EUROPEAN
SPALLATION
SOURCE

McStas - Mantid

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MCSTAS WORKSHOP

May 2021

McStas event-data for data-reduction

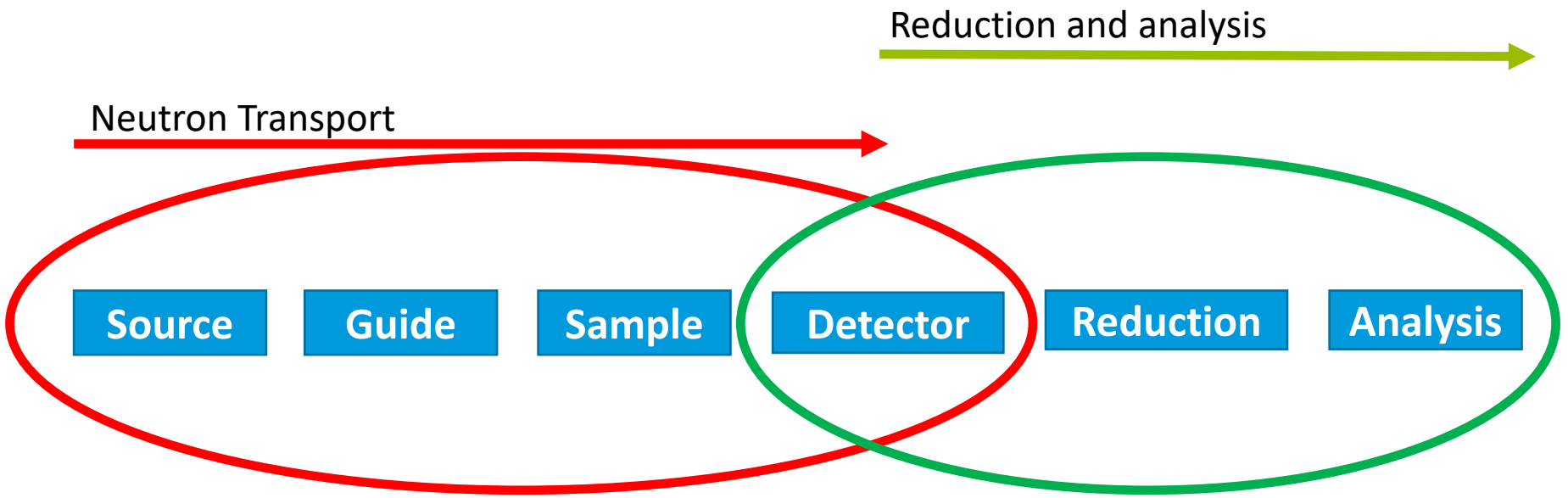
Data-reduction = { Mantid, Scipp }

MCSTAS WORKSHOP

May 2021

McStas-Mantid and the neutron pipeline

Focus: How to analyse McStas data

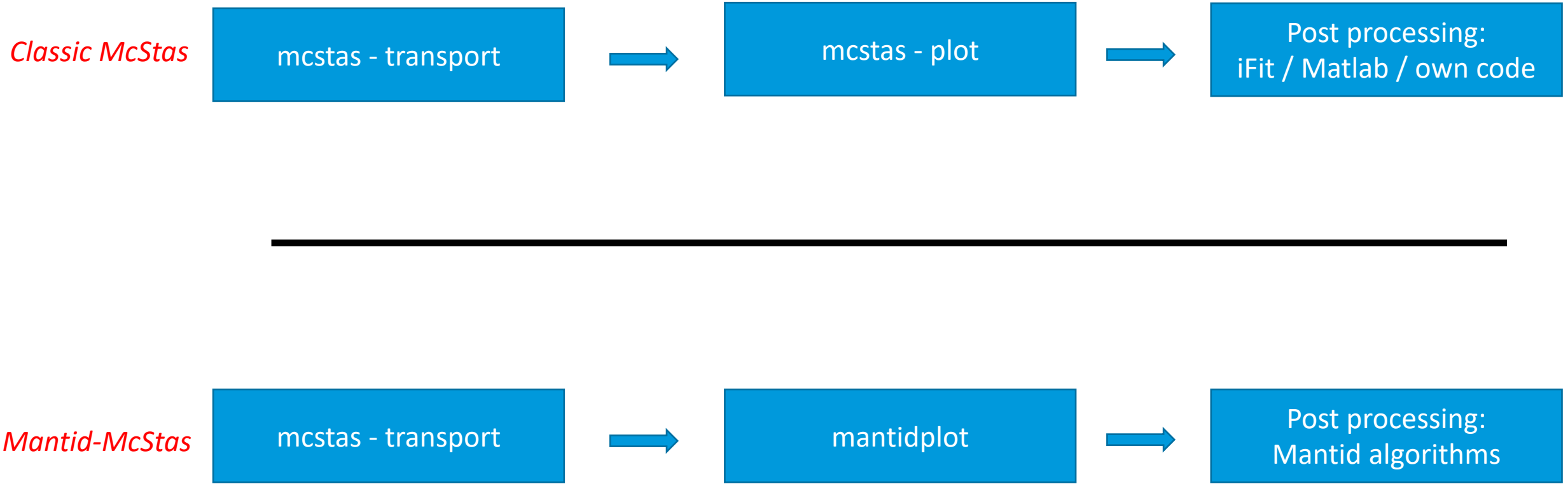


Typical McStas Neutron Transport

Mantid-McStas focus:

How to analyse McStas data

Comparison

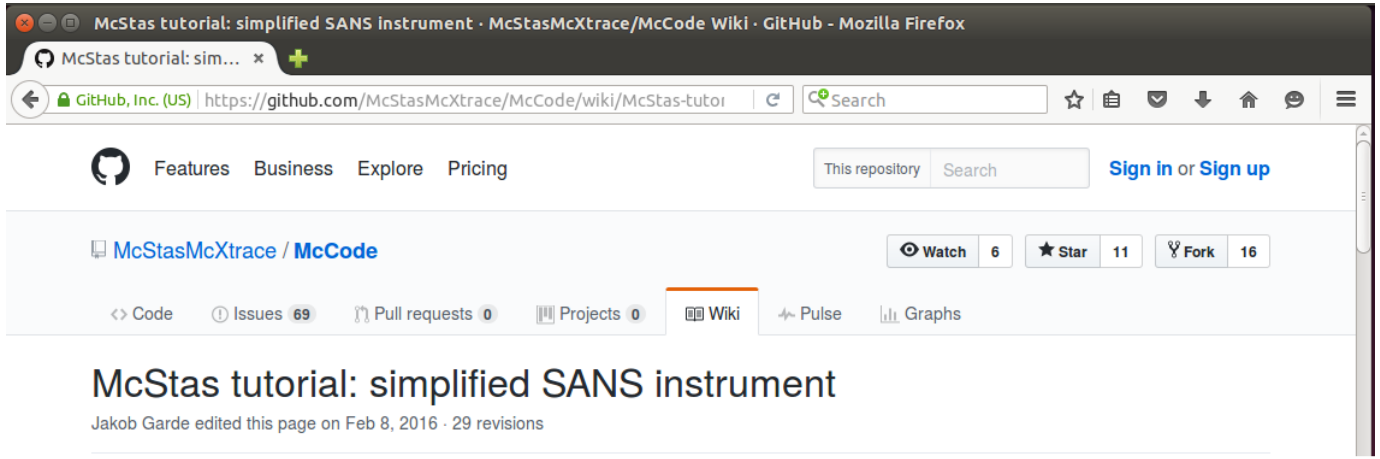

Classic McStas
mcstas - transport
mcstas - plot
Post processing:
iFit / Matlab / own code
Mantid-McStas
mcstas - transport
mantidplot
Post processing:
Mantid algorithms

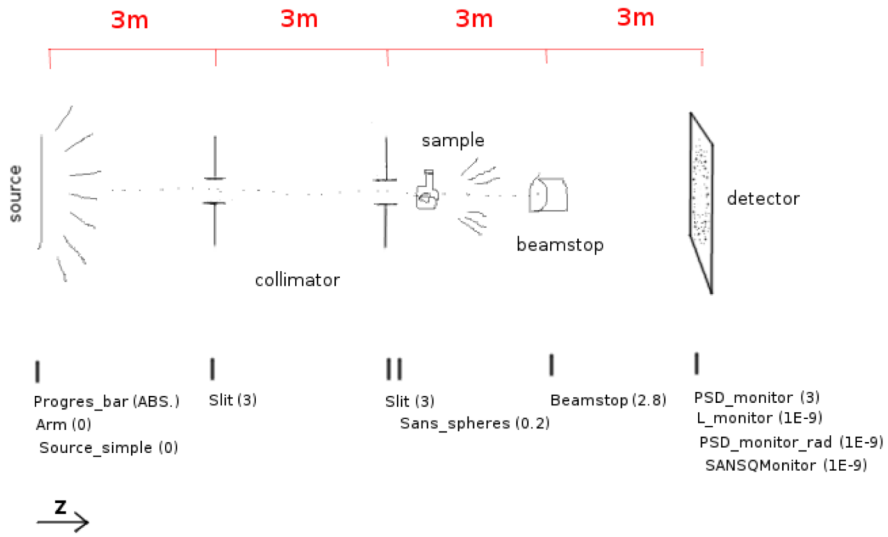
Motivation: new flexible dataflow

1. Combine the reduction framework and the neutron transport framework
2. Neutron transport, reduction and “analysis” in one go
3. View McStas data in Mantid (histogram data)
4. Import McStas event data to Mantid
5. Use already developed and tested algorithms in Mantid to process McStas event data (no need to reinvent methods)
6. Advanced use: Use McStas to quantify (perhaps remove) “spurries” signal on detector (can scatt. – multi. scatt)

Illustration: simplified SANS instrument

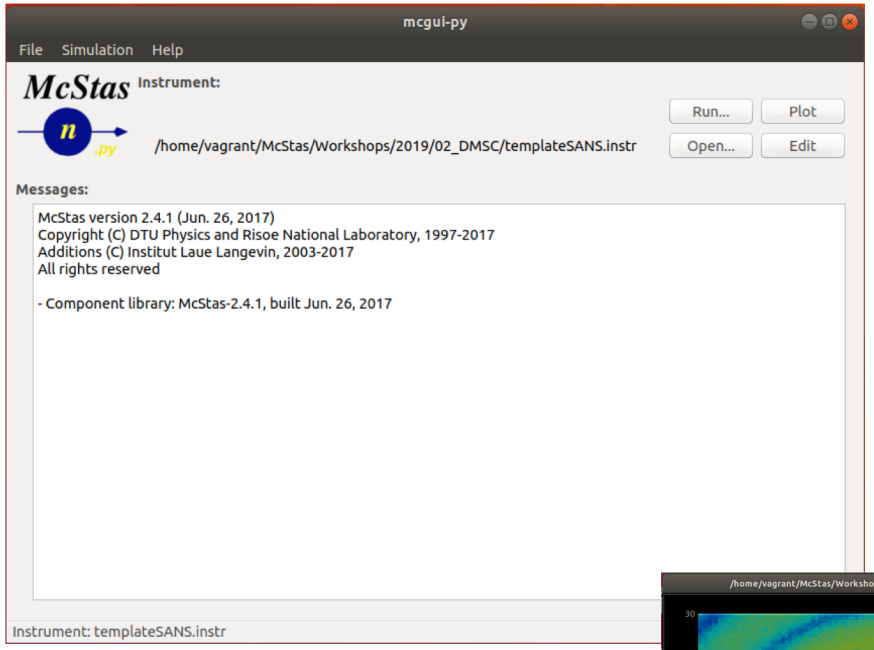
McStas wiki page on Github

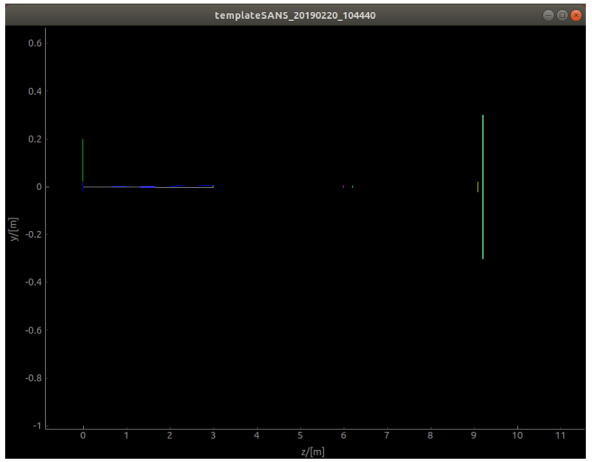


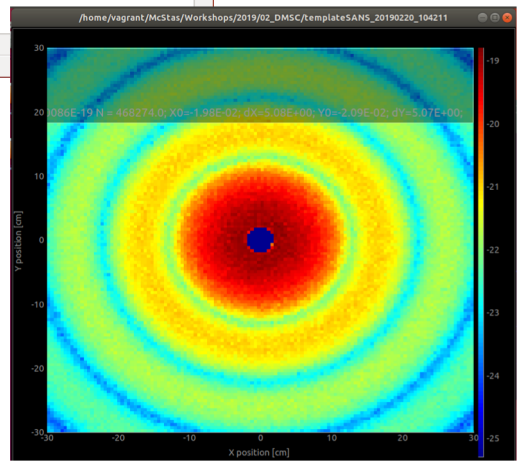


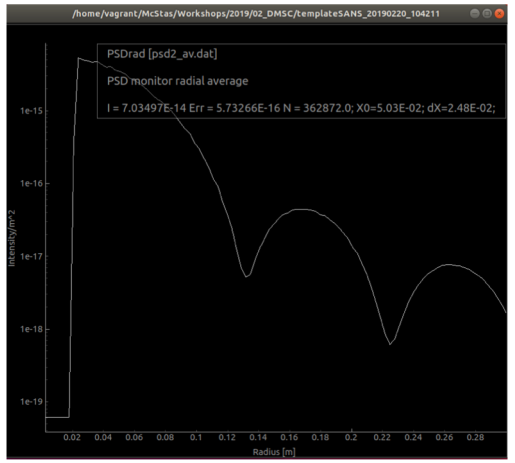
- SANS
- Small angle neutron scattering
- Can give structural information of nano sized particels

McStas GUI: templateSANS.instr







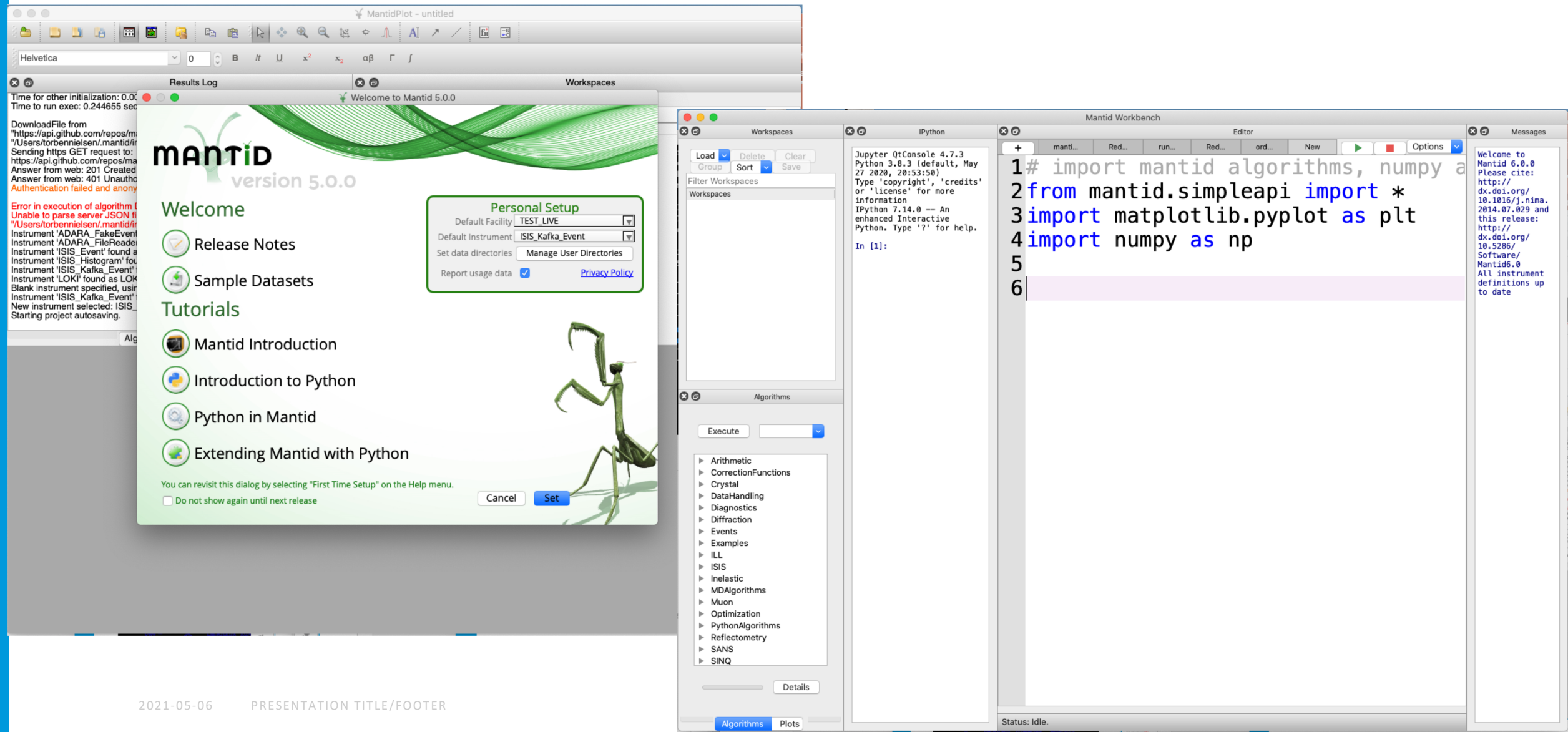


- SANS
- Nano spheres in thin solution

R=150,phi=0.1, d=1,a=0

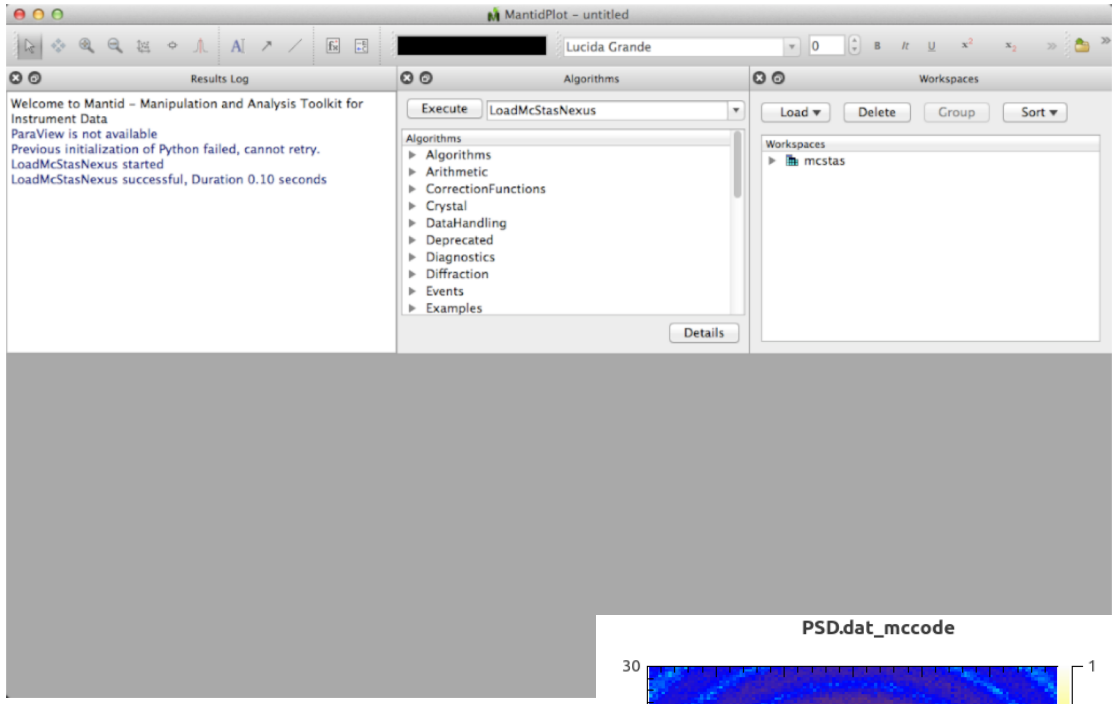
Mantid / MantidWorkBench

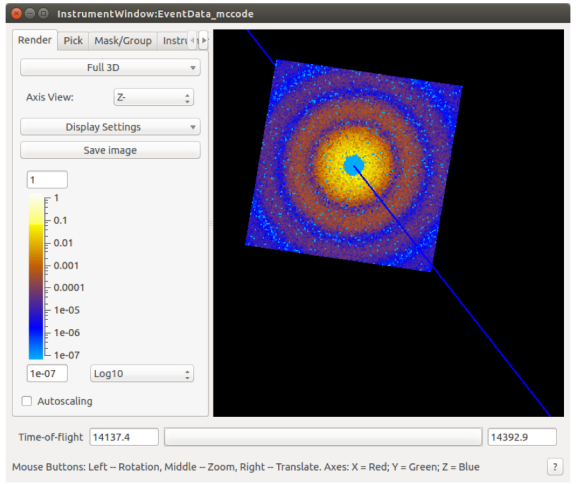
Desktop APP and python CLI: https://www.mantidproject.org

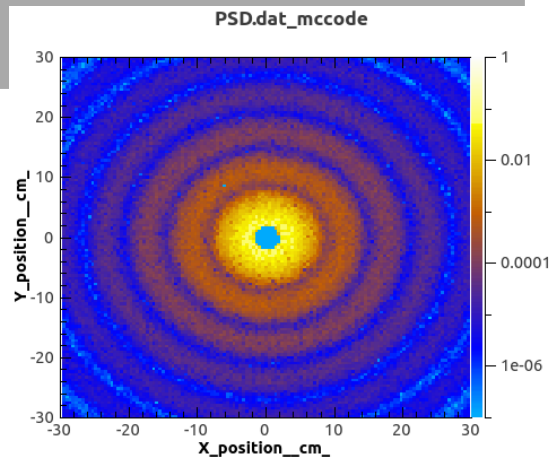


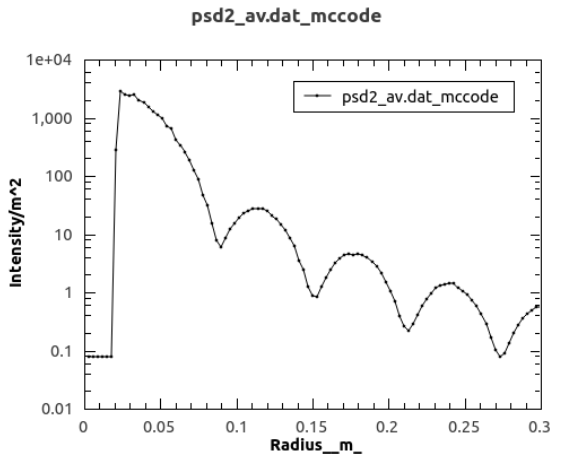
Mantid GUI: templateSANS.instr

Using Mantid 5.0:



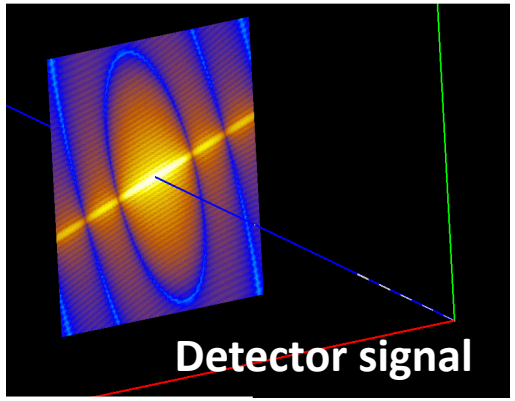


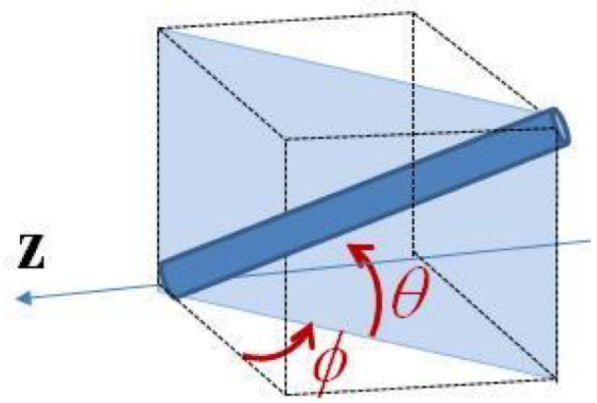




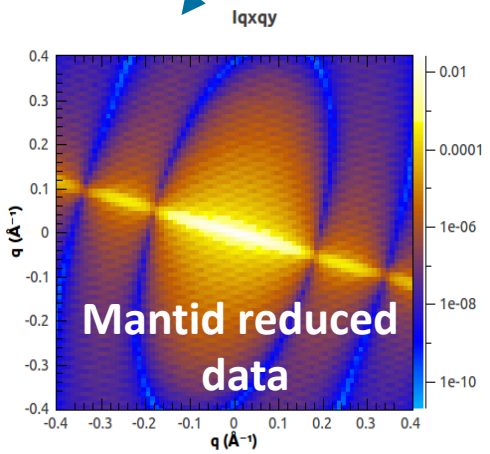
Example: Usage of Mantid algorithms

Let’s try to use a 2D scattering kernel. And use Mantid for data reduction

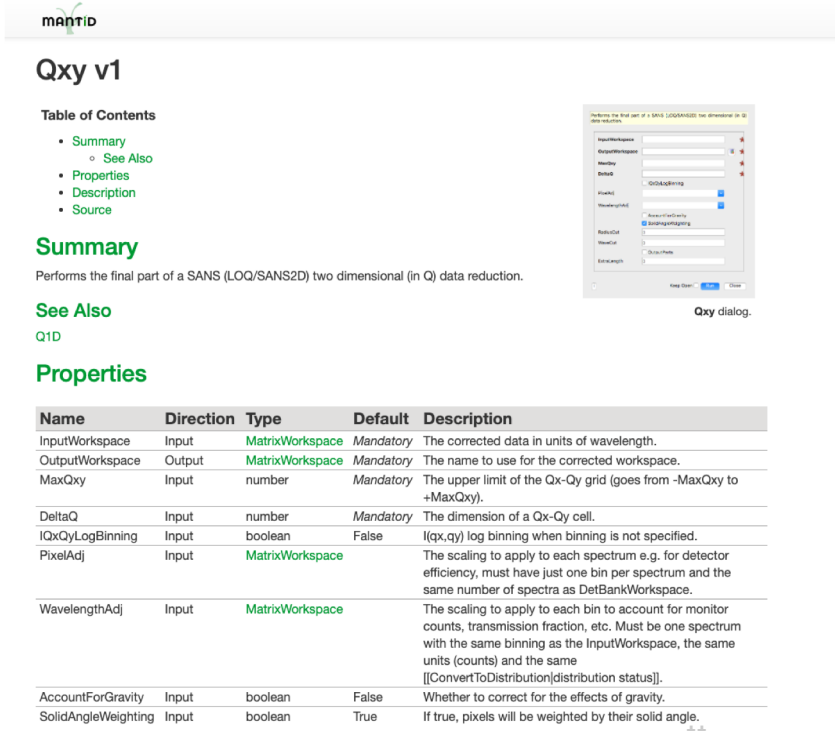




SasView



- SasView_model.comp
- 2D scattering kernel from SasView
- 2D reduction in Mantid: Qxy
- Can be send back to SasView for fitting



mantid

Qxy v1

Table of Contents

- Summary
  - See Also
- Properties
- Description
- Source

Qxy dialog.

Summary

Performs the final part of a SANS (LOQ/SANS2D) two dimensional (in Q) data reduction.

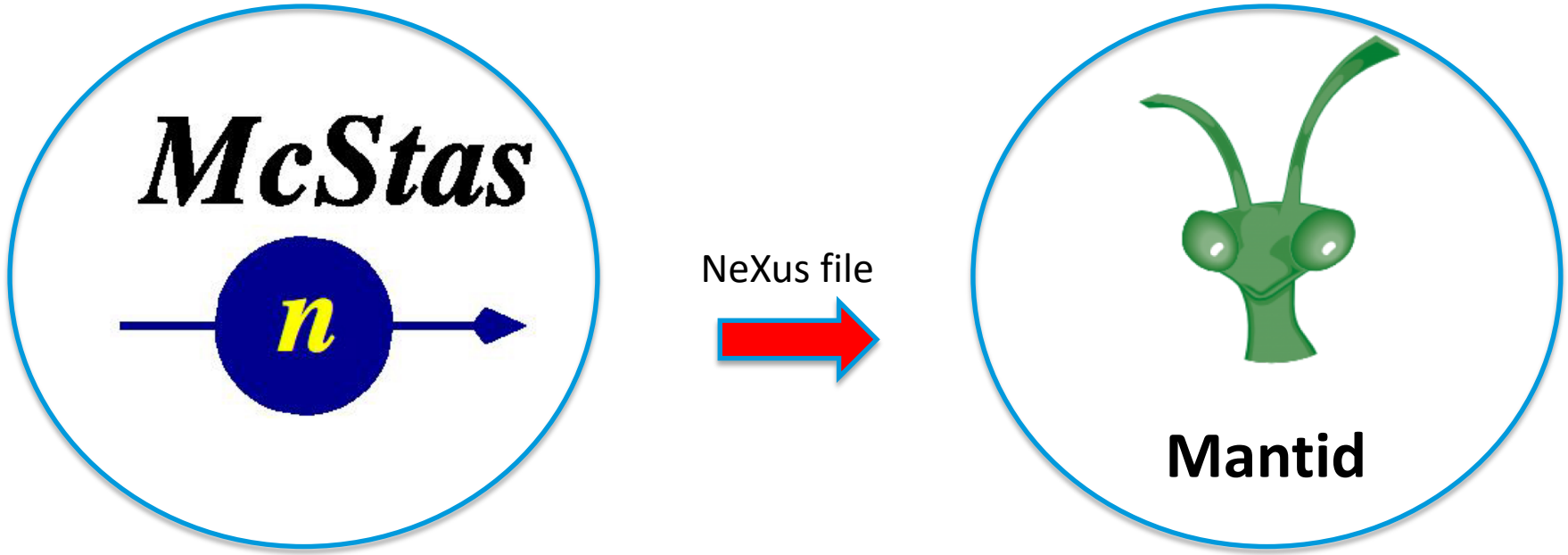
See Also

Q1D

Properties

Name	Direction	Type	Default	Description
InputWorkspace	Input	MatrixWorkspace	*Mandatory*	The corrected data in units of wavelength.
OutputWorkspace	Output	MatrixWorkspace	*Mandatory*	The name to use for the corrected workspace.
MaxQxy	Input	number	*Mandatory*	The upper limit of the Qx-Qy grid (goes from -MaxQxy to +MaxQxy).
DeltaQ	Input	number	*Mandatory*	The dimension of a Qx-Qy cell.
IQxQyLogBinning	Input	boolean	False	I(qx,qy) log binning when binning is not specified.
PixelAdj	Input	MatrixWorkspace		The scaling to apply to each spectrum e.g. for detector efficiency, must have just one bin per spectrum and the same number of spectra as DetBankWorkspace.
WavelengthAdj	Input	MatrixWorkspace		The scaling to apply to each bin to account for monitor counts, transmission fraction, etc. Must be one spectrum with the same binning as the InputWorkspace, the same units (counts) and the same [[ConvertToDistribution|distribution status]].
AccountForGravity	Input	boolean	False	Whether to correct for the effects of gravity.
SolidAngleWeighting	Input	boolean	True	If true, pixels will be weighted by their solid angle.

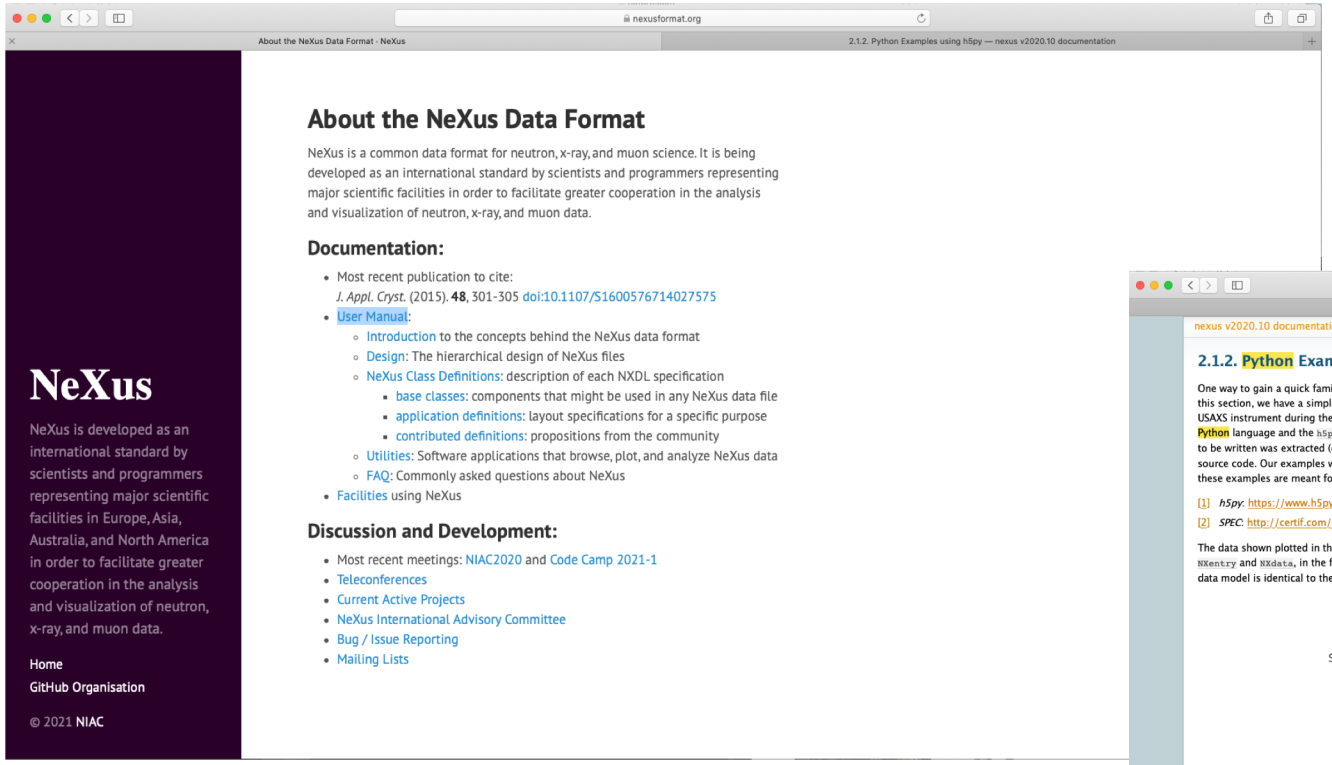
The NeXus file

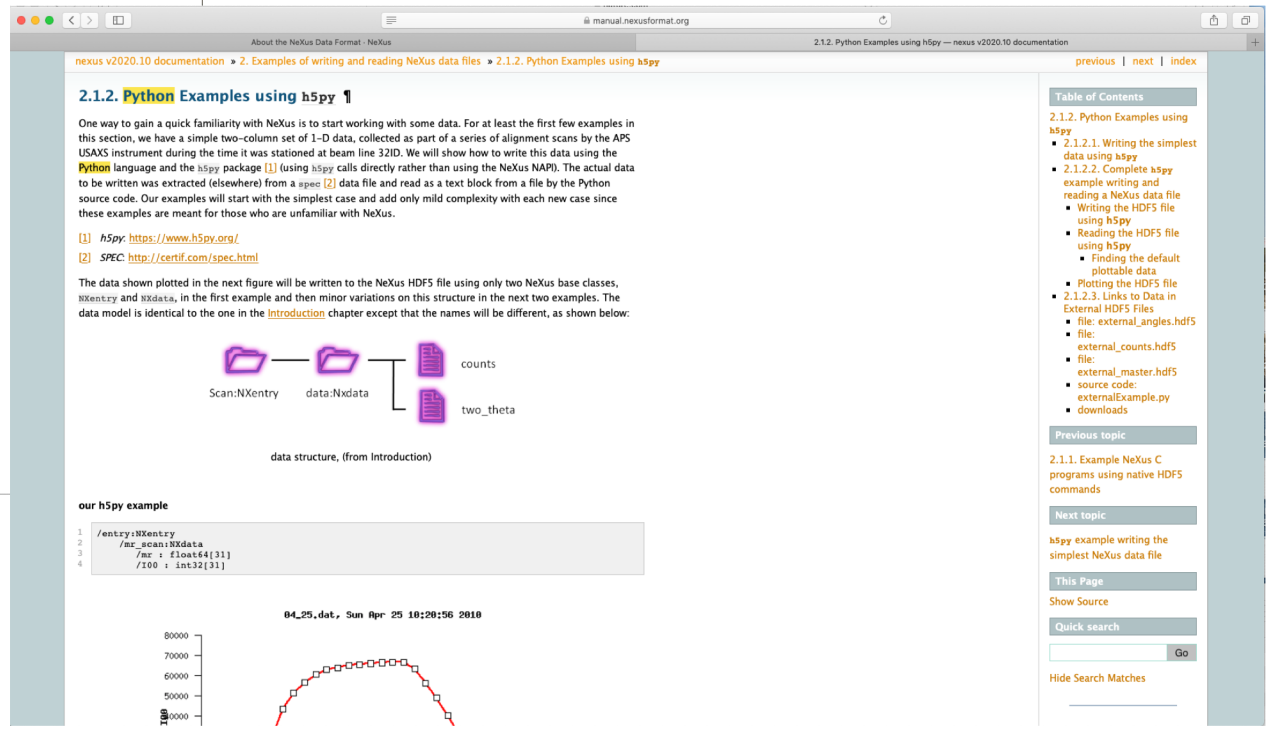


- The McStas Nexus file must contain:
- Event data, i.e. each neutron has a pixel id and a time stamp
- An IDF McStas monitor_nD gives pixle id & time for each event
- *mcdisplay can auto-generate an IDF*

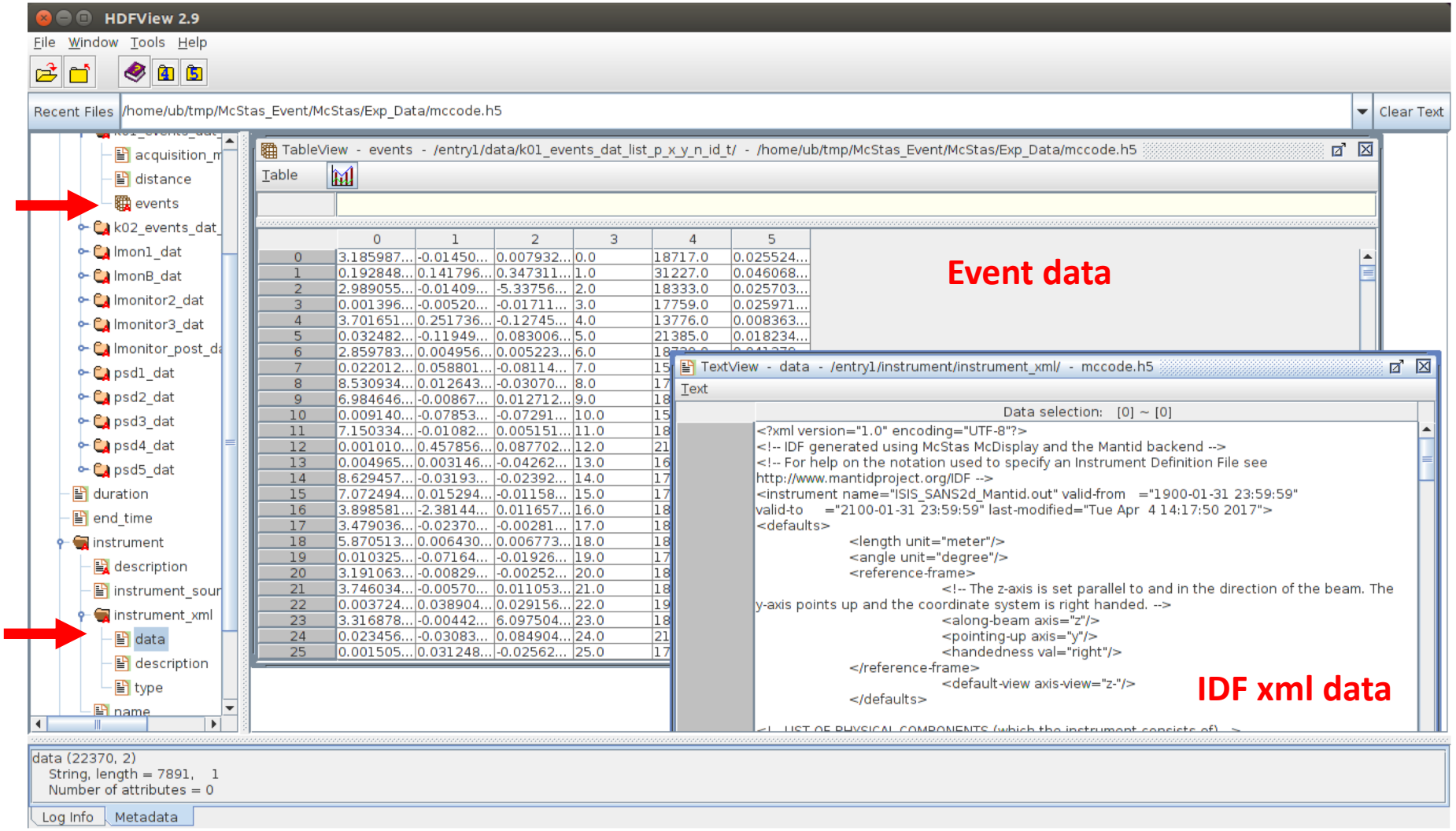
https://www.nexusformat.org

https://manual.nexusformat.org



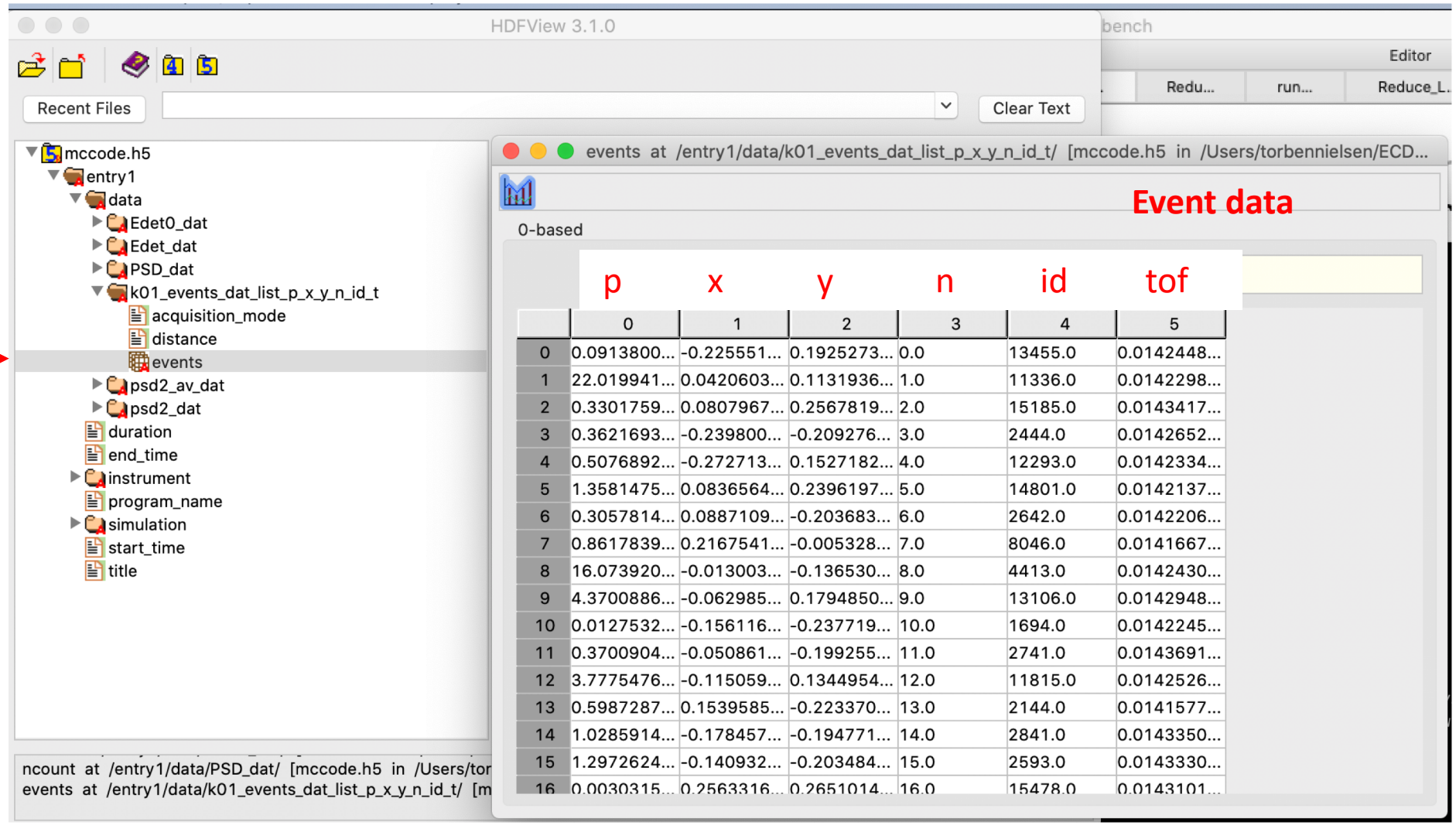


McStas NeXus file



McStas NeXus files (aka. mccode.h5)

Event data (templateSANS_Mantid.instr)



IDF xml data, TOF and pixel ID's

Mantid's IDF store geometry information use in TOF analysis

This implies parsing information about:

- where the neutron source is located,
- where the sample is located,
- where each individual detector pixel is located.

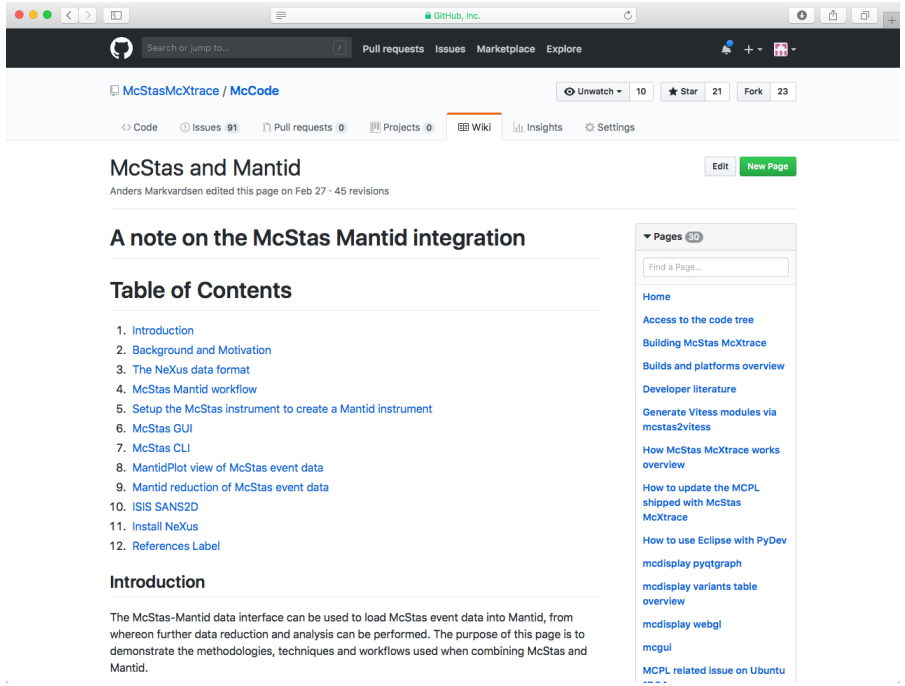
- In other words
- Establising k_i and k_f

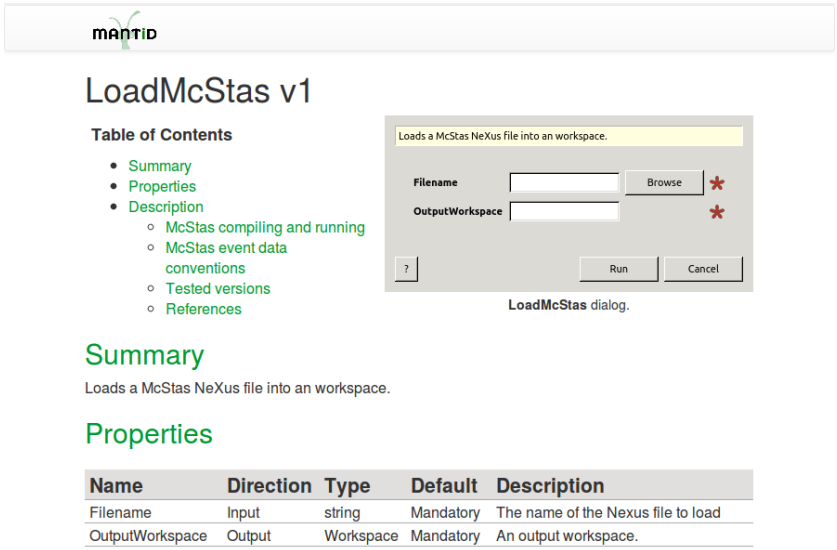
How to use: Online documentation

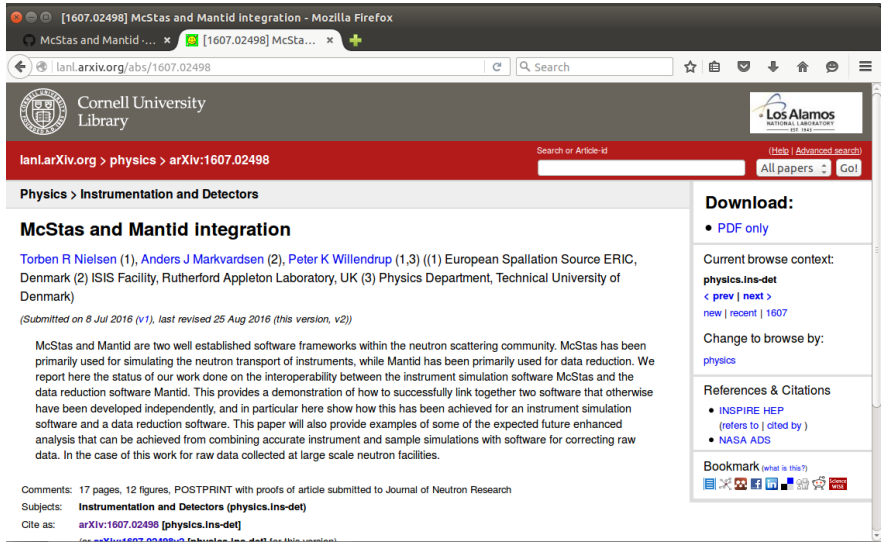
Github McStas wiki pages

Archive - lanl.arXiv.org

Build-in Mantid







McStas event KEYWORDS

1. McStas instrument file name and the McStas defined name of the instrument must be the same:

   E.g. **templateSANS_Mantid.instr** and "**DEFINE INSTRUMENT templateSANS_Mantid**(….)"

2. In the McStas instrument file the source must be named "**sourceMantid**"

   E.g. "**COMPONENT sourceMantid = Source_simple**(….)"

3. In the McStas instrument file the sample must be named "**sampleMantid**"

   E.g. "**COMPONENT sampleMantid = Sans_spheres**(….)"

4. In the McStas instrument file the event monitors must be named "**nD_Mantid_#**"

   E.g. "**COMPONENT nD_Mantid_1 = Monitor_nD**(….)"

templateSANS.inst vs templateSANS_Mantid.inst

templateSANS.instr — UNREGISTERED

templateSANS.instr | templateSANS_Mantid.instr

```
1  DEFINE INSTRUMENT templateSANS(lambda=6, dlambda=0.05, r=100, PHI=1e-
   3, Delta_Rho=0.6, sigma_abs=0.5)
2
3  TRACE
4
5  COMPONENT a1 = Progress_bar()
6    AT (0,0,0) ABSOLUTE
7
8  COMPONENT arm = Arm()
9    AT (0, 0, 0) ABSOLUTE
10
11 COMPONENT source = Source_simple(
12       radius = 0.02, dist = 3, focus_xw = 0.01, focus_yh = 0.01,
13       lambda0 = lambda, dlambda = dlambda, flux = 1e16)
14   AT (0, 0, 0) RELATIVE arm
15
16 COMPONENT coll1 = Slit(
17       radius = 0.005)
18   AT (0, 0, 3) RELATIVE arm
19
20 COMPONENT coll2 = Slit(
21       radius = 0.005)
22   AT (0, 0, 6) RELATIVE arm
23
24
25
26
27
28
29
30 SPLIT COMPONENT sample = Sans_spheres(
31   R=r, Phi=PHI, Delta_rho=Delta_Rho, sigma_abs=sigma_abs,
32   xwidth=0.01, yheight=0.01, zdepth=0.005, focus_xw=0.6, focus_yh=0.
     6, target_index=2)
33    AT (0,0,0.2) RELATIVE coll2
34
35 COMPONENT STOP = Beamstop(
36       radius = 0.02)
37   AT (0, 0, 2.9) RELATIVE sample
```

Line 1, Column 1 — Spaces: 2 — Plain Text

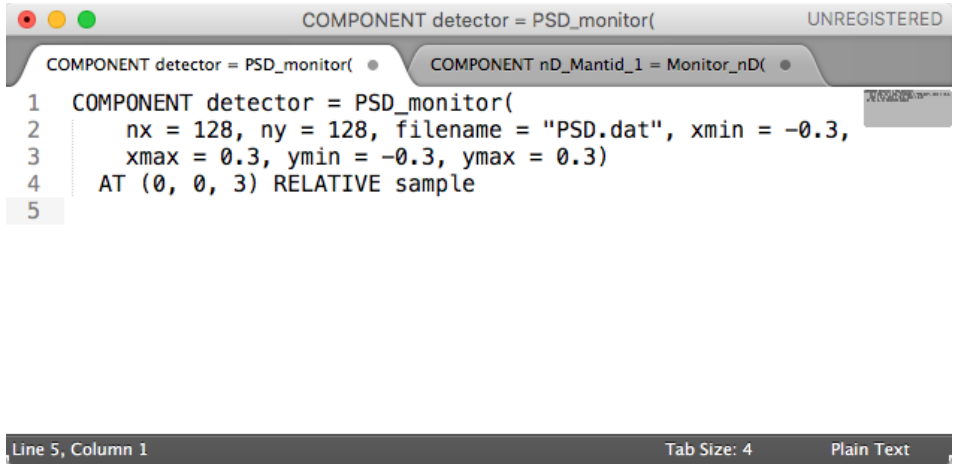
templateSANS_Mantid.instr — UNREGISTERED

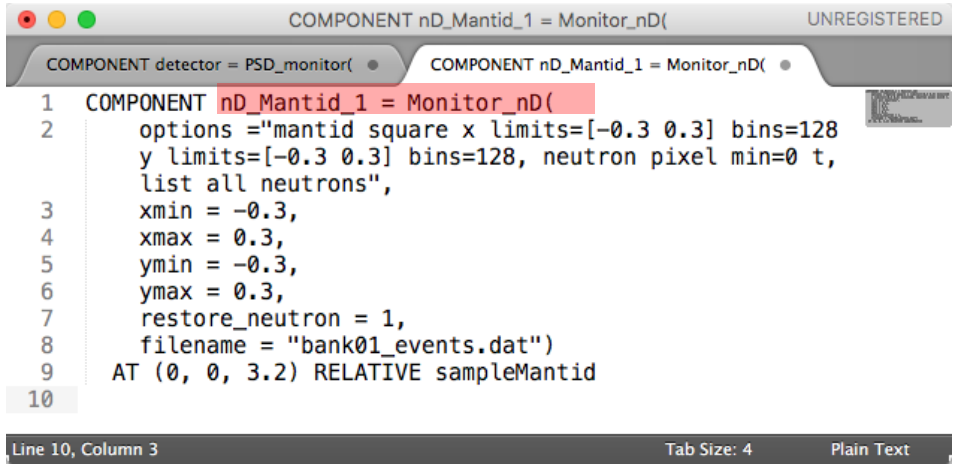
templateSANS.instr | templateSANS_Mantid.instr

```
1  DEFINE INSTRUMENT templateSANS_Mantid(lambda=6, dlambda=0.05, r=150,
   PHI=1e-3, Delta_Rho=0.6, sigma_abs=0.0)
2
3  TRACE
4
5  COMPONENT a1 = Progress_bar()
6    AT (0,0,0) ABSOLUTE
7
8  COMPONENT arm = Arm()
9    AT (0, 0, 0) ABSOLUTE
10
11 COMPONENT sourceMantid = Source_simple(
12       radius = 0.02, dist = 3, focus_xw = 0.01, focus_yh = 0.01,
13       lambda0 = lambda, dlambda = dlambda, flux = 1e16)
14   AT (0, 0, 0) RELATIVE arm
15
16 COMPONENT coll1 = Slit(
17       radius = 0.005)
18   AT (0, 0, 3) RELATIVE arm
19
20 COMPONENT coll2 = Slit(
21       radius = 0.005)
22   AT (0, 0, 6) RELATIVE arm
23
24 COMPONENT LdetectorPRE = L_monitor(
25       nL = 1000, filename = "Edet0.dat", xmin = -0.3,
26       xmax = 0.3, ymin = -0.3, ymax = 0.3, Lmin = 5.5,
27       Lmax = 6.5)
28 AT (0,0,0.05) RELATIVE coll2
29
30 SPLIT COMPONENT sampleMantid = Sans_spheres(
31   R=r, Phi=PHI, Delta_rho=Delta_Rho, sigma_abs=sigma_abs,
32   xwidth=0.01, yheight=0.01, zdepth=0.005)
33    AT (0,0,0.2) RELATIVE coll2
34 EXTEND %{
35           if (!SCATTERED) ABSORB;
36 %}
```

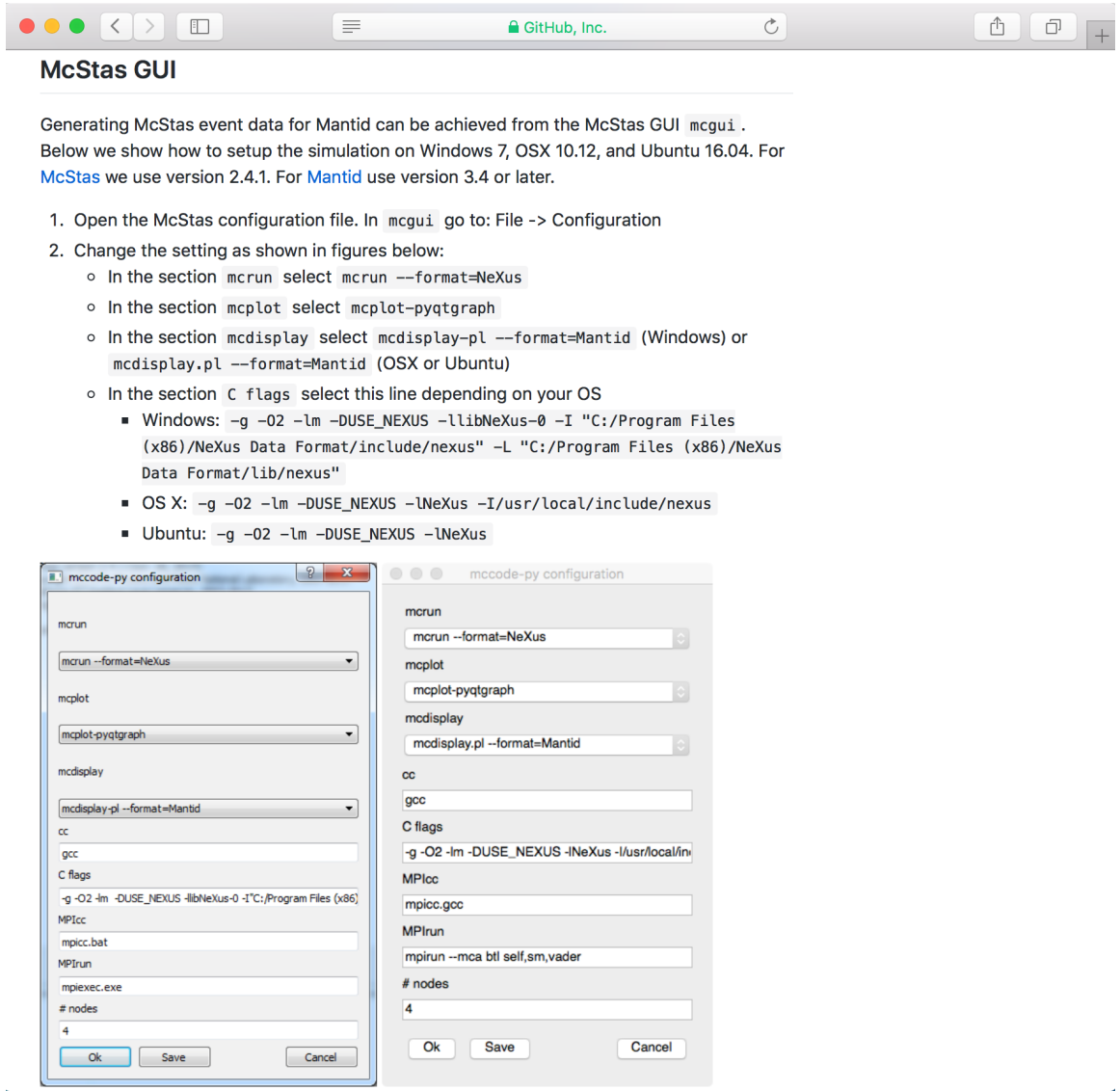
Line 1, Column 1 — Spaces: 2 — Plain Text

templateSANS.inst vs templateSANS_Mantid.inst



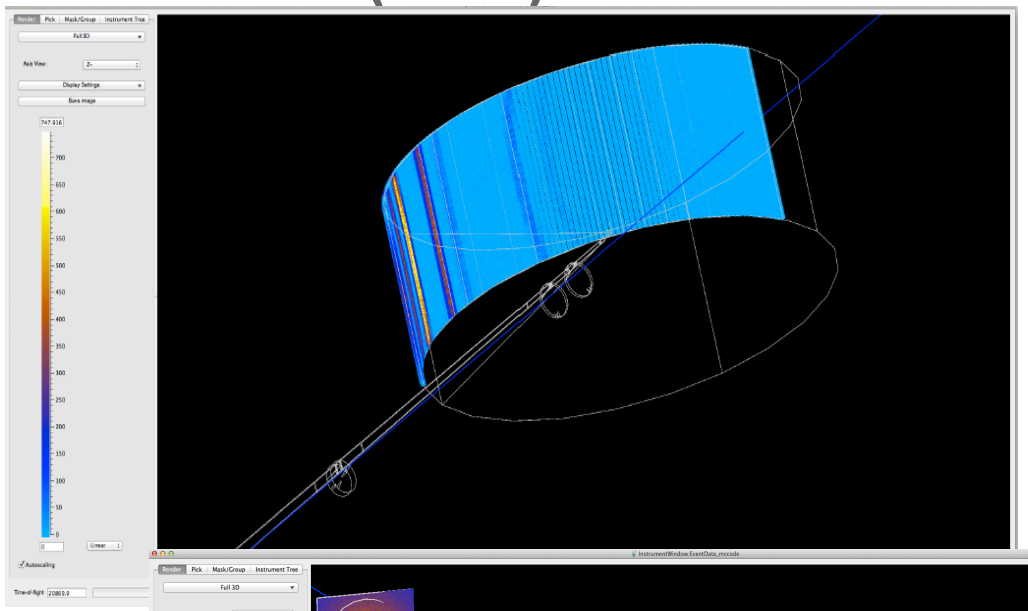


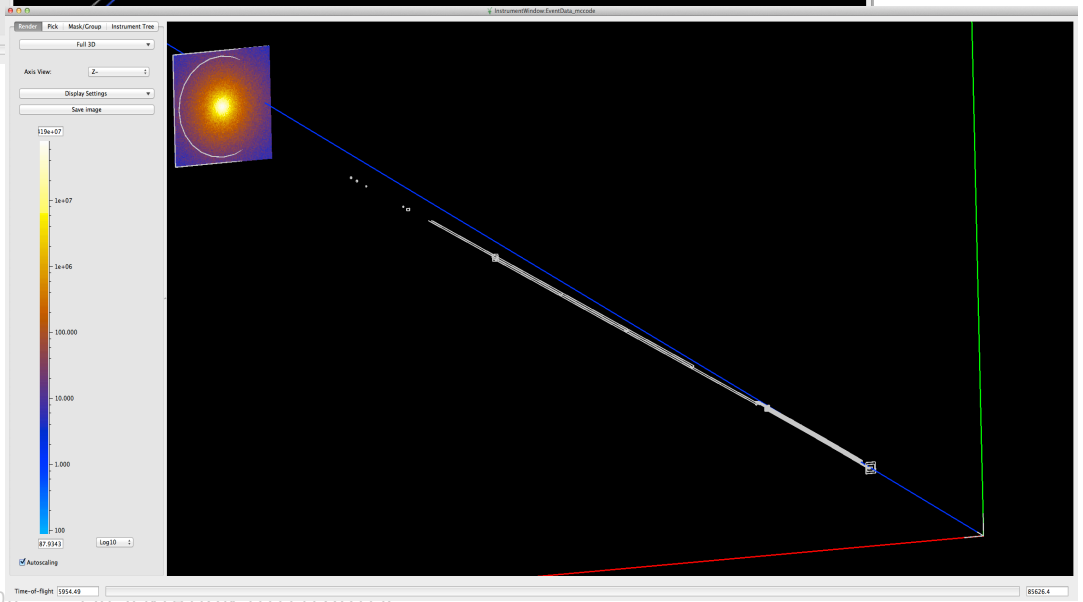
How to run the simulation

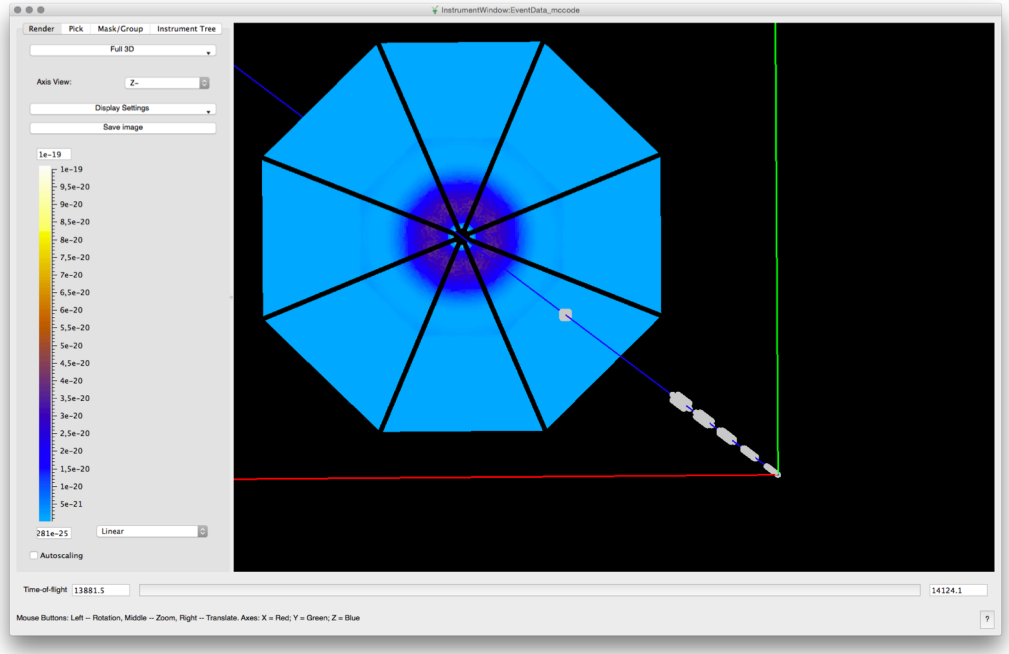


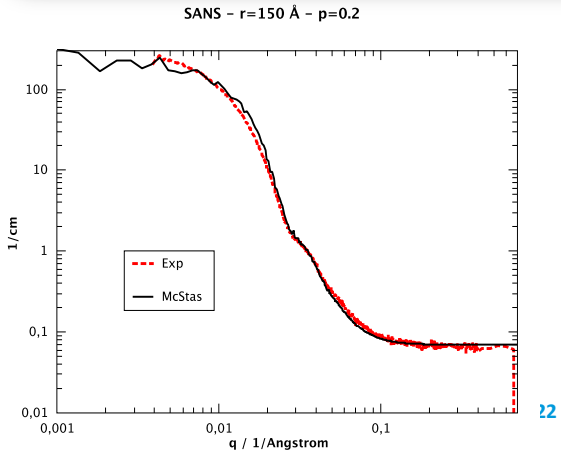
Wiki page on GitHub

Examples of detectors: IN5 (ILL), LoKI (ESS), SANS2D (ISIS)

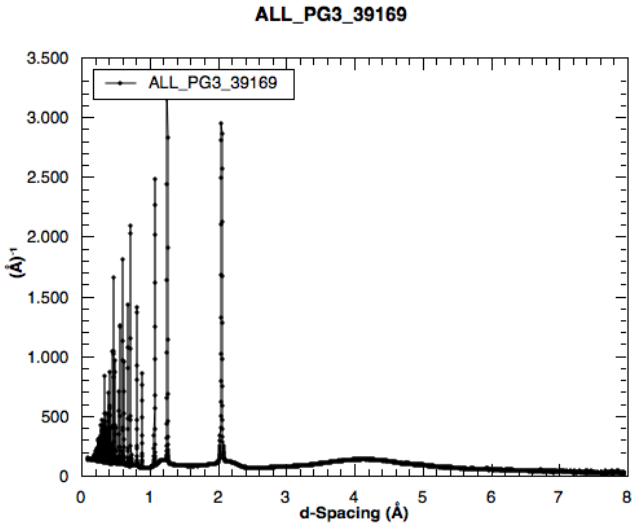


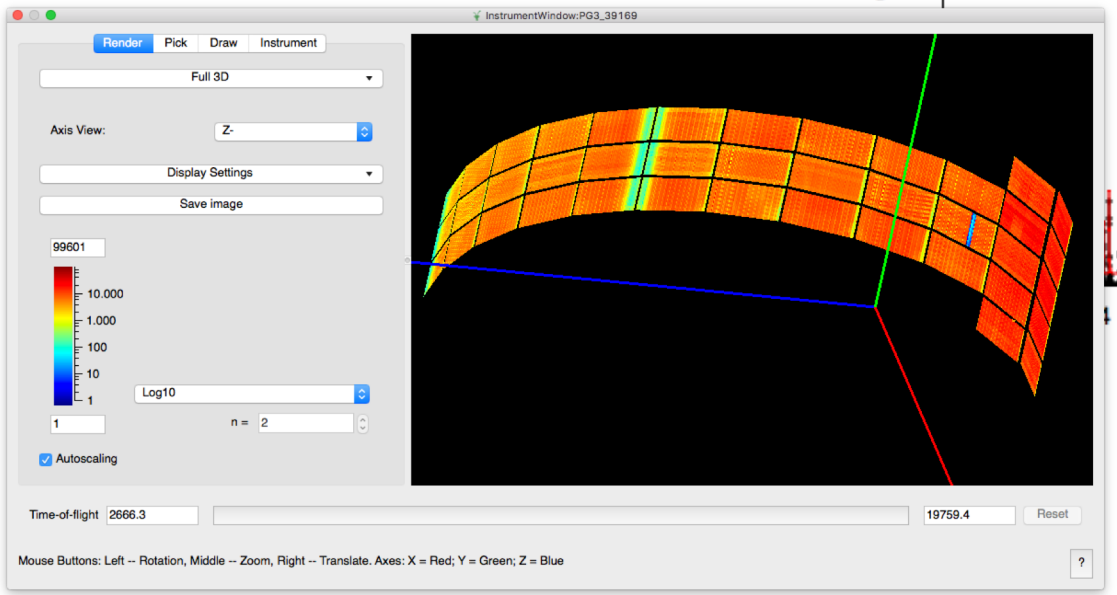


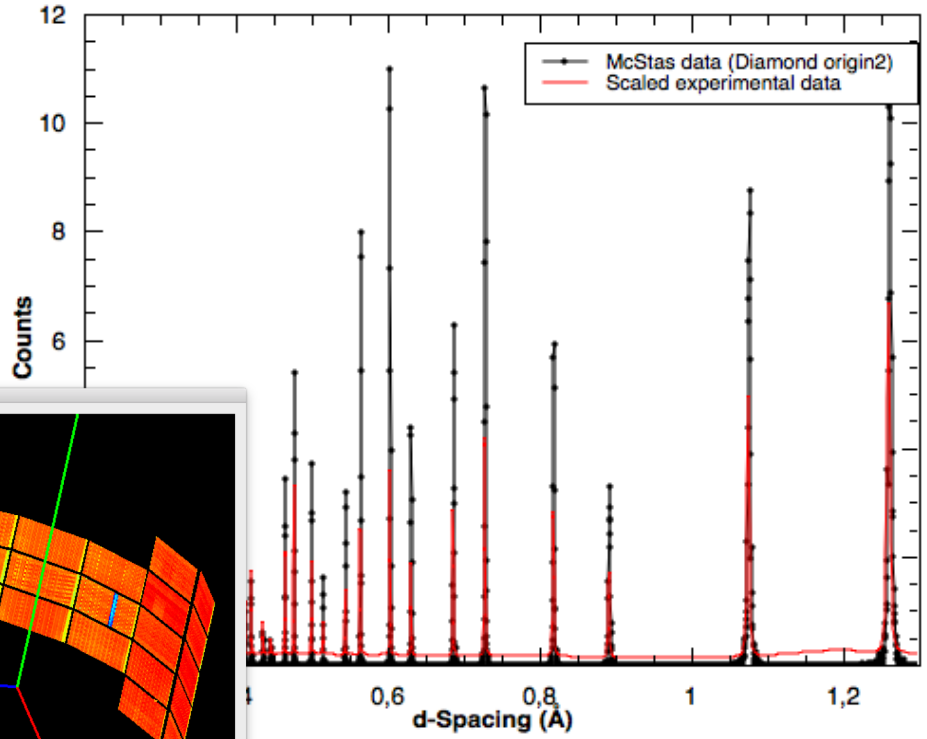




McStas and experimental data: POWGEN

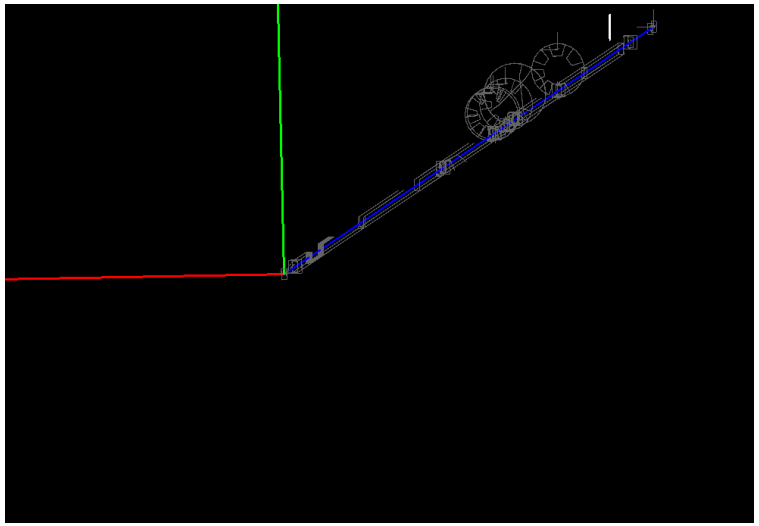


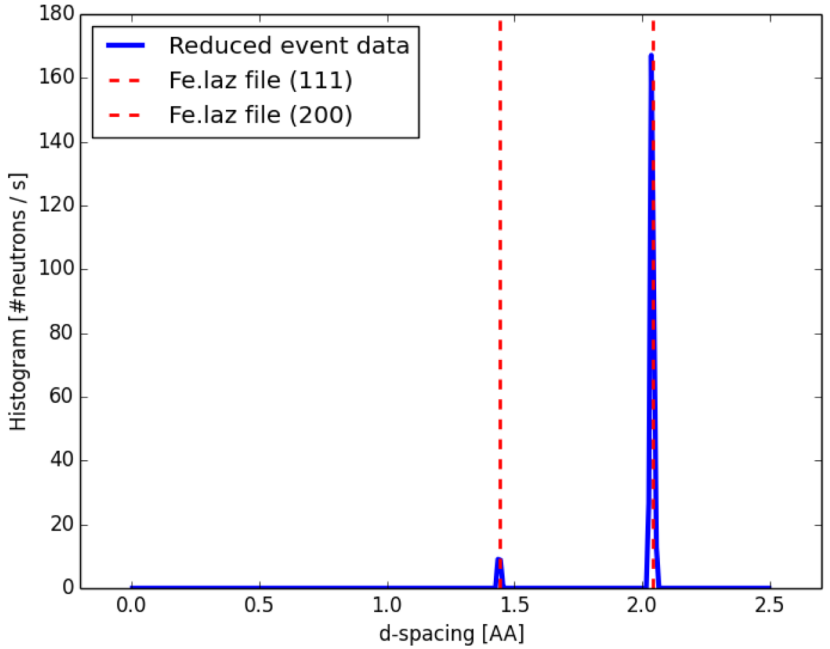




By CelineD @ ESS + SNS collaboration

Example – V20 – Powder diffraction Fe





Summary

1. Easier to post-process (event) data than making a completely new McStas simulation / component
   - E.g.:
   - Rebin as needed
   - Sum selective over detectors
   - Use already developed methods in Mantid

2. Mantid process McStas data as if they were equal to experimental twin data

Presentation headline

Sub-headline to strengthen the headline above

Presentation headline

Sub-headline to strengthen the headline above