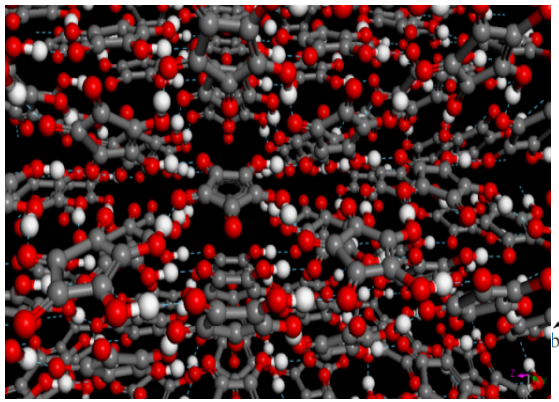
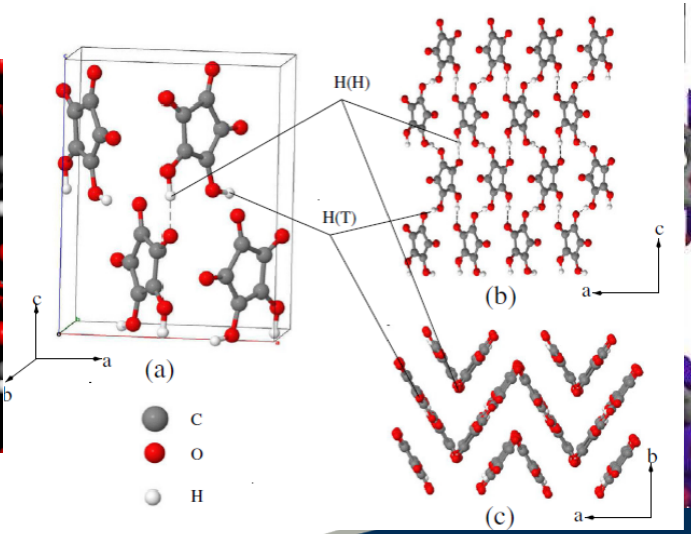
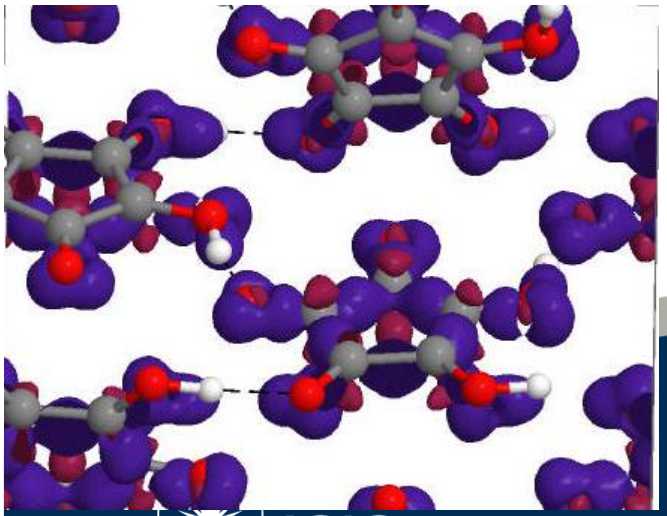
Virtual Experiments: Molecular Spectroscopy

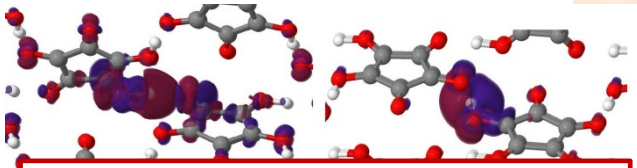
Sanghamitra Mukhopadhyay and Peter Willendrup







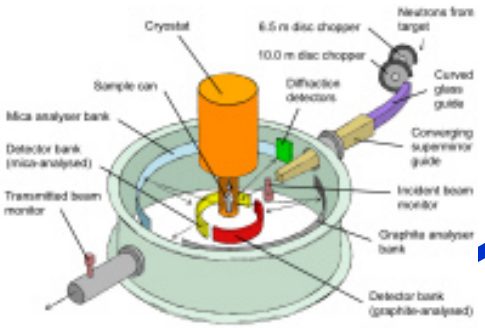
In-Silico Neutron Spectroscopy



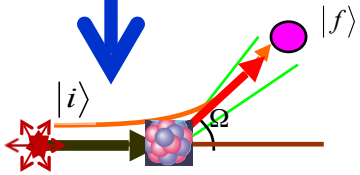
Materials Modelling

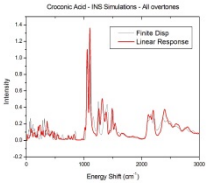
High performance Computers

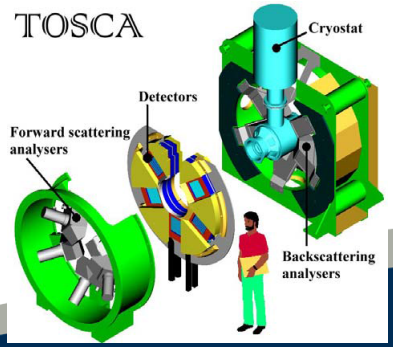
IRIS/OSIRIS



nMoldyn/MDANSE







Python Wrapper

MANTID

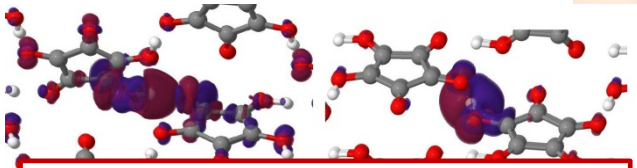
Experiments

MANTID

Experiments

Virtual Experiments: Neutron Spectroscopy

High performance Computers



Materials Modelling

High performance Computers

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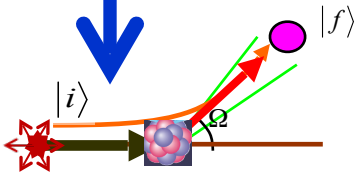
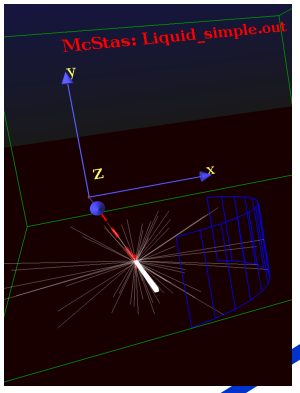
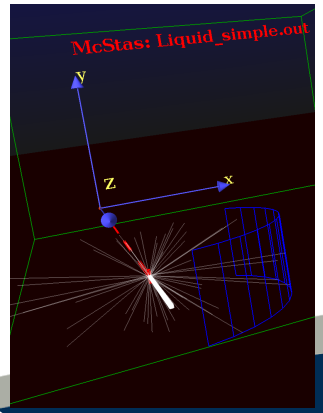
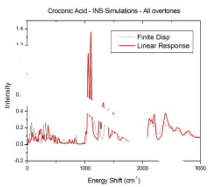








Python Wrapper

MANTID

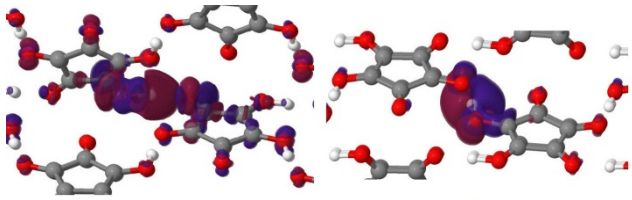
Virtual Experiments

MANTID

Virtual Experiments

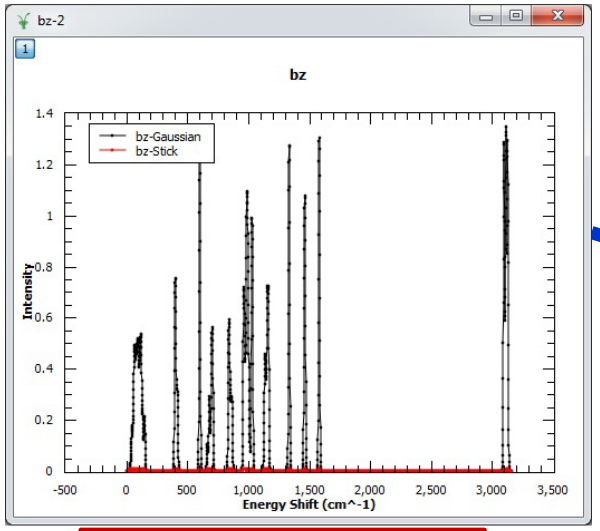
ISIS

Virtual Experiments: Neutron Spectroscopy



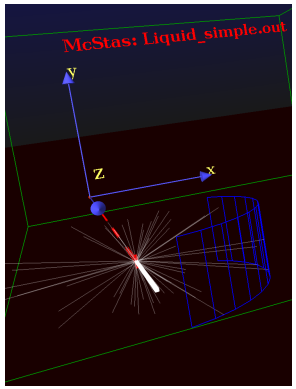
CASTEP DFT Simulations Phonon file

MANTID



VDOS

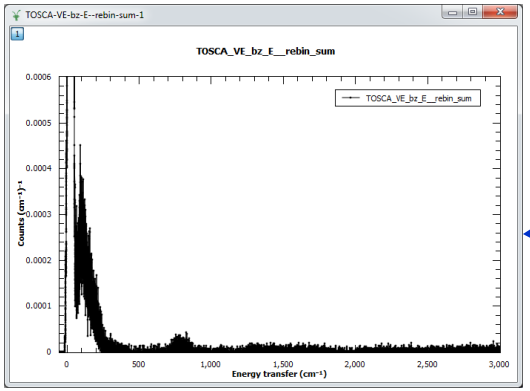
S(Q,W)



McStas Instrument TOSCA

MANTID

Data reduction in MANTID

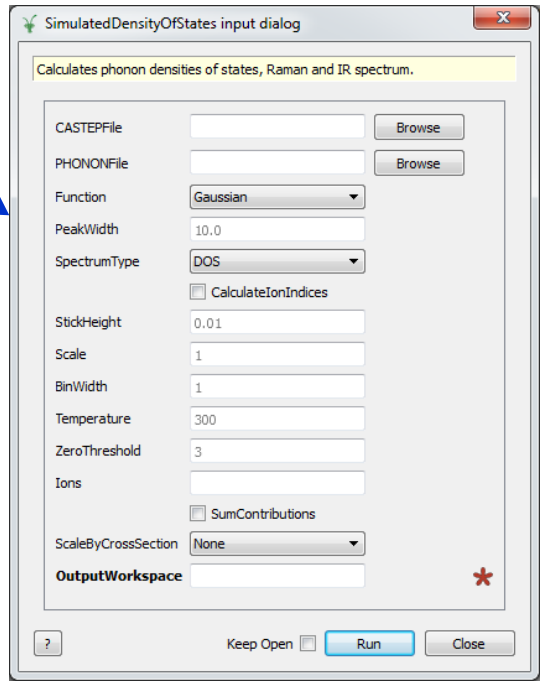


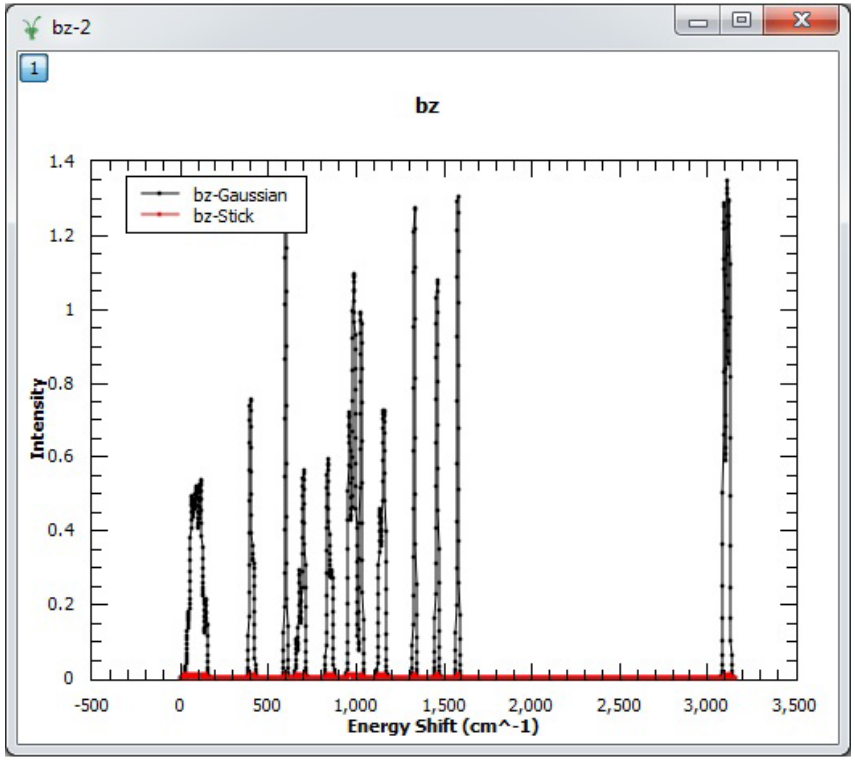
Data Virtual Experiments

Science & Technology Facilities Council
ISIS

Virtual Experiments: Neutron Spectroscopy

CASTEP DFT Simulations Phonon file





VDOS

MANTID

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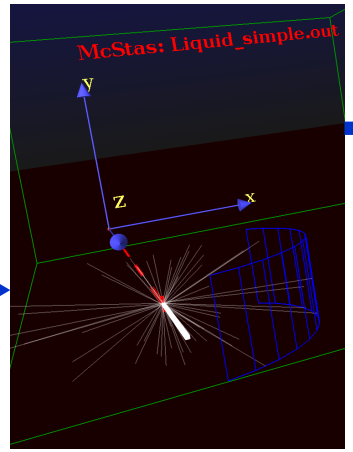
Virtual Experiments: Neutron Spectroscopy

VDOS

S(Q,W)



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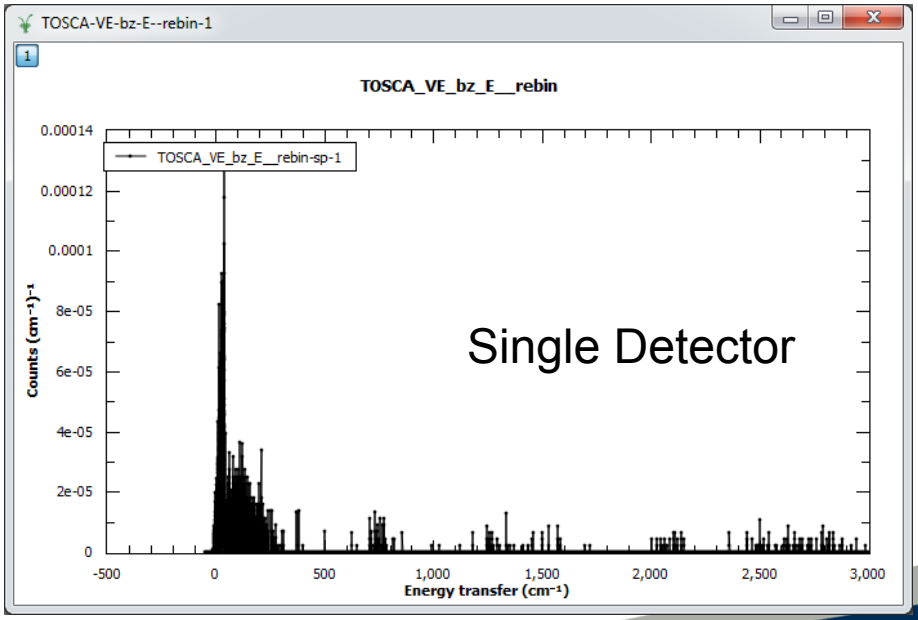

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Virtual Experiments: Neutron Spectroscopy

VDOS

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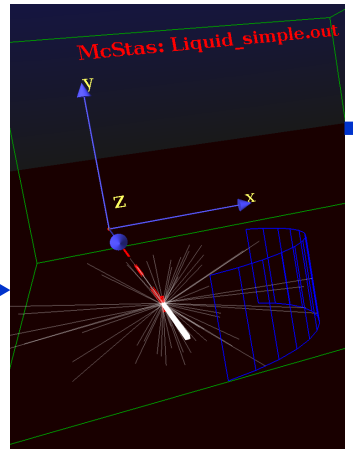

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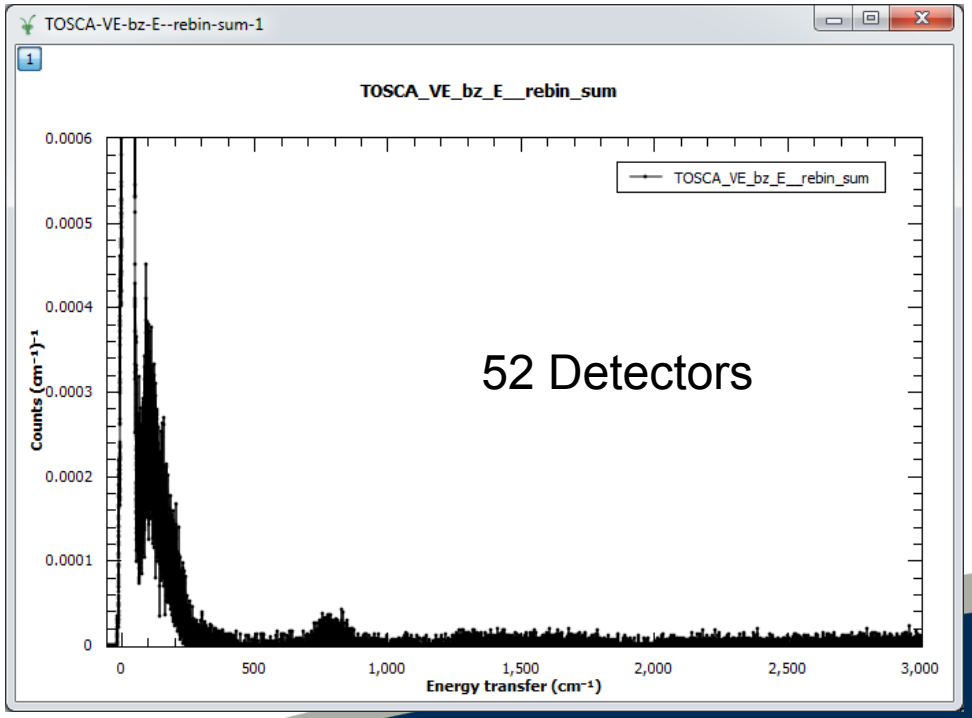

Science & Technology Facilities Council
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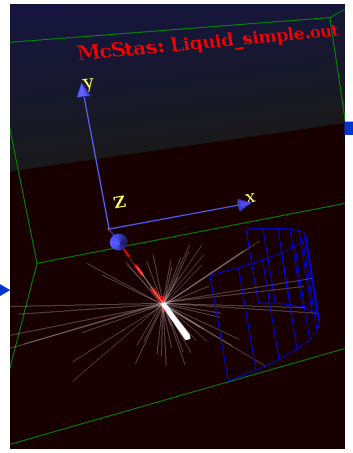
Virtual Experiments: Neutron Spectroscopy

VDOS

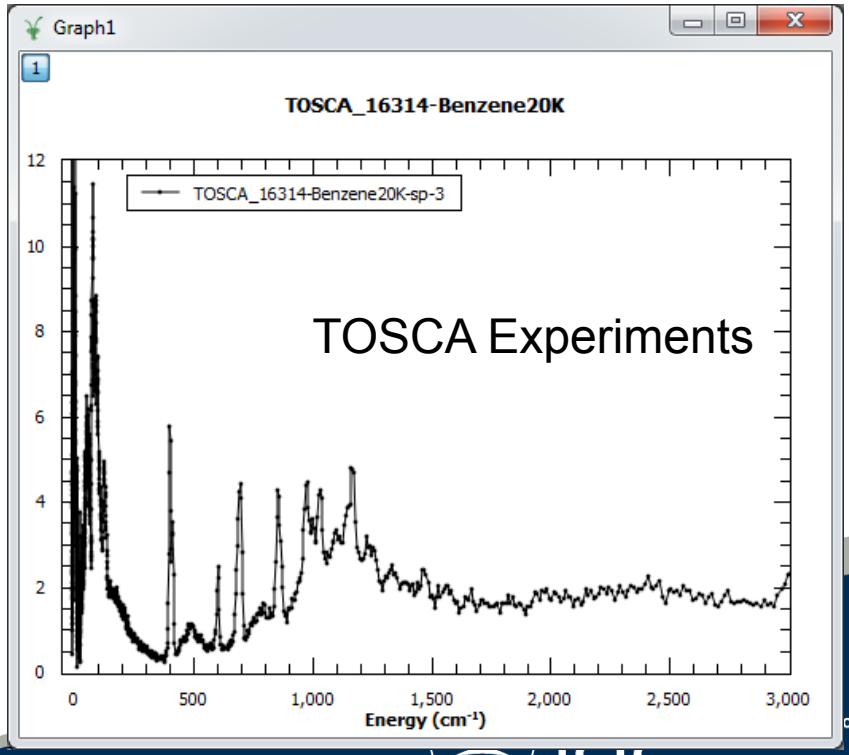
S(Q,W)



McStas Instrument TOSCA

MANTID

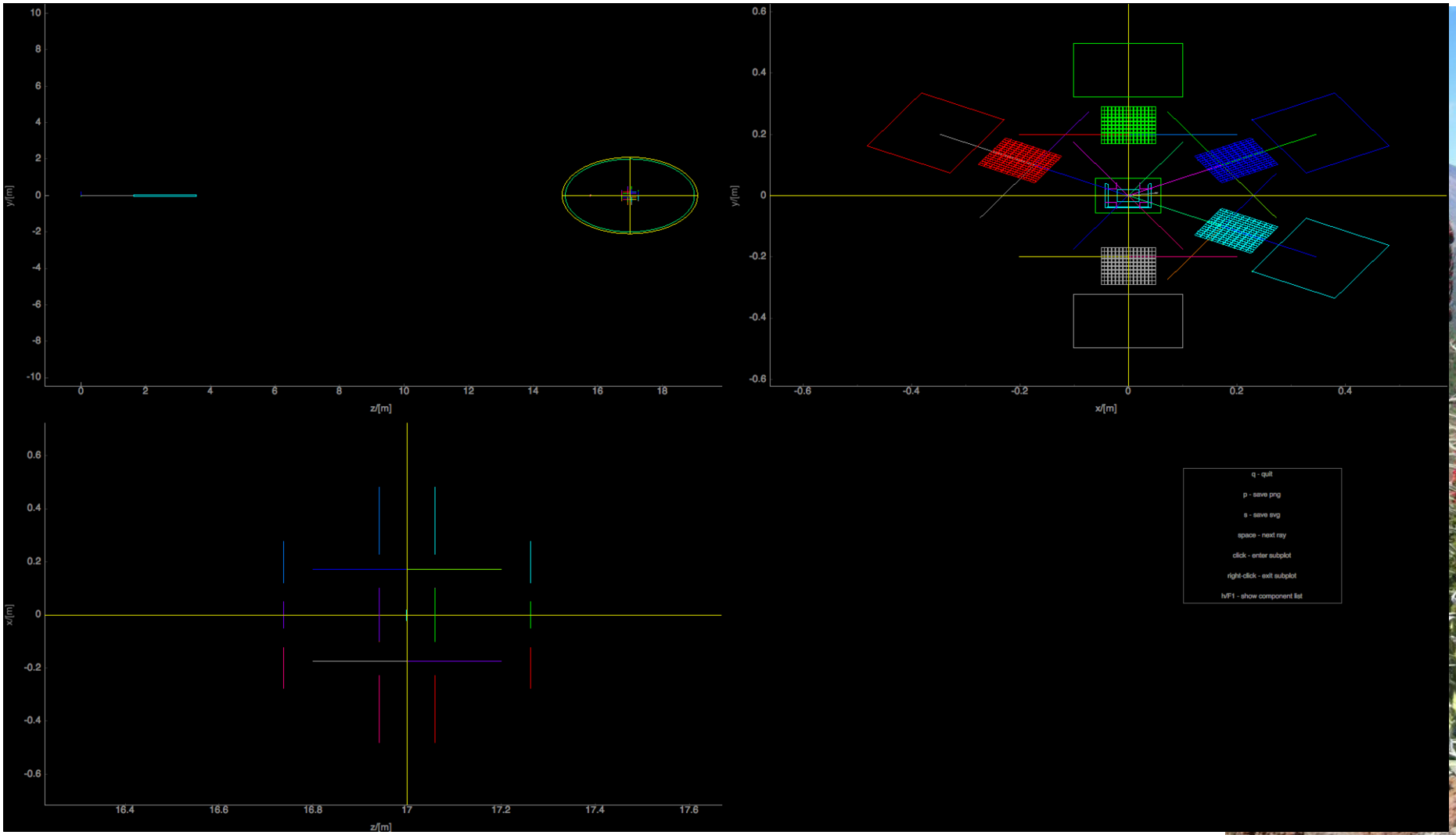
Data reduction in MANTID



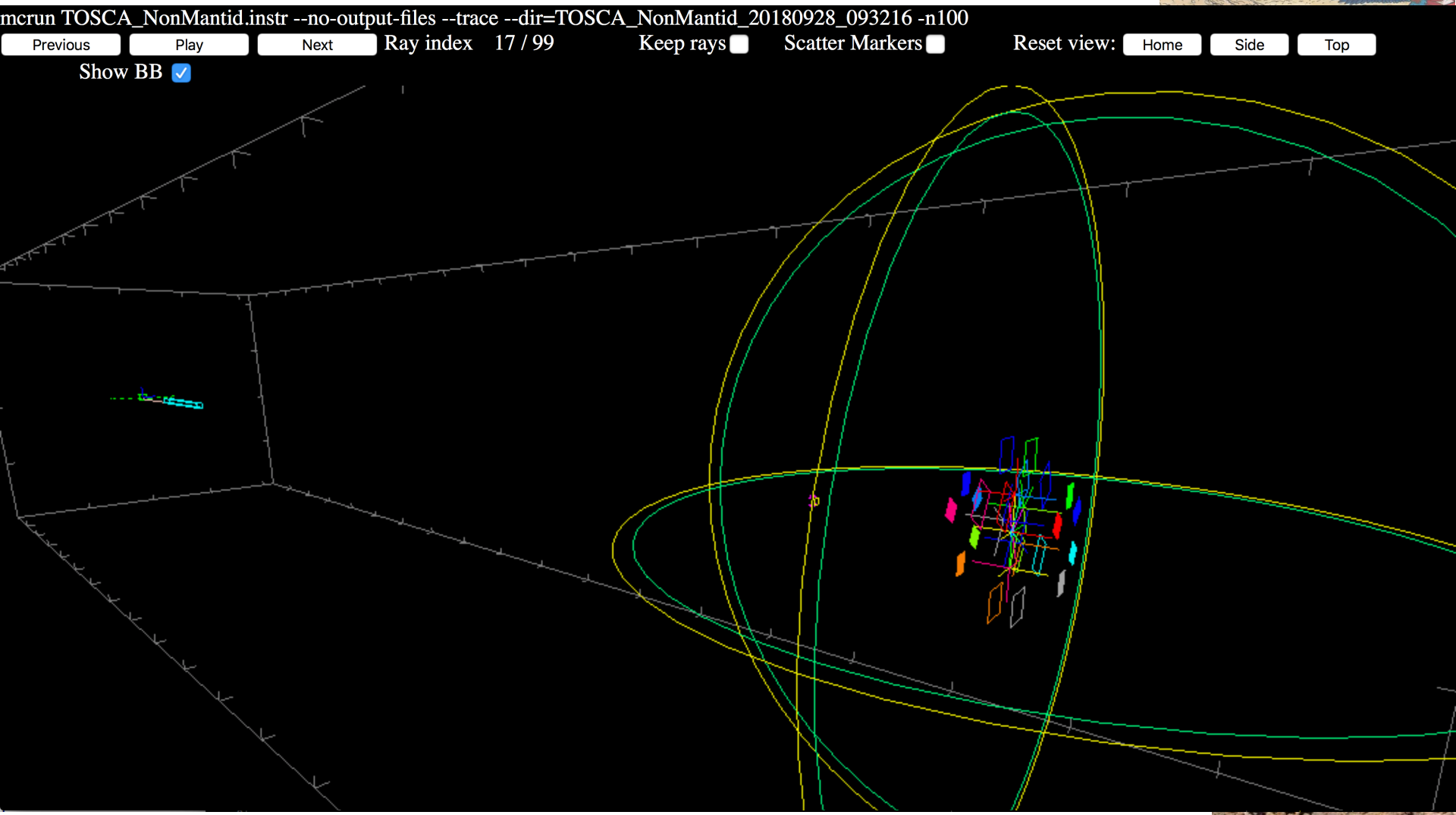
ISIS

TOSCA, McStas → Mantid

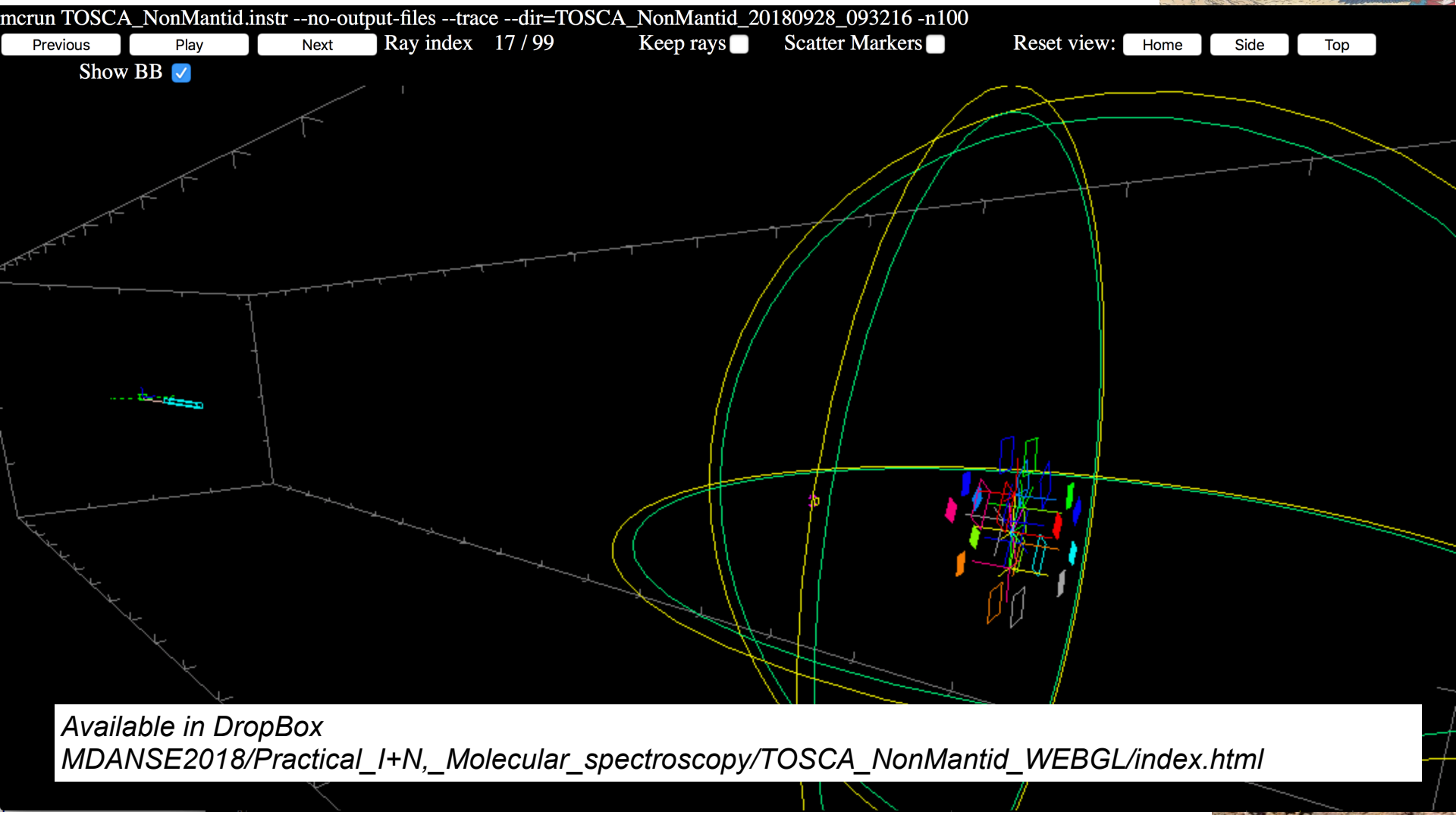
TOSCA in McStas - views along axes



TOSCA in McStas - WEBGL view



TOSCA in McStas - WEBGL view



Available in DropBox
MDANSE2018/Practical_I+N,_Molecular_spectroscopy/TOSCA_NonMantid_WEBGL/index.html

TOSCA transported in Mantid

- *(General recipe available in https://github.com/McStasMcXtrace/McCode/wiki/McStas-and-Mantid)*

- *1. Mantid needs to know where the source is located*

```
//————————MODERATOR
COMPONENT moder=ViewModISIS(Face="TS1_N08_Tosca.mcstas", E0 = 0.01, E1 = 500.0,
 modPosition=0, xw=0.12, yh = 0.115,  xw = 0.04, yh = 0.04, dist = 17)    // New I
AT (0, 0, 0.00001) RELATIVE arm1

  COMPONENT sourceMantid = Arm()
  AT (0,0,0) RELATIVE moder
```

- *2. … and where the sample is located*

```
//————————SAMPLE

SPLIT 1000 COMPONENT powder=Isotropic_Sqw(
  thickness=0, xwidth=0.04, yheight = 0.04, zdepth=zdepth,
  Sqw_coh="NULL", Sqw_inc=inc, p_interact=0.9, d_phi=105
) AT (0, 0, 0) RELATIVE arm_sample
EXTEND
%{
  if (!SCATTERED) ABSORB;
%}

COMPONENT sampleMantid = Arm()
  AT (0,0,0) RELATIVE powder
```

TOSCA transported in Mantid

- *3. Addition of a special series of event monitors - here first backward banks*

```
COMPONENT nD_Mantid_1 = Monitor_nD(xwidth=0.2, yheight=0.1762, user1=t-t_minE/1e6,
        options="mantid square x limits=[-0.1 0.1] bins=2 y limits=[-0.0881 0.0881] bins=13, neutron pixel user1, list all neutrons",
        filename="Bbank")
  WHEN (eventmode==1) AT (0, 0.4165+0.09-0.18/13*7, -0.46548) RELATIVE arm_bank1  GROUP detectors

COMPONENT TOF2 = Monitor_nD(xwidth=0.2, yheight=0.1762, user1=t-t_minE/1e6,
        options="square x limits=[-0.1 0.1] bins=2 y limits=[-0.0881 0.0881] bins=13, neutron pixel user1, list all neutrons",
        filename="Bbank")
  WHEN (eventmode==1) AT (0, 0.4165+0.09-0.18/13*7, -0.46548) RELATIVE arm_bank2  GROUP detectors
```

...

- *4. Geometrical trick - since Mantid directly uses distance between sample and detector for k_f calculation - the analysers are tricked to transmit the reflected beam*

```
//————————BACKWARD BANKS
COMPONENT monocr_b1 = Monochromator_curved( order=1, mosaich = 150,
mosaicv = 150, width = 0.10, height = 0.12, DM = 3.354, reflect="HOPG.rfl",
NH = 15, NV = 10, RH = 0, gap = 0.001)
AT (0, 0.23, -0.2625) RELATIVE arm_bank1 ROTATED (0, 90, 0) RELATIVE arm_bank1
GROUP Monos
EXTEND %{
     if (SCATTERED) vx=-vx;
%}
```

- *5. And detectors then placed behind the analysers instead of toward sample…*
- *6. Recorded ToF is made relative to beam onset at sample*

TOSCA transported in Mantid

- *3. Addition of a special series of event monitors - here first backward banks*

```
xwidth=0.2, yheight=0.1762, user1=t-t_minE/1e6,
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  GROUP Monos
  EXTEND %{
       if (SCATTERED) vx=-vx;
  %}
```

- *5. And detectors then placed behind the analyzers instead of toward sample…*
- *6. Recorded ToF is made relative to beam onset at sample*

TOSCA transported in Mantid

- *6. Instrument must be compiled with NeXus capability*
  - *export MCSTAS_CFLAGS="-g -lm -O2 -DUSE_NEXUS -lNeXus"*
  - *(MCSTAS_CFLAGS_OVERRIDE if using python tools)*

- *7. IDF in xml format must be generated using mcdisplay.pl*
  - *mcdisplay TOSCA_Mantid_2.instr —format=Mantid -n0*
  - *-> TOSCA_Mantid_2.instr.xml*

- *8. Simulation should generate NeXus output, i.e.*

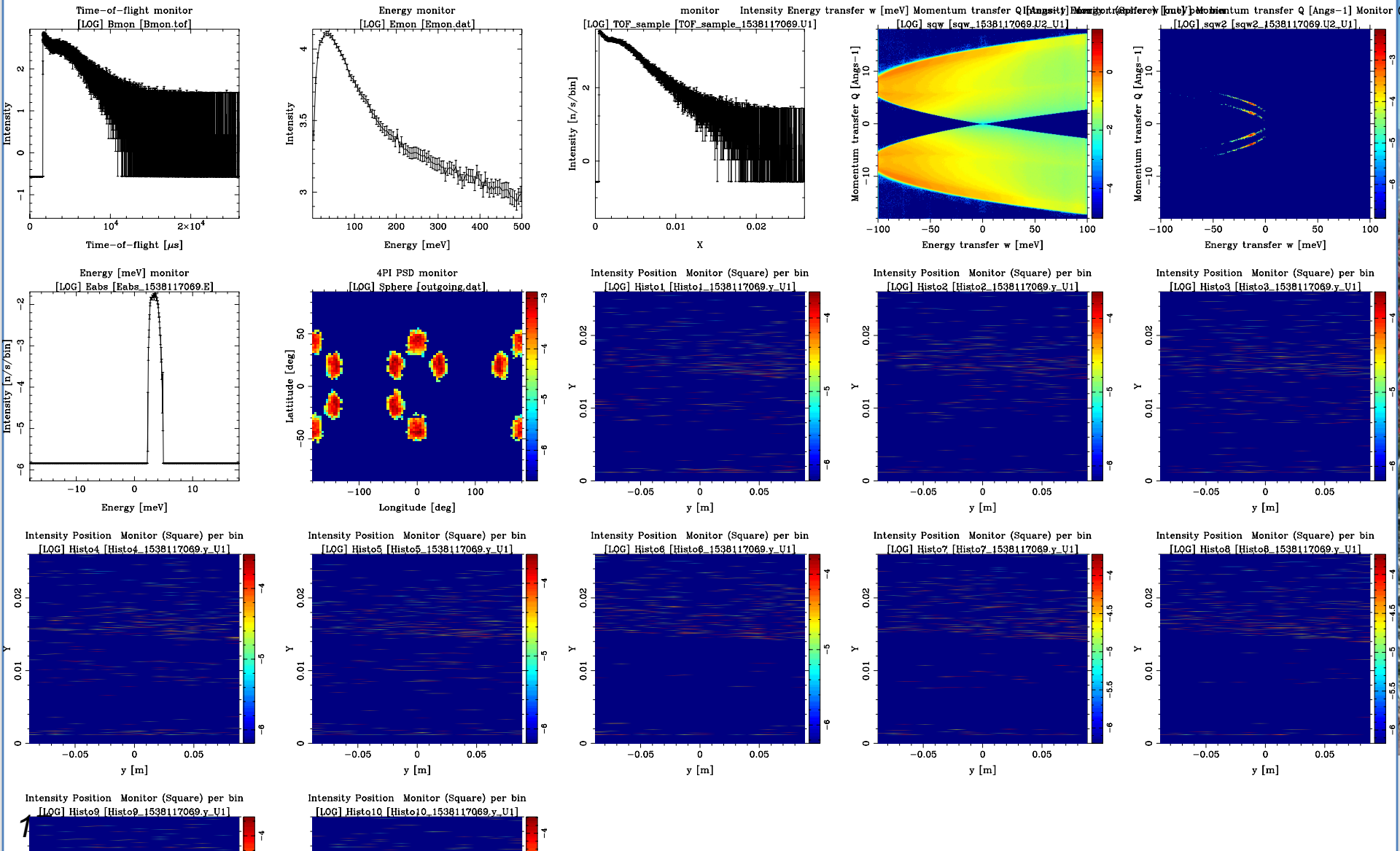
```
mcrun TOSCA_Mantid_2.instr inc=bz_inc_castep2.sqw eventmode=1 -n1e7 --format=NeXus
```

Energy range 0.01 - 500 meV

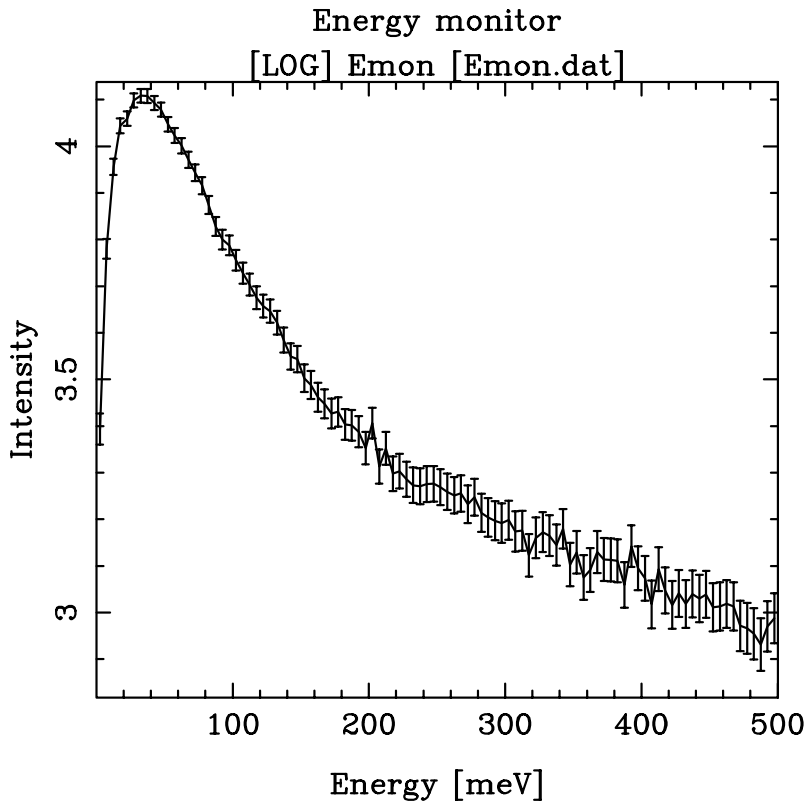
- *… demanding, required 4 hours using MPI on Quad-Core Intel i7 last night…*

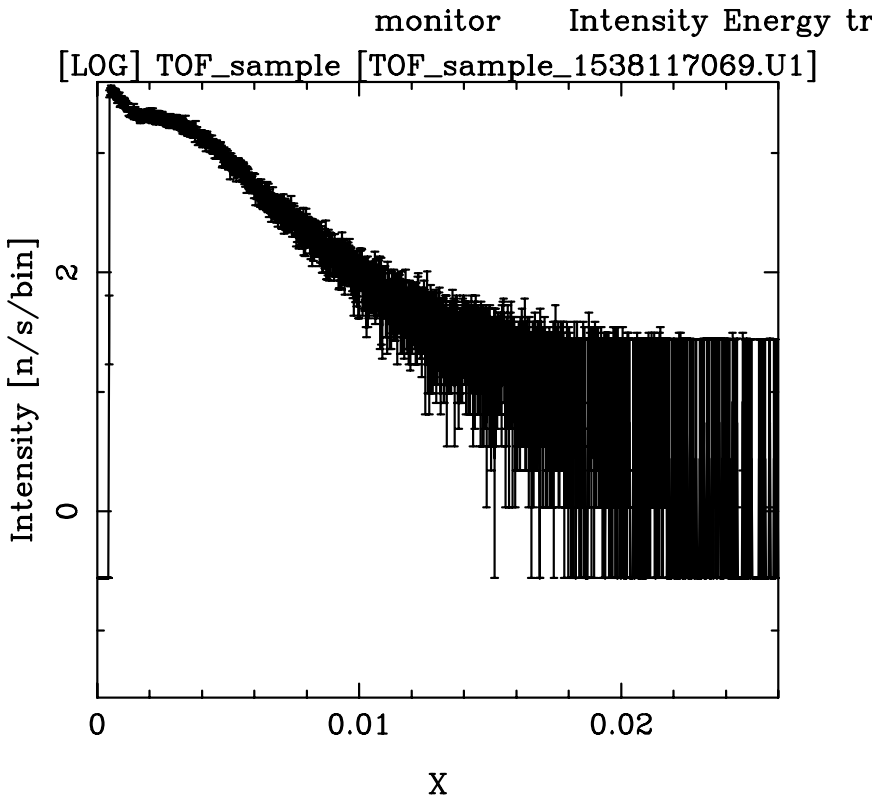
--ncount 1e6

McStas output outside Mantid



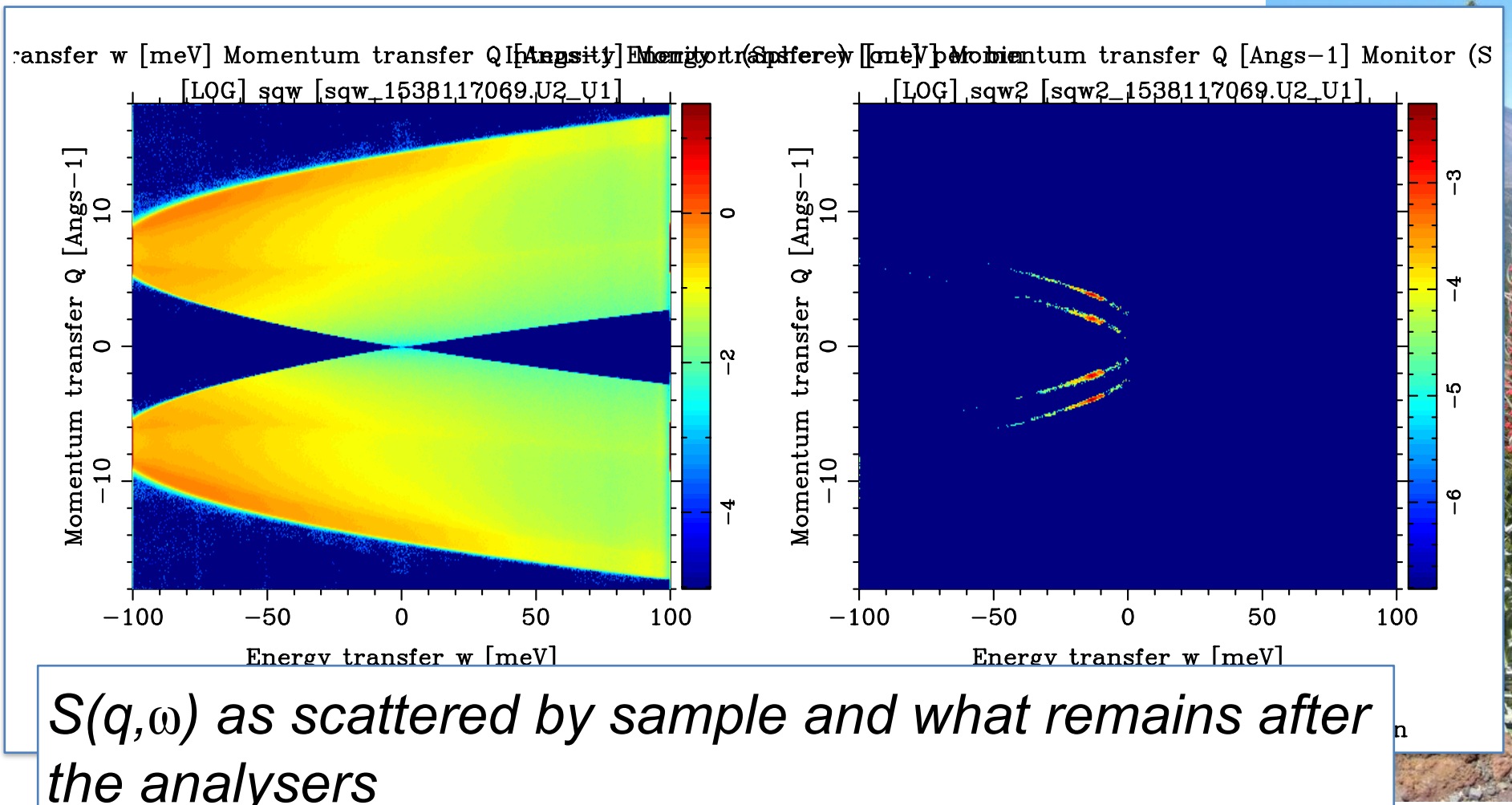
McStas output outside Mantid





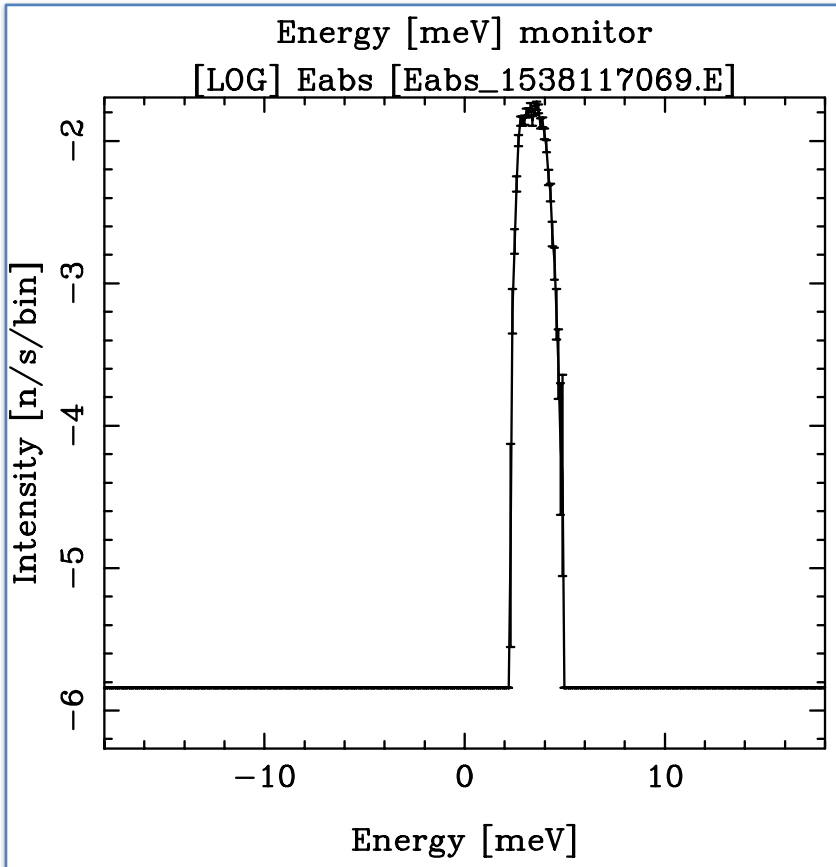
Spectrum and ToF at sample position…

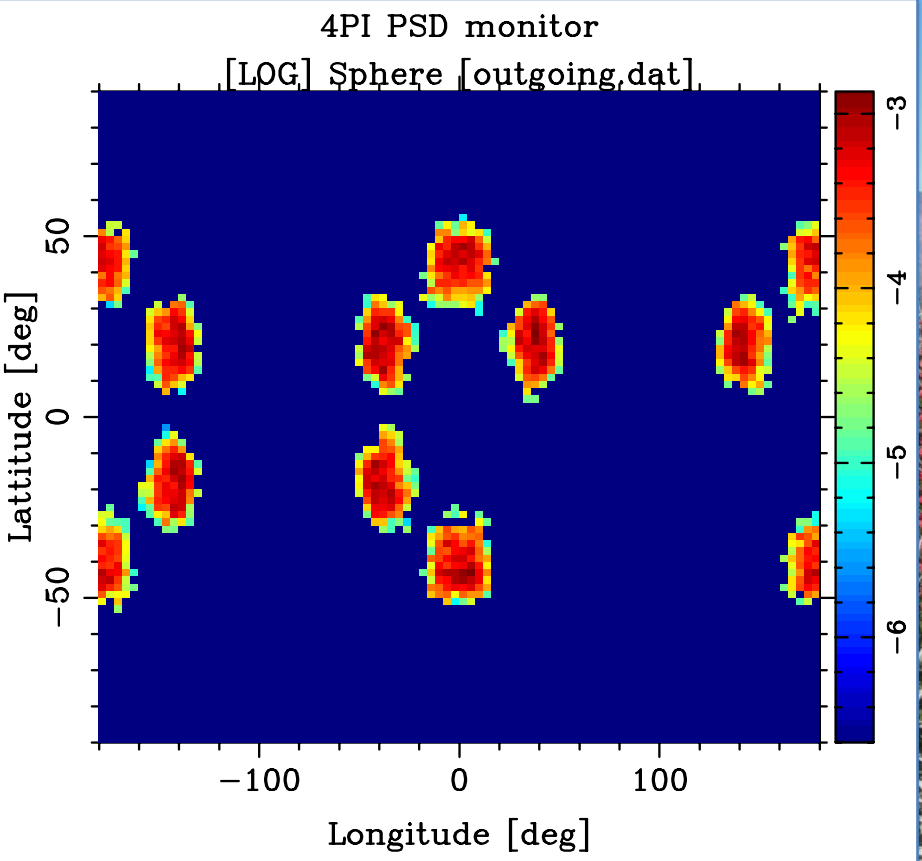
McStas output outside Mantid



S(q,ω) as scattered by sample and what remains after the analysers

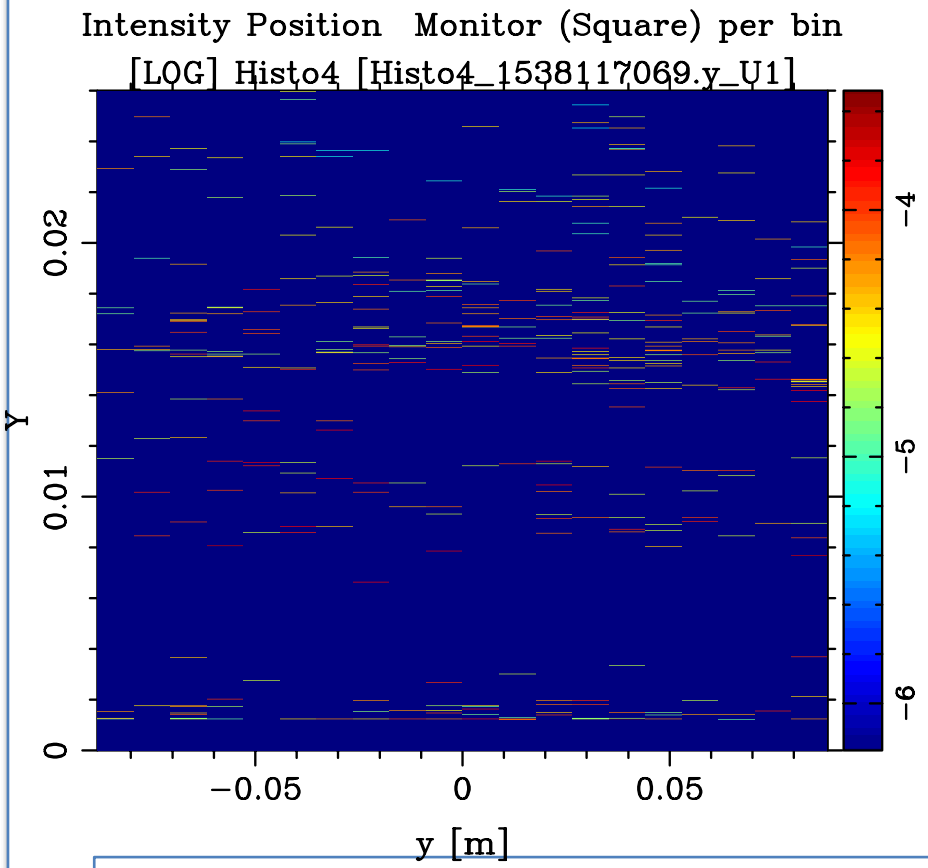
McStas output outside Mantid

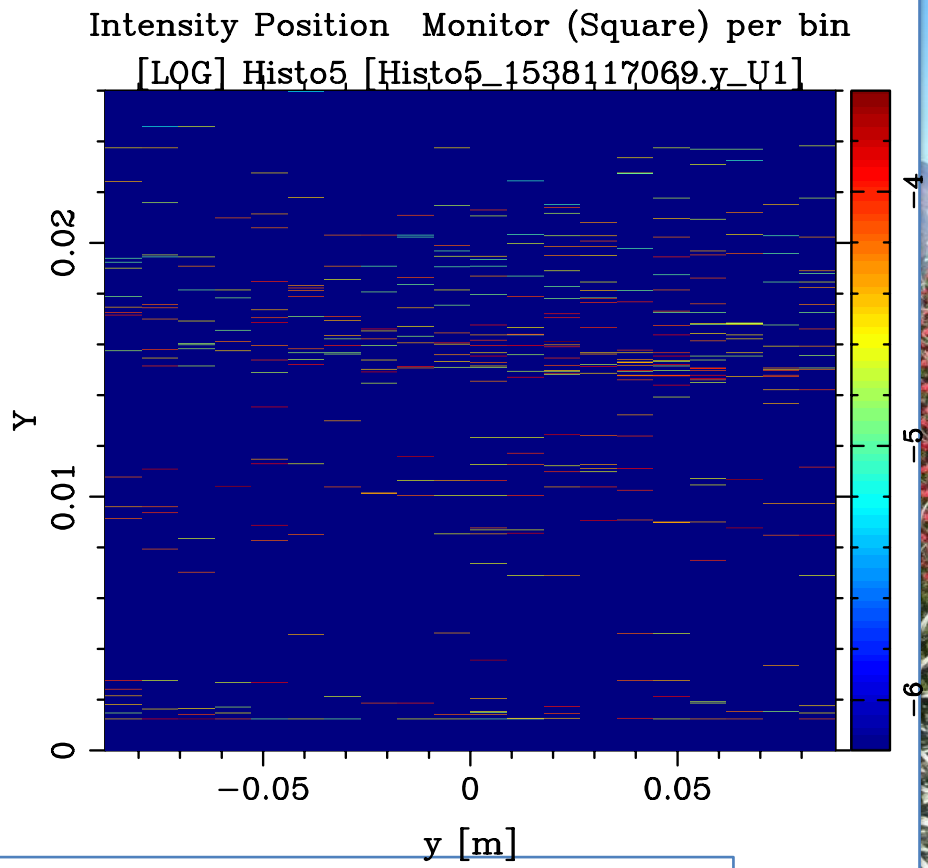




Absolute neutron energy and spatial location of beams on 4PI monitor…

McStas output outside Mantid





… result is relatively sparse in ToF on the individual panels…

DTU ess EUROPEAN SPALLATION SOURCE

The event data are then reduced in Mantid

- Steps:
  - ConvertUnits on event dataset, indirect geometry and Efixed of 1.85
  - Rebin dataset to achieve spectra
  - SumSpectra to get the final reduced dataset