r'/Users/jon/Work-computing/mantid_test_data/mari/mari_res.map',Behaviour='Average')
```

WB Integral workspace

Solid Angle Correction

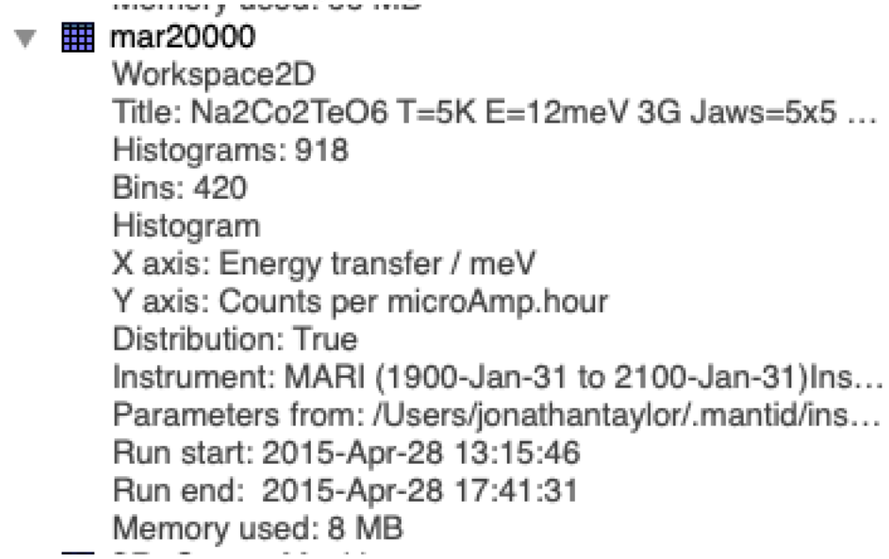
```
Divide(LHSWorkspace='_wksp.spe',RHSWorkspace='_wksp.spe-white',OutputWorkspace='_wksp.spe')
```



Processed workspace includes processing history

Workspace
+ data
+ Instrument information
+ log information

- **No real sample info - just what is in data file i.e. title str**
- **instrument geometry only partial**
- **not always upto date**



Experiment logs and history

```
from qtiGenie import *
from PySlice2 import *

inst='mar'
iliad_setup(inst)
ext='.raw'
#mapfile='mari_res2013'
mapfile='/Users/jonathantaylor/Dropbox/MantidScriptRepository/direct_inelastic/MARI/MapFiles/mari_121_cor'

#det_cal_file must be specified if the reduction sends out put to a workpsace
cal_file='MAR19717.raw'
#hard mask file
#mask_file='/home/mari/Users/taylor/mask.msk'
#load vanadium file
whitebeamfile='19717'
LoadRaw(Filename=whitebeamfile,OutputWorkspace="wb_wksp",LoadLogFiles="0")
#-------
```

1

```
#load a run
############ normal reduction####################


#runs=[19984]; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @5K
#runs=[19985]; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @17K
#runs=[19986]; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @19K
#runs=[19987]; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @22K
#runs=['19988']; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @35K
#runs=['19989']; ei=35; rebin_params='-10,.1,34'; sum=False#Co3TeO6 @50K
#runs=[19990]; ei=19; rebin_params='-10,.05,18'; sum=False#Co3TeO6 @5K 19mev
#runs=[19991]; ei=19; rebin_params='-10,.05,18'; sum=False#Co3TeO6 @22K 19mev
#runs=[19992]; ei=19; rebin_params='-10,.05,18'; sum=False#Co3TeO6 @50K 19mev

#runs=[19993]; ei=50; rebin_params='-10,.1,47'; sum=False#CoCl2.2D2O @cooling 50mev
#runs=[19994]; ei=50; rebin_params='-10,.1,47'; sum=False#CoCl2.2D2O @5K 50mev
#runs=[19995]; ei=50; rebin_params='-10,.1,47'; sum=False#CoCl2.2D2O @100K 50mev
#runs=[19996]; ei=50; rebin_params='-10,.1,47'; sum=False#CoCl2.2D2O @100K 50mev 450 Hz
#runs=[19997]; ei=19; rebin_params='-10,.05,18'; sum=False#Na2Co2TeO6 @cooling 19mev 200 Hz
#runs=[19998]; ei=19; rebin_params='-10,.05,18'; sum=False#Na2Co2TeO6 @5K 19mev 200 Hz
runs=[20000]; ei=12; rebin_params='-10,.05,11'; sum=False#Na2Co2TeO6 @5K 12mev 200 Hz
#runs=[20001]; ei=12; rebin_params='-10,.05,11'; sum=False#Na2Co2TeO6 @13K 12mev 200 Hz
#runs=[20002]; ei=12; rebin_params='-10,.05,11'; sum=False#Na2Co2TeO6 @35K 12mev 200 Hz
#runs=[20003]; ei=7; rebin_params='-10,.05,6.5'; sum=False#Na2Co2TeO6 @5K 7mev 100 Hz
#runs=[20004]; ei=70; rebin_params='-10,.1,68'; sum=False#Na2Co2TeO6 @50K 70mev 200 Hz
#runs=[20005]; ei=70; rebin_params='-10,.1,68'; sum=False#Na2Co2TeO6 @5K 70mev 200 Hz
#runs=[20006]; ei=12; rebin_params='-10,.05,11.5'; sum=False#Na2Co2TeO6 @17K 12mev 150 Hz
#runs=[20007]; ei=50; rebin_params='-10,.1,48'; sum=False#Ni3TeO6 @cooling 50mev 200 Hz
#runs=[20008]; ei=50; rebin_params='-10,.1,48'; sum=False#Ni3TeO6 @5K 50mev 200 Hz
#runs=[20009]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @5K 35mev 200 Hz
#runs=[20010]; ei=50; rebin_params='-10,.1,48'; sum=False#Ni3TeO6 @5K 50mev 200 Hz
#runs=[20011]; ei=50; rebin_params='-10,.1,48'; sum=False#Ni3TeO6 @70K 50mev 200 Hz
#runs=[20012]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @70K 70mev 200 Hz
#runs=[20013]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @10K 35mev 200 Hz
#runs=[20014]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @15K 35mev 200 Hz
#runs=[20015]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @20K 35mev 200 H3z
#runs=[20016]; ei=35; rebin_params='-10,.1,34'; sum=False#Ni3TeO6 @25K 35mev 200 Hz

#
```

2

```
if sum == True:
        nxsp_file=inst+str(runs[0])+'sum.nxspe'
        for i in range(len(runs)):
            if str(runs[i]) == 'live':
                StartLiveData(UpdateEvery='0.0',Instrument='MARI',AccumulationMethod='Replace',OutputWorkspace="w"+str(i+1))
            else:LoadRaw(Filename=str(runs[i]),OutputWorkspace="w"+str(i+1),LoadLogFiles="0")
            if i == 0: run_wksp = mtd['w1']
            else: run_wksp = run_wksp+mtd['w'+str(i+1)]
        #w1=iliad("wb_wksp","run_wksp",ei,rebin_params,mapfile,fixei=False,det_cal_file=cal_file,norm_method='current',hardmaskOnly=mask_file)
        w1=iliad("wb_wksp","run_wksp",ei,rebin_params,mapfile,fixei=False,det_cal_file=cal_file,norm_method='current')
        RenameWorkspace(InputWorkspace='w1',OutputWorkspace=inst+str(runs[0])+'sum')
#       SaveNXSPE(InputWorkspace='mar'+str(runs[0])+'sum',Filename=nxspe_file, KiOverKfScaling=True)
else:

        for runfile in runs:
            LoadRaw(Filename=whitebeamfile,OutputWorkspace="wb_wksp",LoadLogFiles="0")
            if runfile == 'live':
                StartLiveData(UpdateEvery='0.0',Instrument='MARI',AccumulationMethod='Replace',OutputWorkspace='run_wksp')
        else:
                LoadRaw(Filename=str(runfile),OutputWorkspace="run_wksp",LoadLogFiles="0")

            #w1=iliad("wb_wksp","run_wksp",ei,rebin_params,mapfile,fixei=False,det_cal_file=cal_file,norm_method='current',hardmaskOnly=mask_file)
            w1=iliad("wb_wksp","run_wksp",ei,rebin_params,mapfile,fixei=False,det_cal_file=cal_file,norm_method='current')
            RenameWorkspace(InputWorkspace='w1',OutputWorkspace=inst+str(runfile))
    SaveNXSPE(InputWorkspace='mar'+str(runs[0]),Filename=inst+str(runfile)+'.nxspe', KiOverKfScaling=True)
```

3

1. Instrument setup and normalisation data
2. Digital log of runs taken during beamtime.
3. data reduction workflow

Ipad + evernote

Co2MnSi Spring8 Dec 2013

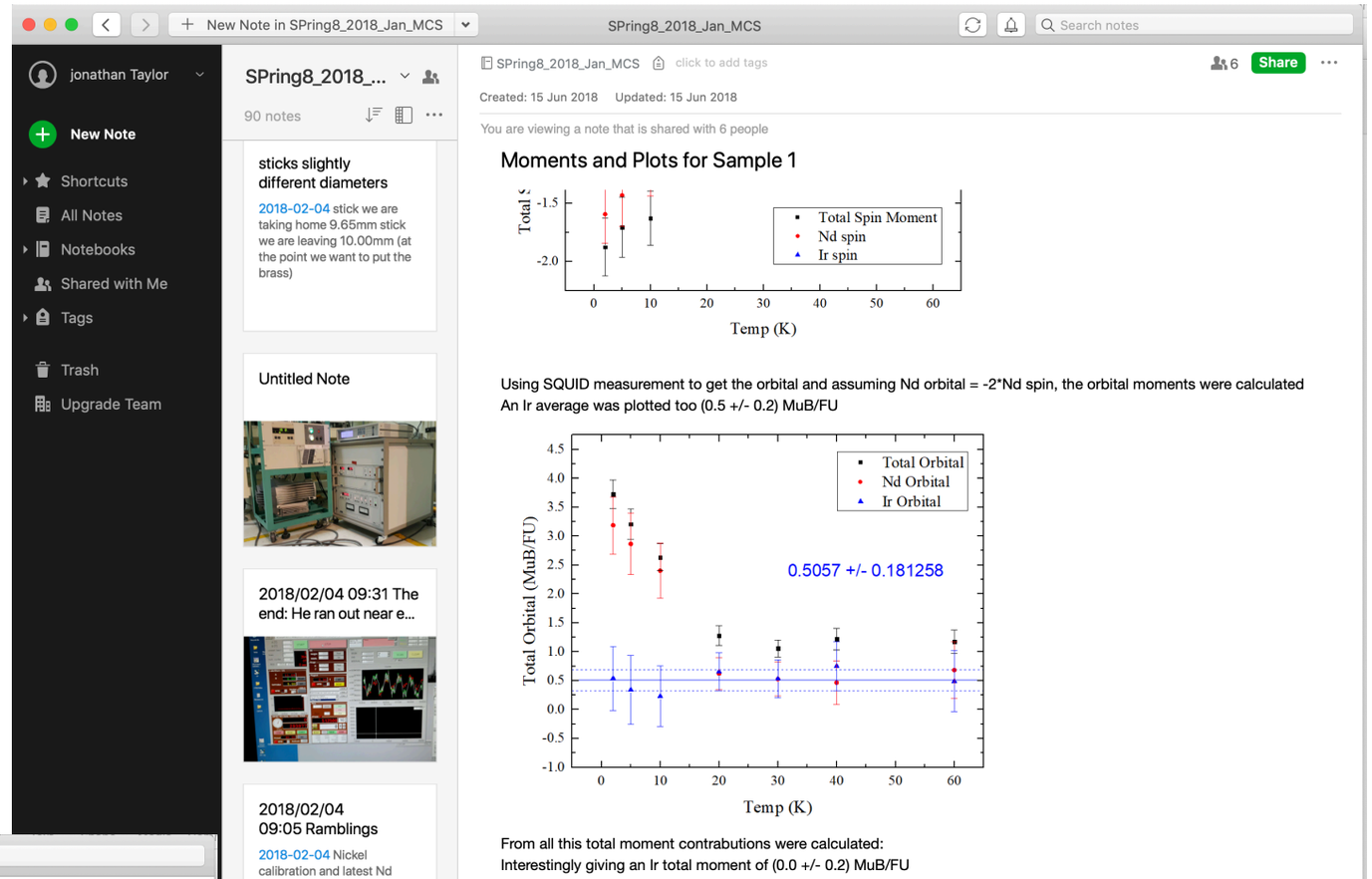
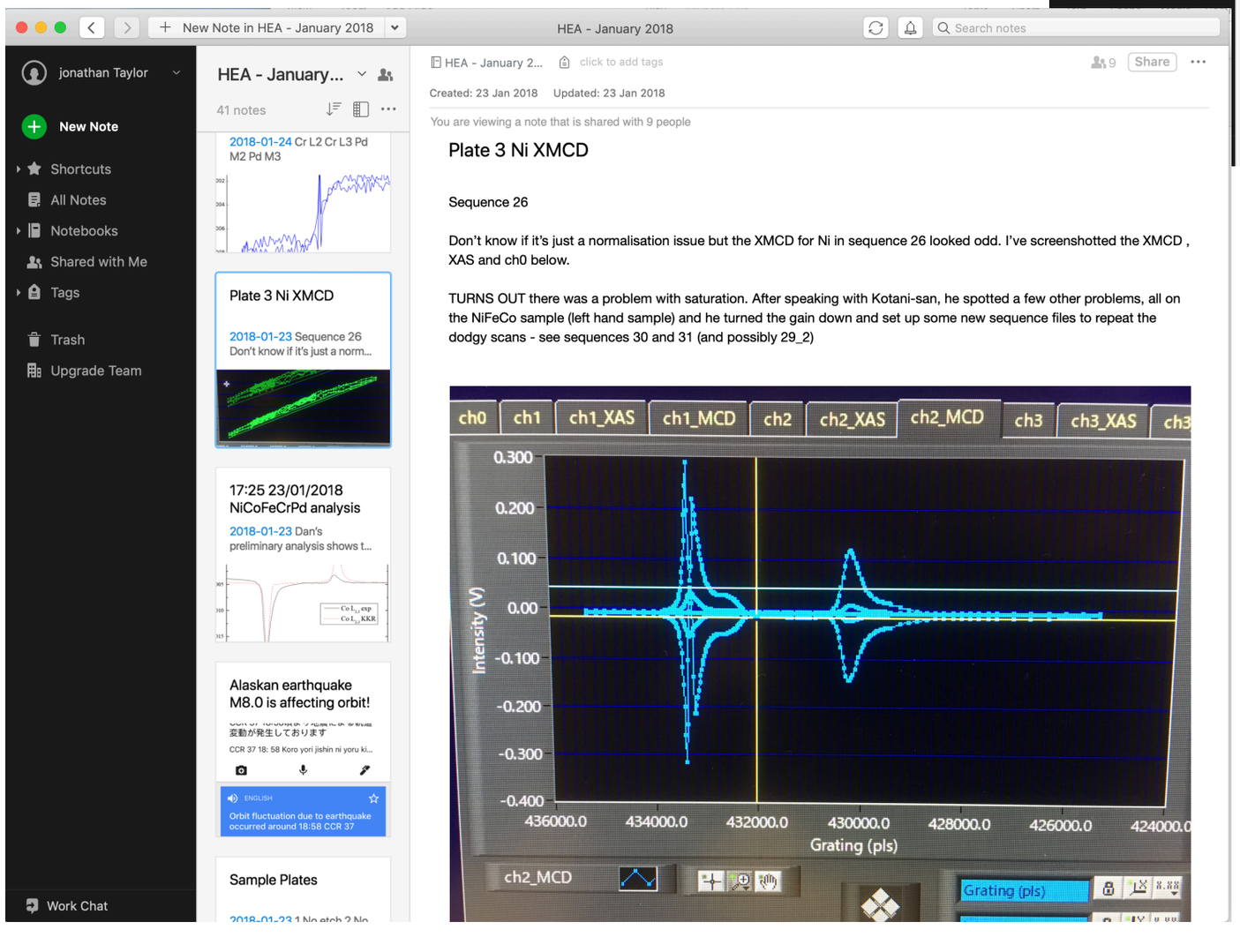
→ purge He bath / VTi Lift He
2.30 pm → fill N_2 Jacket.
3.15 pm → full.

3.30 → fill He bath with N_2

13/12/2013

14th. Dec.

Pt magnet into hotel

Evernote as a e-log

+ Easy to use
+ Can add pictures etc etc
+ easy to share
- Data policy
- cost
- Does not keep notes in time order