

# McStas - Mantid

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- Motivation
- Illustration of the Mantid-McStas interface
  - A simple toy model: `templateSANS.instr`
- TOF, IDF, and NeXus files
- How to use – a little more explanation
- Demo time
- A few other examples

# Motivation: I - Highlevel



1. Mantid is well established software – long history
2. McStas is well established software – long history
3. Wanted to combine the reduction framework and the neutron transport framework
4. So users can do transport, reduction and “analysis” in one go

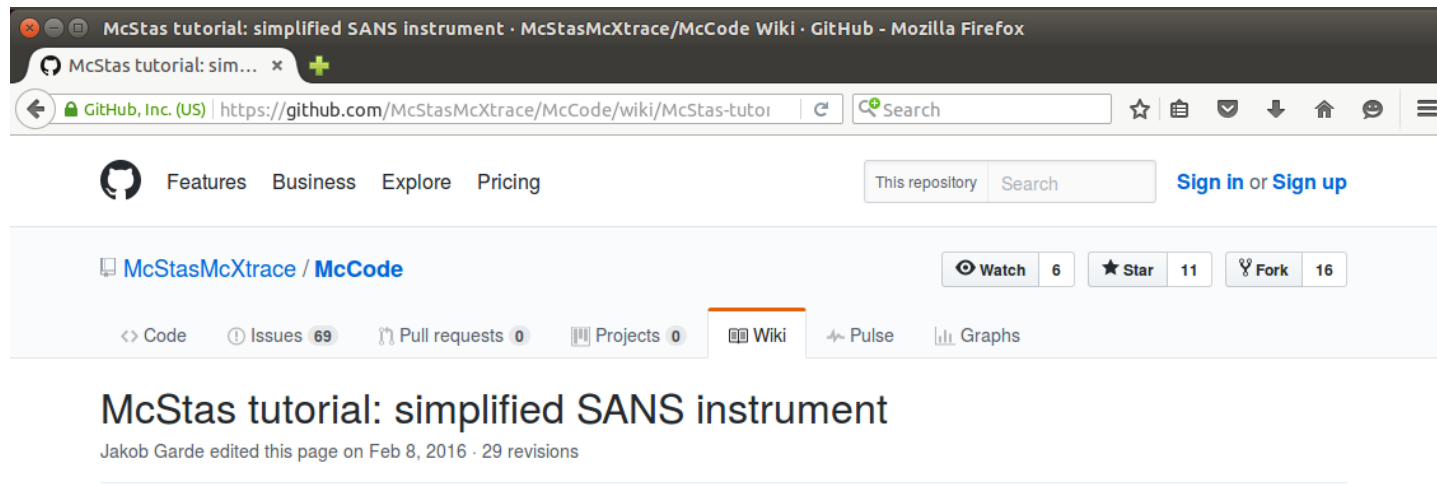
## Motivation: II - Benefits for users

1. View McStas data in Mantid (simple – but nice to have)
2. Import McStas event data to Mantid
3. Use already developed and tested algorithms in Mantid to process McStas event data (no need to reinvent stuff!!!)
4. Advanced use: Use McStas to quantify (perhaps remove) “spurries” signal on detector (can scatt. – multi. scatt )

# Motivation: II - Benefits for users

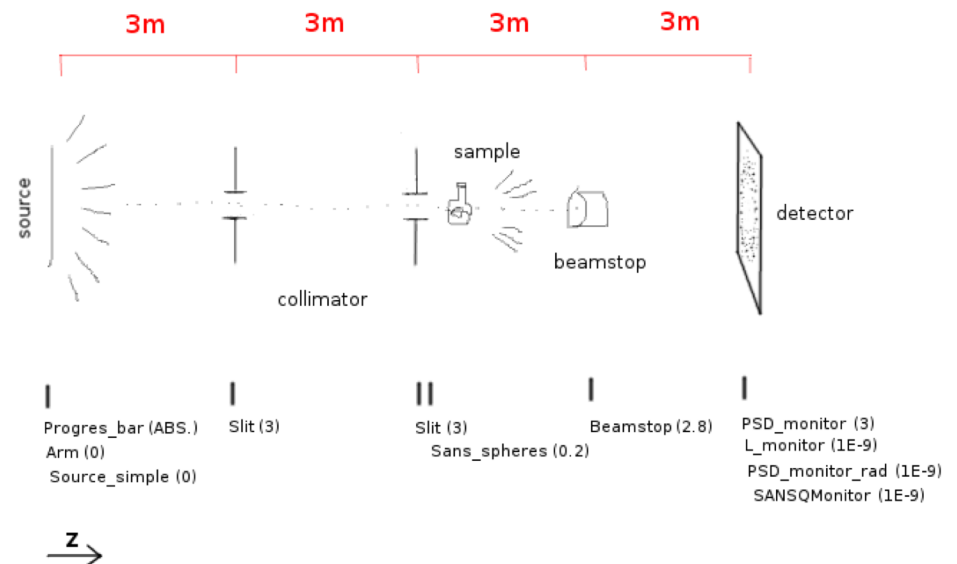
1. View McStas data in Mantid (simple – but nice to have)
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# Illustration: simplified SANS instrument

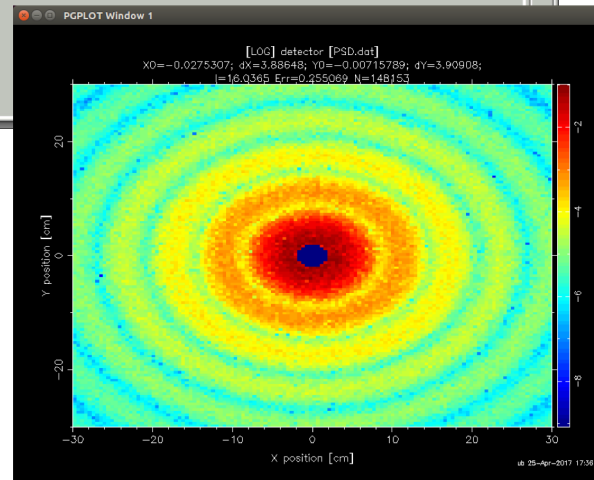
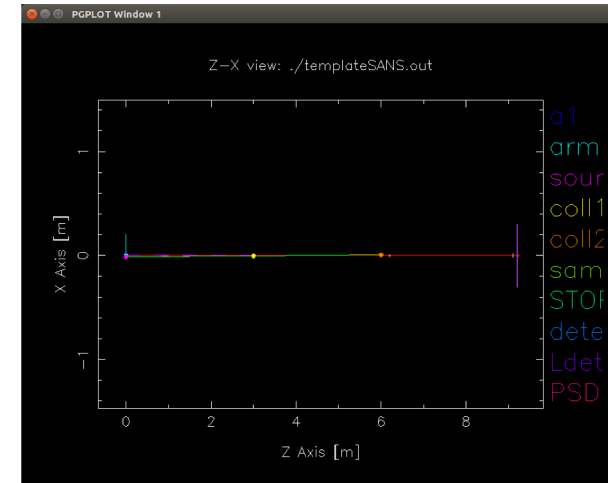
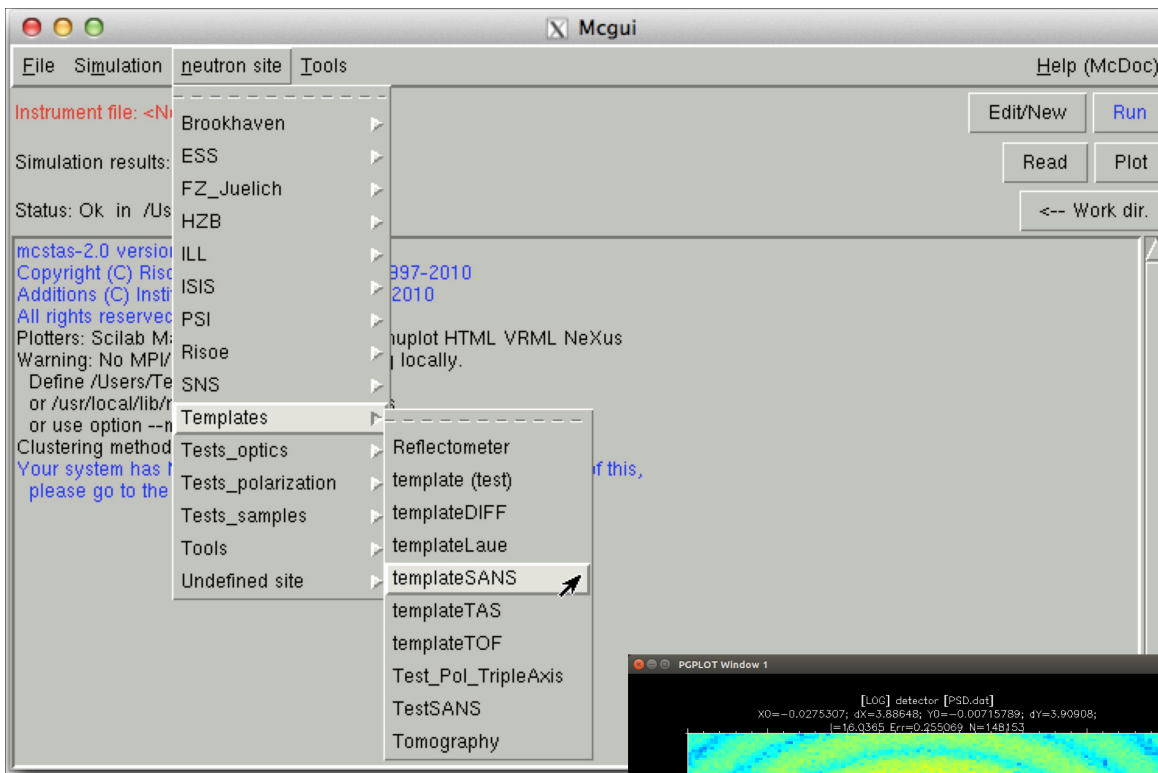


In this tutorial, you will write a simplified SANS instrument. When you have completed this tutorial, you will have learned the basics of mcstas.

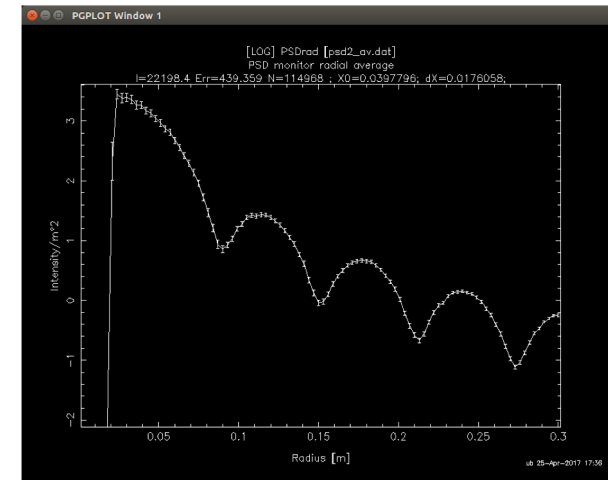
- Requirements: mcstas 2.2a.



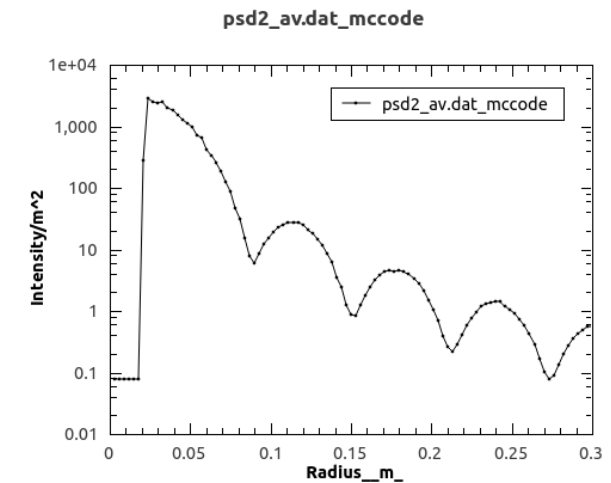
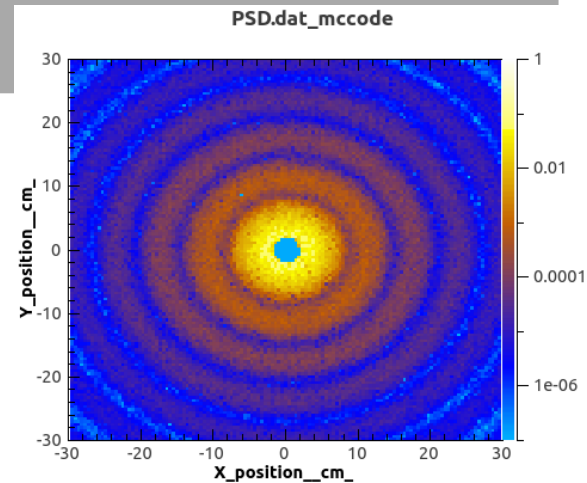
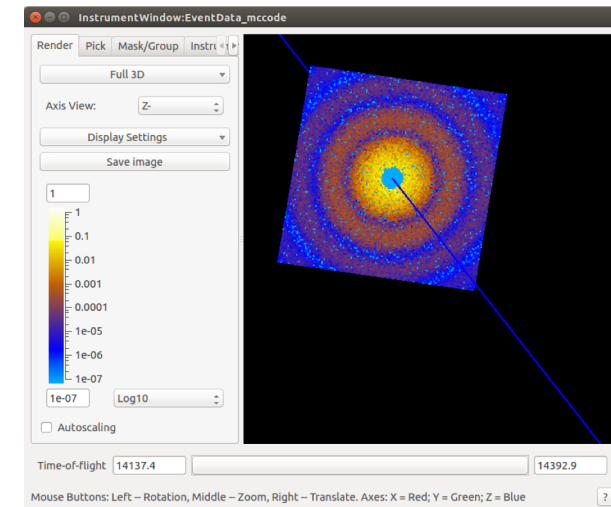
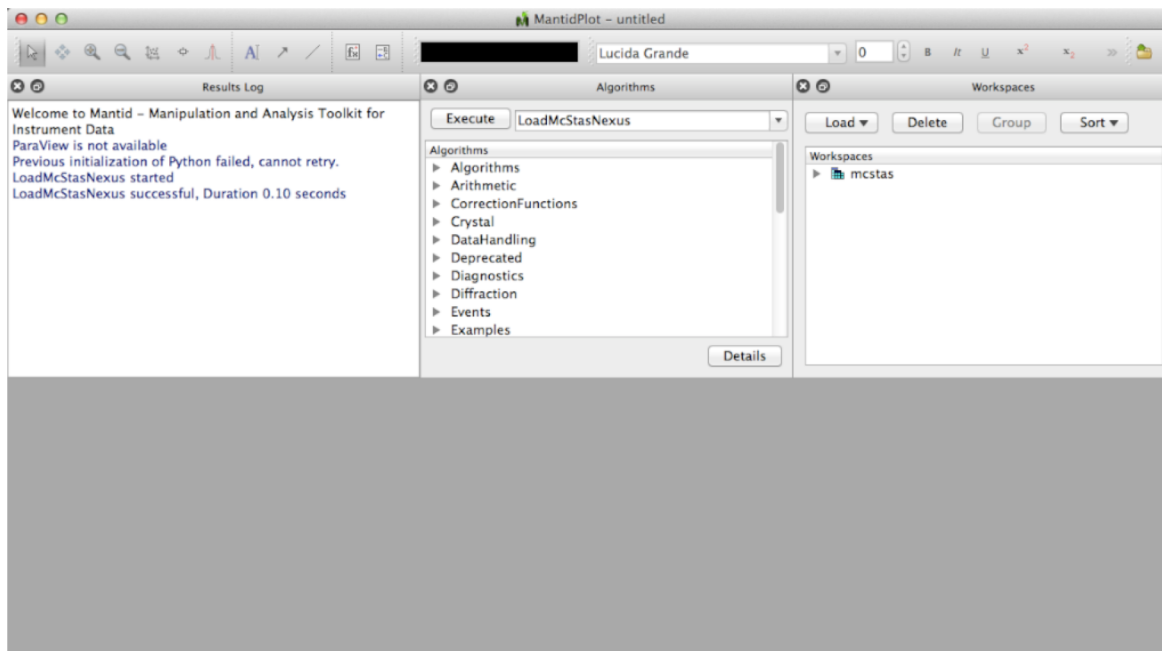
# McStas GUI: templateSANS



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



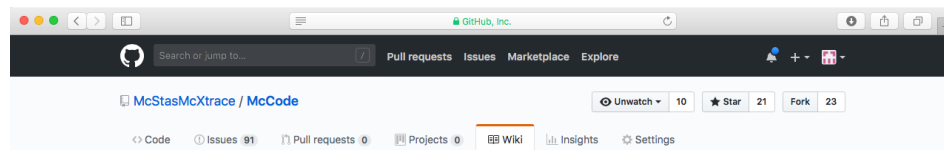
# Mantid GUI: templateSANS McStas data



# How to use: Online documentation



- Built-in Mantid
- Github McStas
- Archive - lanl.arXiv.org



## McStas and Mantid

Anders Markvardsen edited this page on Feb 27 · 45 revisions

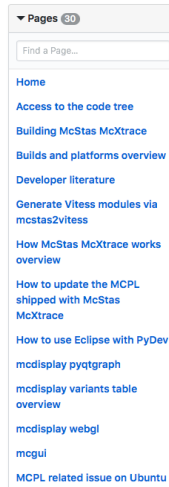
### A note on the McStas Mantid integration

#### Table of Contents

1. Introduction
2. Background and Motivation
3. The NeXus data format
4. McStas Mantid workflow
5. Setup the McStas instrument to create a Mantid instrument
6. McStas GUI
7. McStas CLI
8. MantidPlot view of McStas event data
9. Mantid reduction of McStas event data
10. ISIS SANS2D
11. Install NeXus
12. References Label

#### Introduction

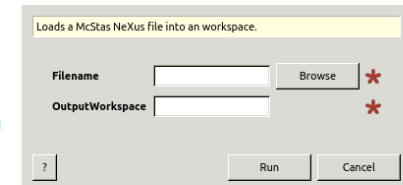
The McStas-Mantid data interface can be used to load McStas event data into Mantid, from where further data reduction and analysis can be performed. The purpose of this page is to demonstrate the methodologies, techniques and workflows used when combining McStas and Mantid.



## LoadMcStas v1

### Table of Contents

- Summary
- Properties
- Description
  - McStas compiling and running
  - McStas event data conventions
  - Tested versions
  - References



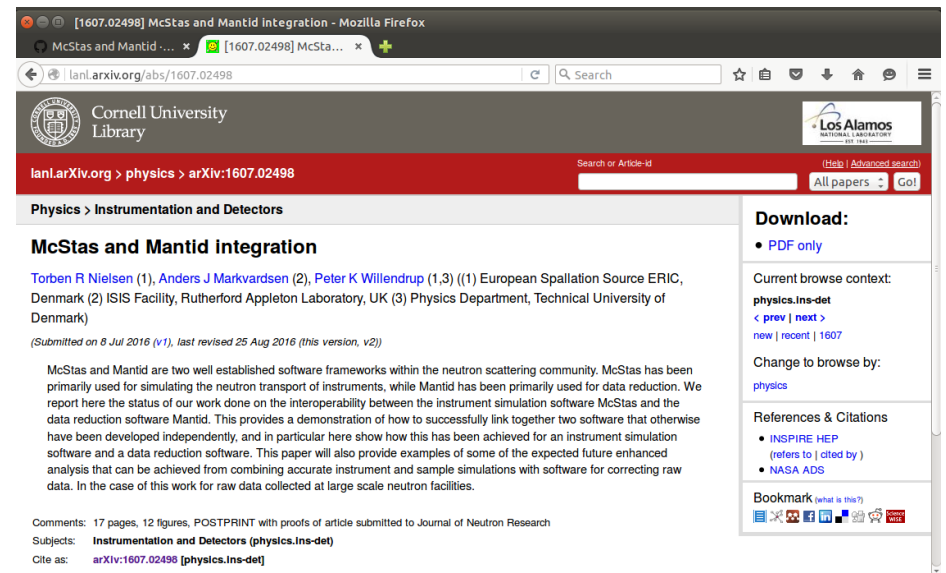
LoadMcStas dialog.

### Summary

Loads a McStas NeXus file into a workspace.

### Properties

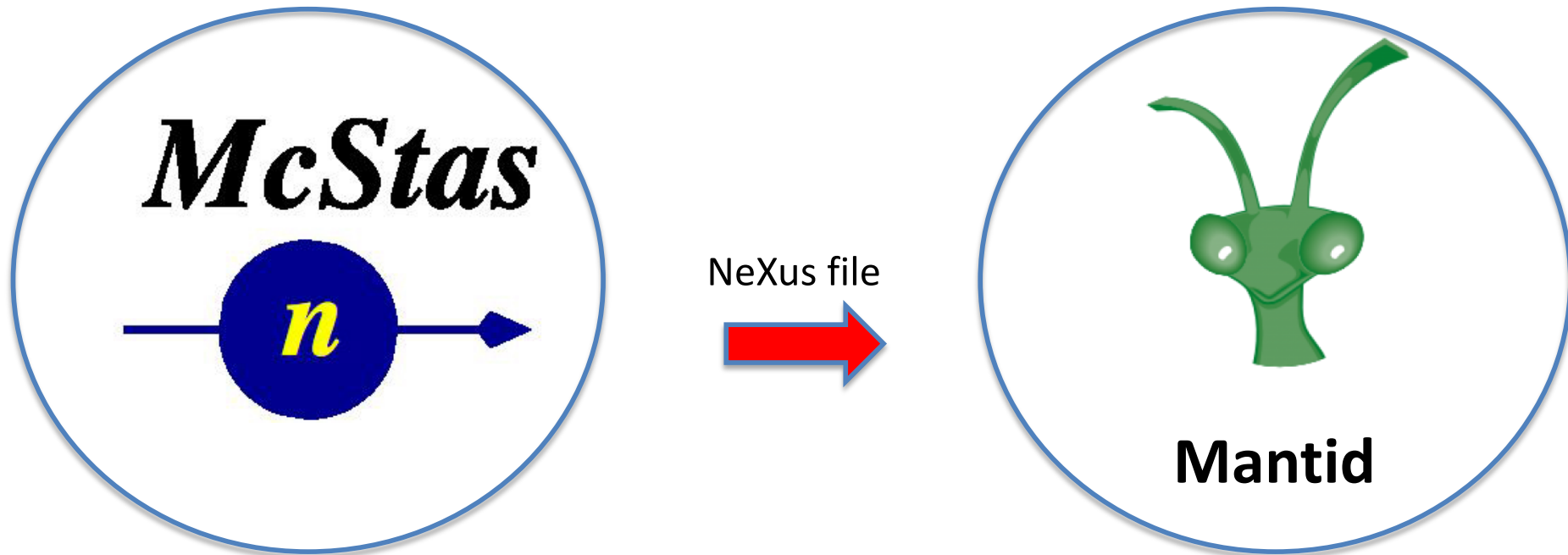
Name	Direction	Type	Default	Description
Filename	Input	string	Mandatory	The name of the Nexus file to load
OutputWorkspace	Output	Workspace	Mandatory	An output workspace.



# TOF and pixel ID's

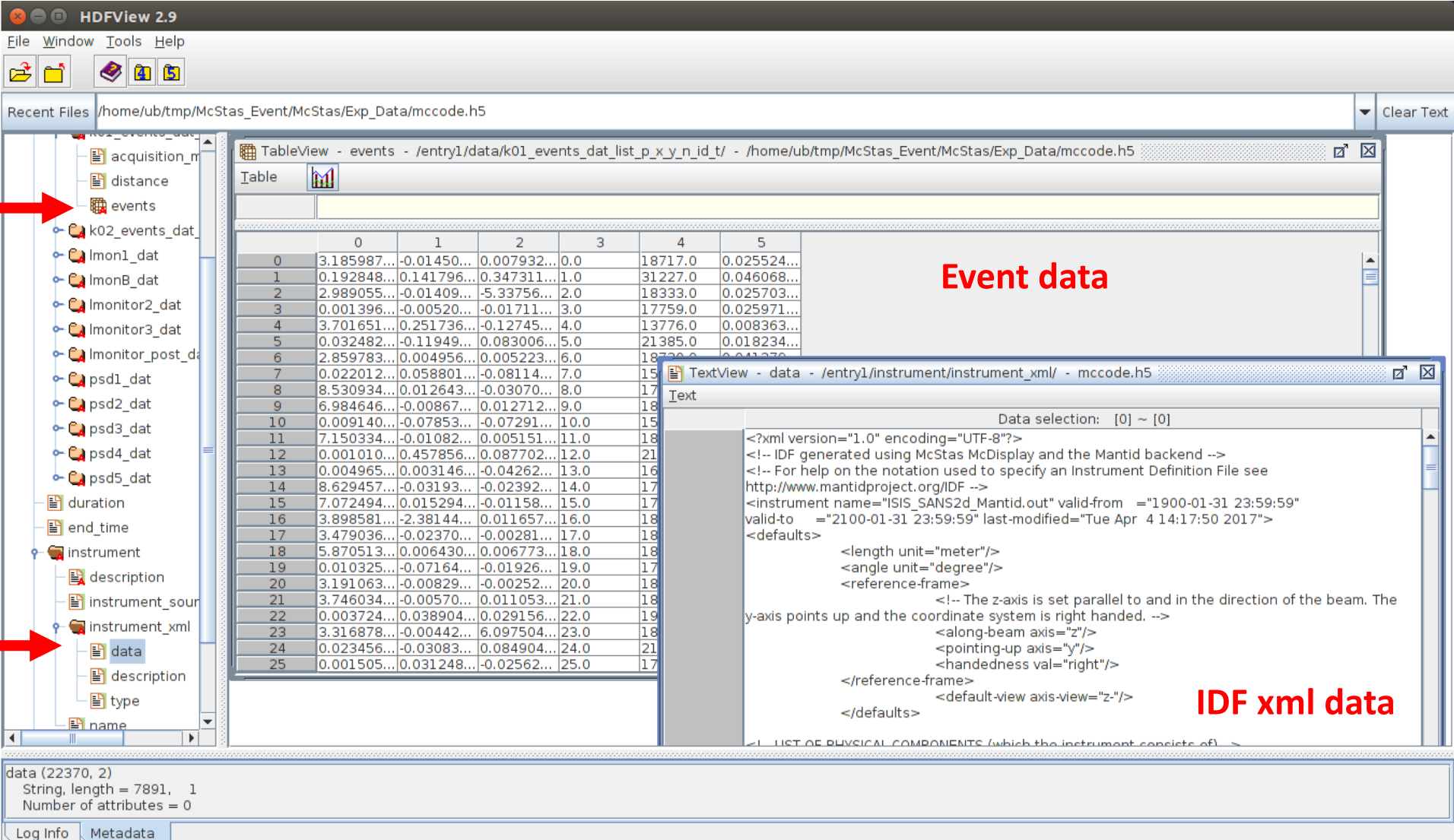
- Mantid was designed for data reduction at TOF spallation neutron sources
- Mantid's IDF store geometry information use in TOF analysis
- This implies parsing information about:
  - where the neutron source is located,
  - where the sample is located,
  - where each individual detector pixel is located.

# 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

# McStas NeXus file



The screenshot shows the HDFView 2.9 interface. The left sidebar displays a tree view of the NeXus file structure. Two red arrows point to the 'events' and 'instrument' folders. The main window is divided into two panes:

- Event data:** A TableView window showing a table of event data. The table has 6 columns (0-5) and 26 rows (0-25). The data is as follows:

	0	1	2	3	4	5
0	3.185987...	-0.01450...	0.007932...	0.0	18717.0	0.025524...
1	0.192848...	0.141796...	0.347311...	1.0	31227.0	0.046068...
2	2.989055...	-0.01409...	-5.33756...	2.0	18333.0	0.025703...
3	0.001396...	-0.00520...	-0.01711...	3.0	17759.0	0.025971...
4	3.701651...	0.251736...	-0.12745...	4.0	13776.0	0.008363...
5	0.032482...	-0.11949...	0.083006...	5.0	21385.0	0.018234...
6	2.859783...	0.004956...	0.005223...	6.0	18739.0	0.041276...
7	0.022012...	0.058801...	-0.08114...	7.0	15739.0	0.041276...
8	8.530934...	0.012643...	-0.03070...	8.0	17739.0	0.041276...
9	6.984646...	-0.00867...	0.012712...	9.0	18739.0	0.041276...
10	0.009140...	-0.07853...	-0.07291...	10.0	15739.0	0.041276...
11	7.150334...	-0.01082...	0.005151...	11.0	18739.0	0.041276...
12	0.001010...	0.457856...	0.087702...	12.0	21739.0	0.041276...
13	0.004965...	0.003146...	-0.04262...	13.0	16739.0	0.041276...
14	8.629457...	-0.03193...	-0.02392...	14.0	17739.0	0.041276...
15	7.072494...	0.015294...	-0.01158...	15.0	17739.0	0.041276...
16	3.898581...	-2.38144...	0.011657...	16.0	18739.0	0.041276...
17	3.479036...	-0.02370...	-0.00281...	17.0	18739.0	0.041276...
18	5.870513...	0.006430...	0.006773...	18.0	18739.0	0.041276...
19	0.010325...	-0.07164...	-0.01926...	19.0	17739.0	0.041276...
20	3.191063...	-0.00829...	-0.00252...	20.0	18739.0	0.041276...
21	3.746034...	-0.00570...	0.011053...	21.0	18739.0	0.041276...
22	0.003724...	0.038904...	0.029156...	22.0	19739.0	0.041276...
23	3.316878...	-0.00442...	6.097504...	23.0	18739.0	0.041276...
24	0.023456...	-0.03083...	0.084904...	24.0	21739.0	0.041276...
25	0.001505...	0.031248...	-0.02562...	25.0	17739.0	0.041276...

- IDF xml data:** A TextView window showing the XML content of the instrument definition file. The XML includes metadata and instrument parameters such as units, reference frame, and axis orientations.

At the bottom of the interface, a status bar shows: data (22370, 2) String, length = 7891, 1 Number of attributes = 0. Buttons for 'Log Info' and 'Metadata' are visible.

# templateSANS.inst vs templateSANS\_Mantid.inst



```
templateSANS.instr UNREGISTERED
templateSANS.instr x templateSANS_Mantid.instr x
1 DEFINE INSTRUMENT templateSANS(lambda=6, dlambd=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, dlambd = dlambd, 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 x templateSANS_Mantid.instr x
1 DEFINE INSTRUMENT templateSANS_Mantid(lambda=6, dlambd=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, dlambd = dlambd, 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



```
COMPONENT detector = PSD_monitor( UNREGISTERED
COMPONENT detector = PSD_monitor(
COMPONENT nD_Mantid_1 = Monitor_nD(
1 COMPONENT detector = PSD_monitor(
2     nx = 128, ny = 128, filename = "PSD.dat", xmin = -0.3,
3     xmax = 0.3, ymin = -0.3, ymax = 0.3)
4     AT (0, 0, 3) RELATIVE sample
5
```

Line 5, Column 1      Tab Size: 4      Plain Text

```
COMPONENT nD_Mantid_1 = Monitor_nD( UNREGISTERED
COMPONENT detector = PSD_monitor(
COMPONENT nD_Mantid_1 = Monitor_nD(
1 COMPONENT nD_Mantid_1 = Monitor_nD(
2     options ="mantid square x limits=[-0.3 0.3] bins=128
3     y limits=[-0.3 0.3] bins=128, neutron pixel min=0 t,
4     list all neutrons",
5     xmin = -0.3,
6     xmax = 0.3,
7     ymin = -0.3,
8     ymax = 0.3,
9     restore_neutron = 1,
10    filename = "bank01_events.dat")
11    AT (0, 0, 3.2) RELATIVE sampleMantid
```

Line 10, Column 3      Tab Size: 4      Plain Text

# McStas event KEYWORDS

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(... )**”

In the McStas instrument file the source must be named “**sourceMantid**”

- E.g. “**COMPONENT sourceMantid = Source\_simple(... )**”

In the McStas instrument file the sample must be named “**sampleMantid**”

- E.g. “**COMPONENT sampleMantid = Sans\_spheres(... )**”

In the McStas instrument file the event monitors must be named “**nD\_Mantid\_#**”

- E.g. “**COMPONENT nD\_Mantid\_1 = Monitor\_nD(... )**”

# How to run simulation



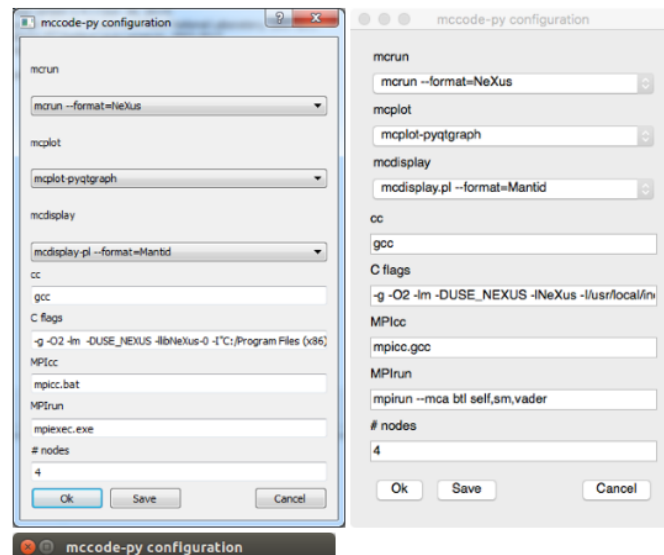
## McStas GUI

Generating McStas event data for Mantid can be achieved from the McStas GUI `mcgui`. Below we show how to setup the simulation on Windows 7, OSX 10.12, and Ubuntu 16.04. For [McStas](#) we use version 2.4.1. For [Mantid](#) use version 3.4 or later.

**Windows users** need to download the latest version of [mccode-r.c](#) in order to generate IDF data in the `mccode.h5` file which Mantid can read. Copy the downloaded file to the directory where your McStas instrument file is located.

1. Open the McStas configuration file. In `mcgui` go to: File -> Configuration
2. Change the setting as shown in figures below:
  - o In the section `mcrun` select `mcrun --format=NeXus`
  - o In the section `mcplot` select `mcplot-pyqtgraph`
  - o In the section `mcdisplay` select `mcdisplay-pl --format=Mantid` (Windows) or `mcdisplay.pl --format=Mantid` (OSX or Ubuntu)
  - o In the section `C flags` select this line depending on your OS
    - Windows: `-g -O2 -lm -DUSE_NEXUS -llibNeXus-0 -I "C:/Program Files (x86)/NeXus Data Format/include/nexus" -L "C:/Program Files (x86)/NeXus Data Format/lib/nexus"`
    - OS X: `-g -O2 -lm -DUSE_NEXUS -lNeXus -I/usr/local/include/nexus`
    - Ubuntu: `-g -O2 -lm -DUSE_NEXUS -lNeXus`

Wiki page on GitHub

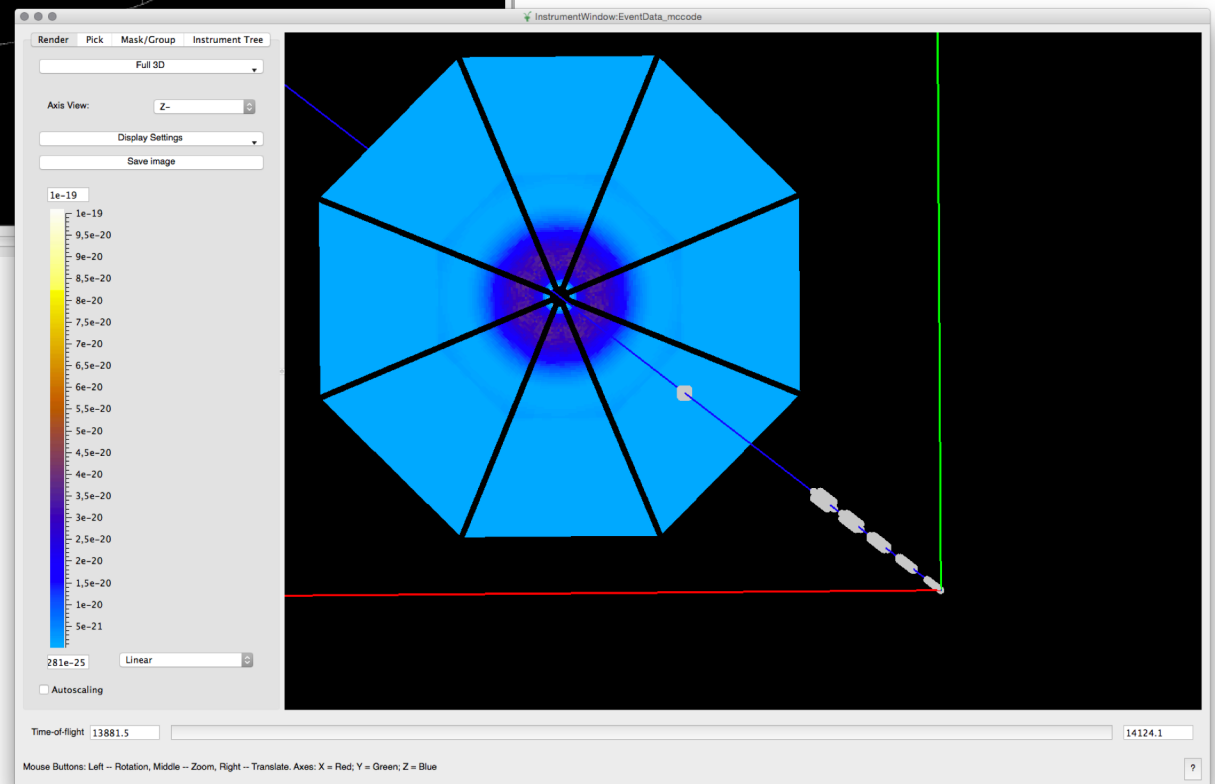
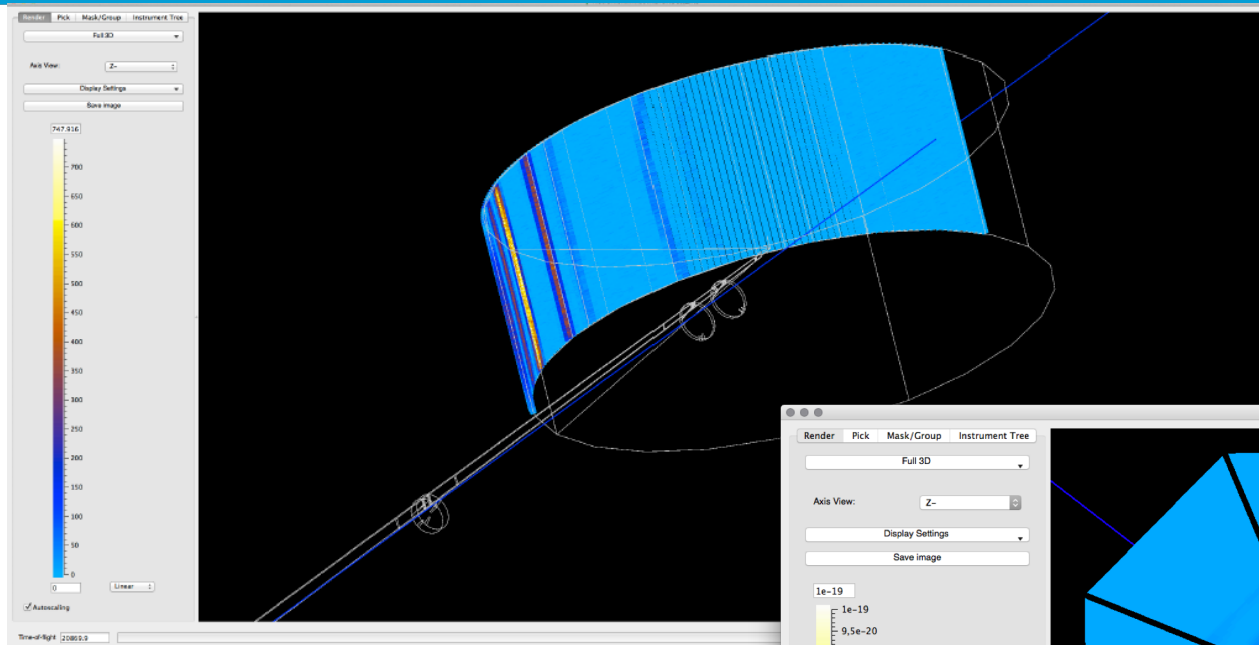


# McStas – Mantid: Demo Time

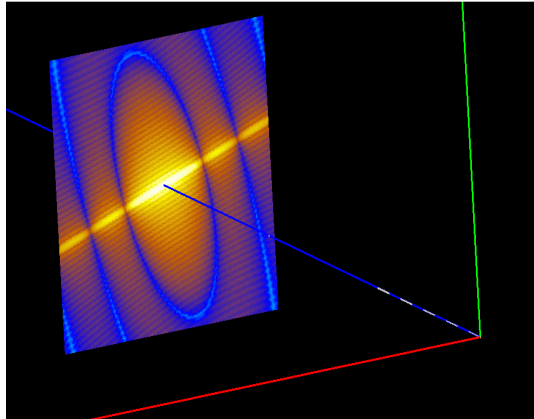


- See how to use Mantid – McStas interface

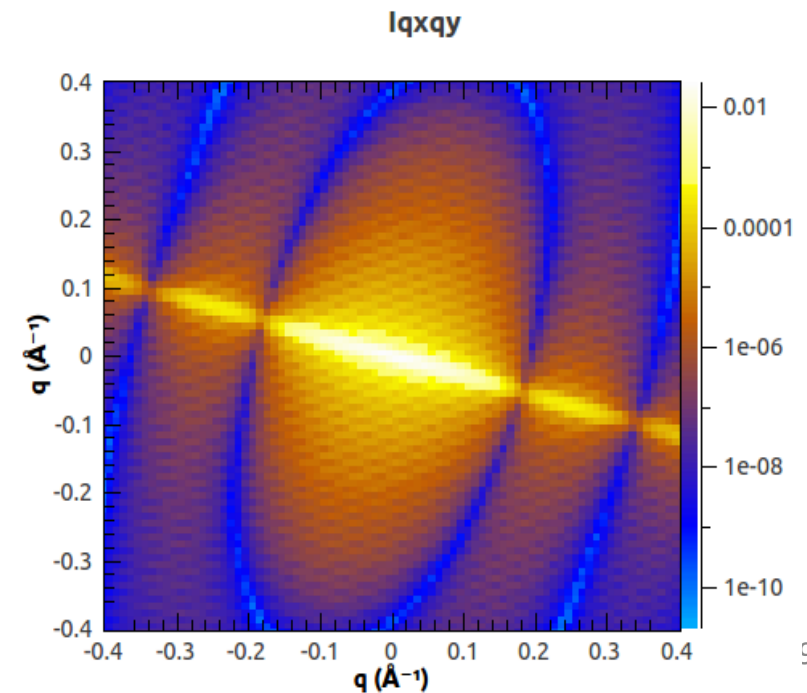
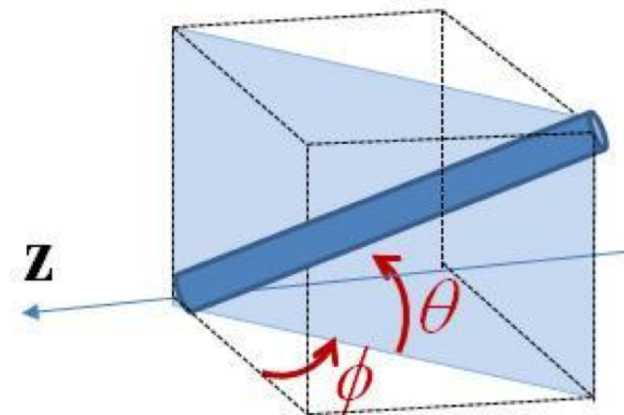
# Examples of detectors: IN5 (ILL) and LoKI (ESS)



# Example: Usage of Mantid algorithms

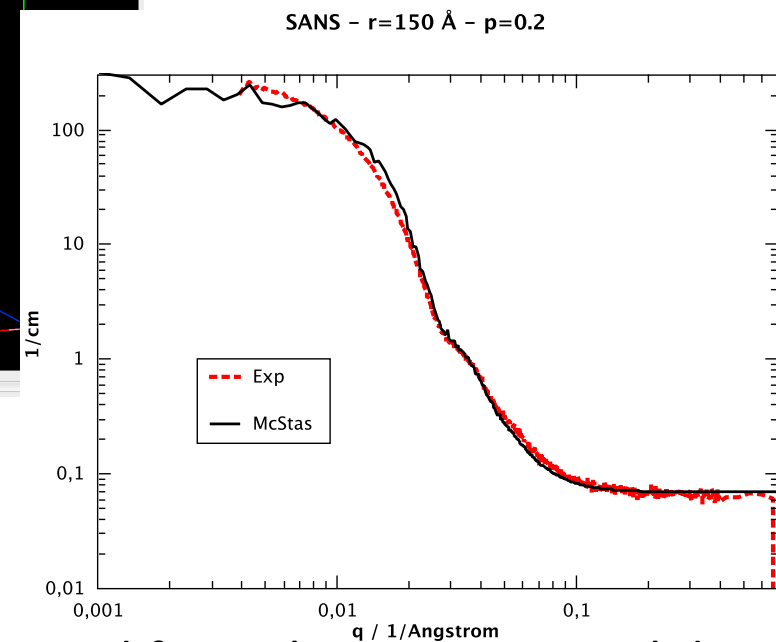
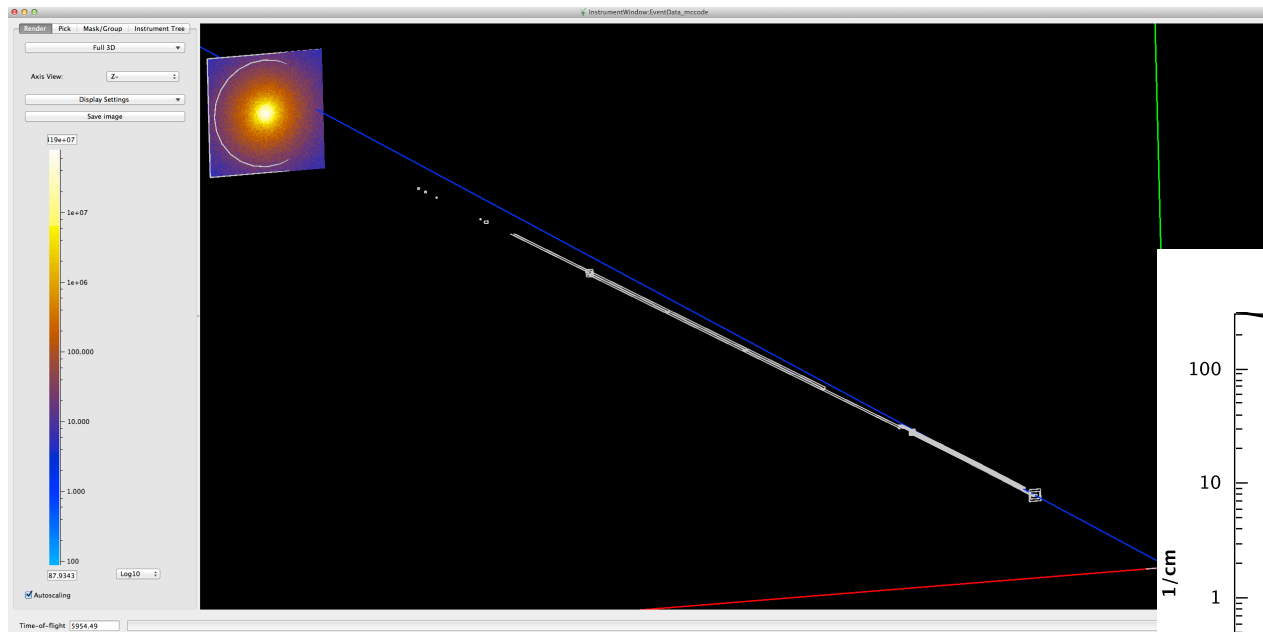


- McStas – Mantid
- 2D scattering kernel from SasView
- 2D reduction in Mantid: Qxy
- Can be send back to SasView fitting



# McStas and experimental data: SANS2D

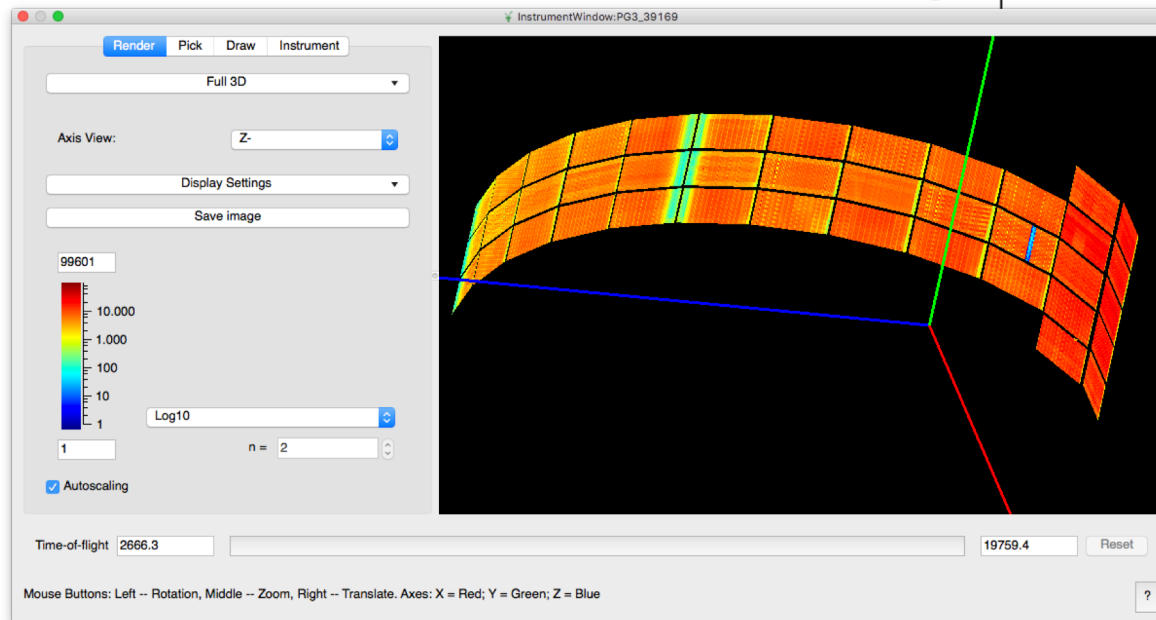
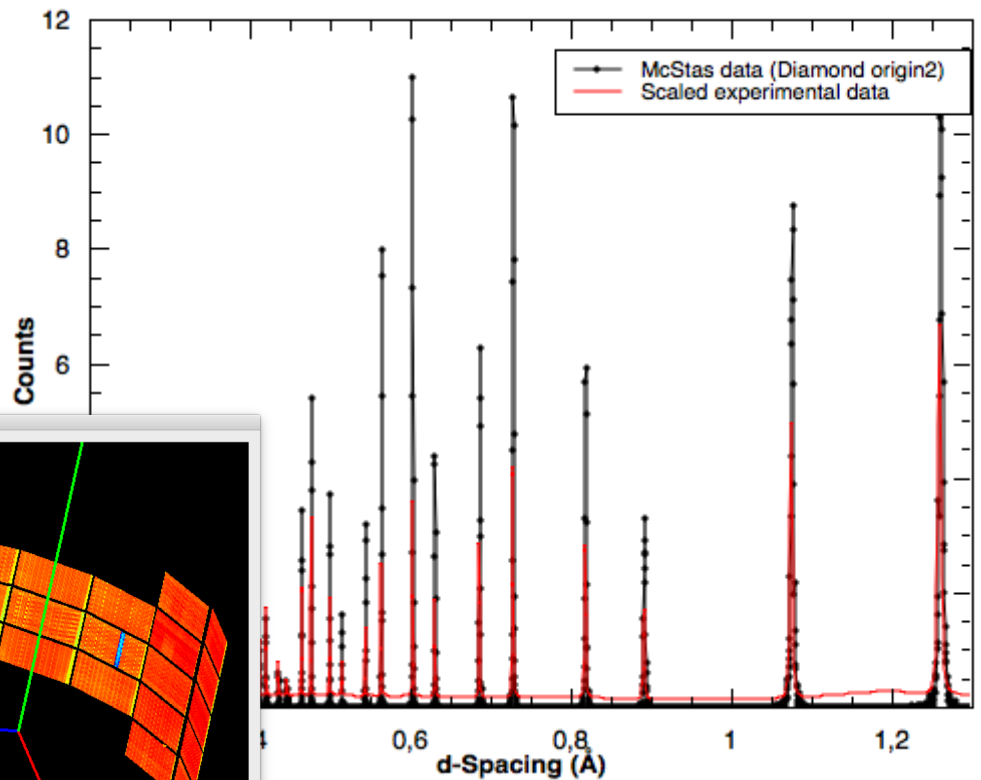
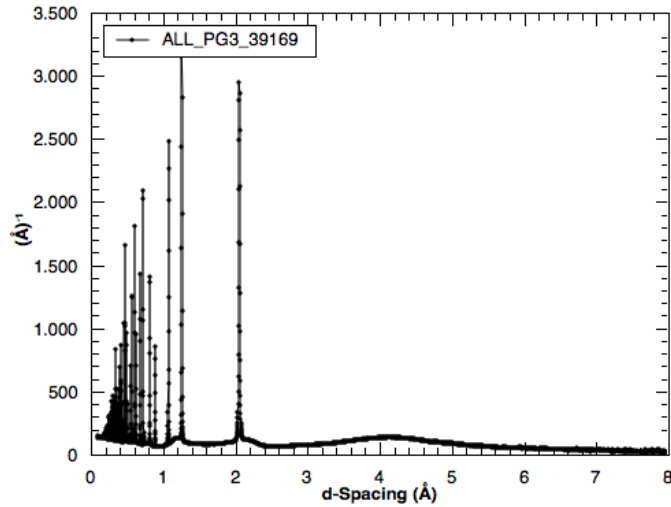
Mantid view of the McStas event data generated for the ISIS\_SANS2d.instr file.



Comparison of rescaled scattering intensity  $I(q)$  derived from the experimental data and a McStas simulation. Nanospheres of radius  $150 \text{ \AA}$ , polydispersion 0.2.

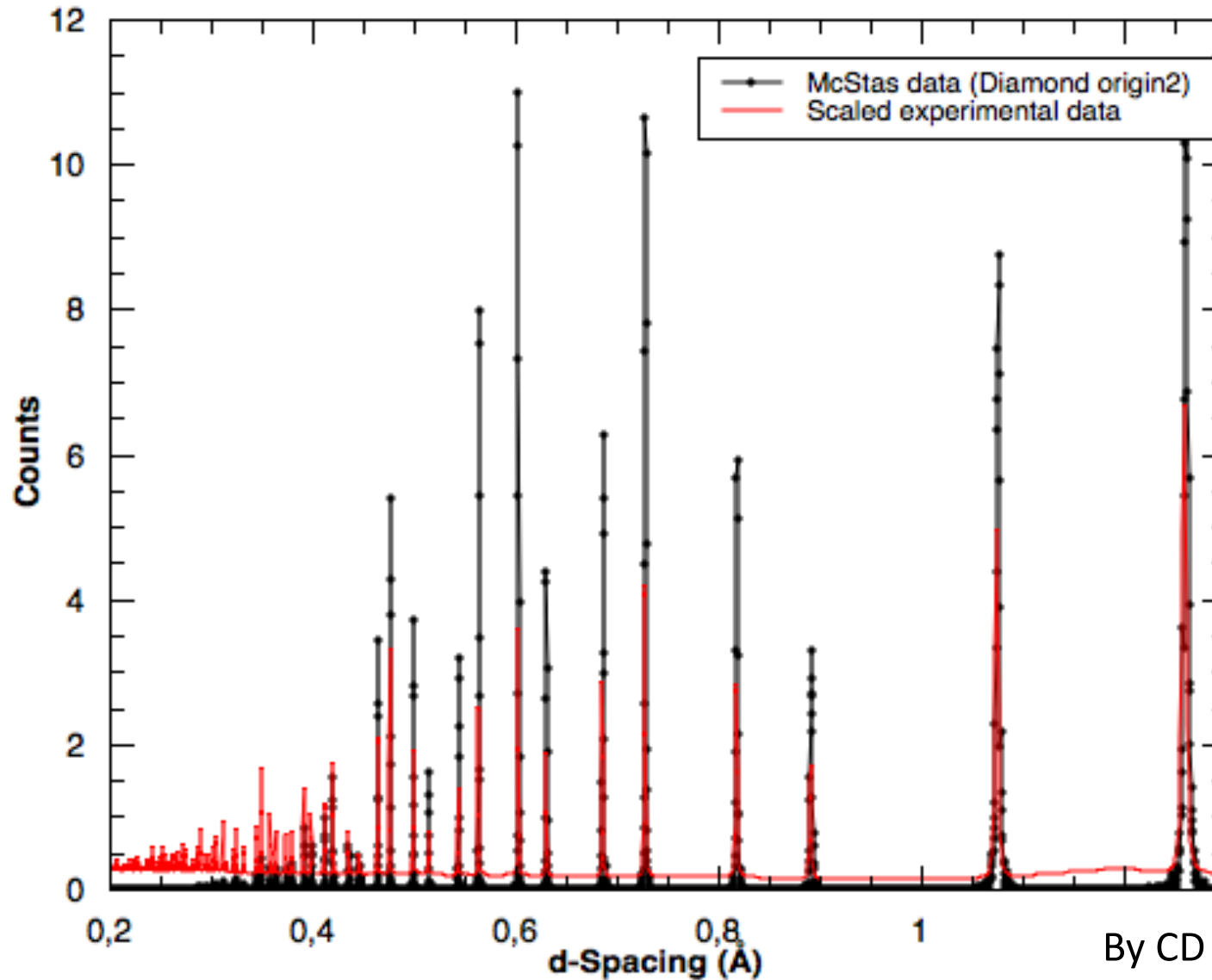
# McStas and experimental data: POWGEN

ALL\_PG3\_39169



By CD @ ESS + SNS collaboration

# McStas and experimental data: POWGEN



- The end .....

# How to use: Generate the IDF

How-to generate McStas event data for Mantid

Step 1. Generate IDF:

- `mcdisplay templateSANS_Mantid.instr --format=Mantid -n0`

**A new xml IDF file is then generated on disk**

# How to use: Make NeXus file for Mantid



How-to generate McStas event data for Mantid

Step 1. Compile c code:

- `gcc -o templateSANS_Mantid.out templateSANS_Mantid.c -DUSE_NEXUS -lNeXus -lm`

Step 2. Run simulation:

- `templateSANS_Mantid.out --format=Nexus`

Now IDF is embedded in the NeXus file to be read by Mantid