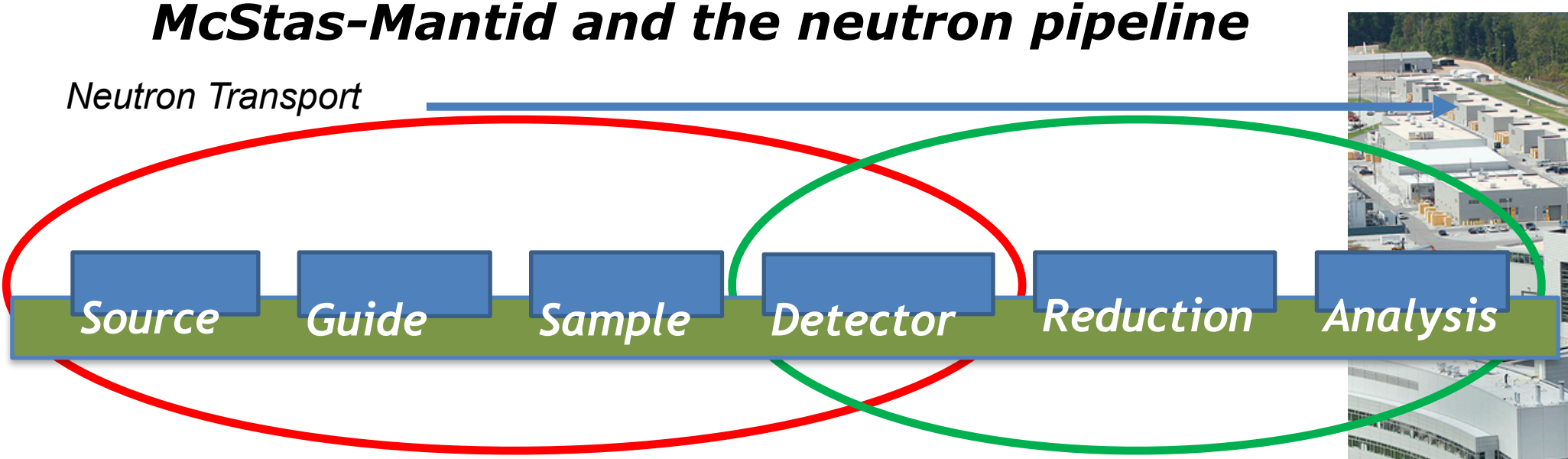
Using the McStas + Mantid interface

Presenter: Peter Willendrup
(slides from Torben Nielsen, ESS)

McStas-Mantid and the neutron pipeline

Neutron Transport



Typical McStas Neuron Transport

Mantid-McStas focus:

How to analyse McStas data

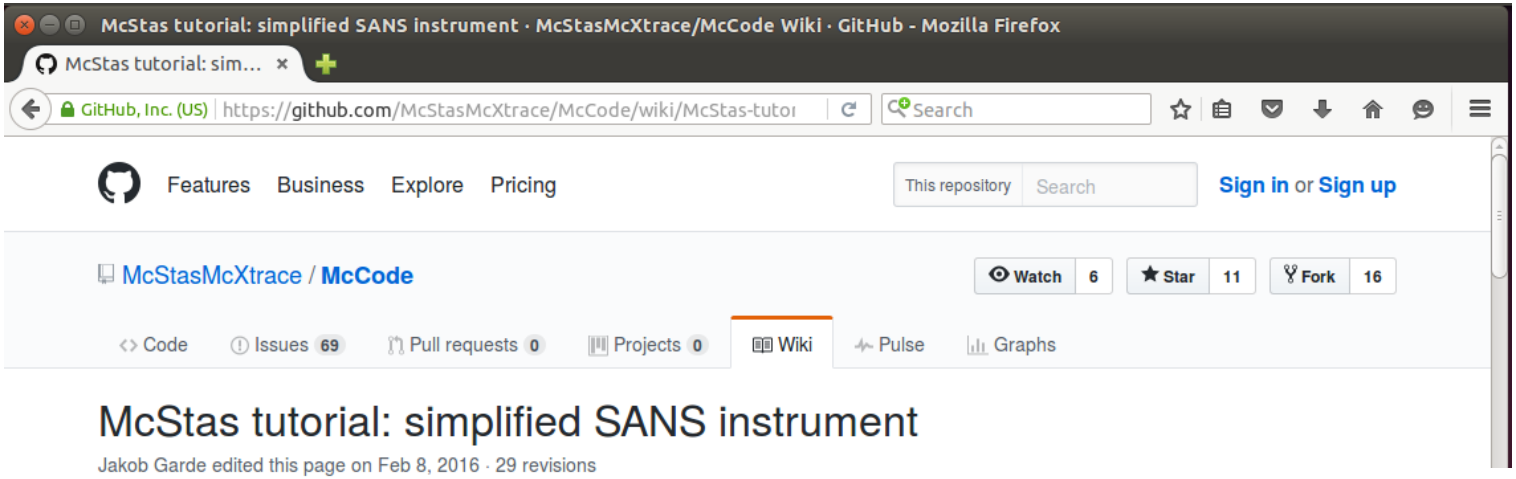
Motivation: I - Highlevel

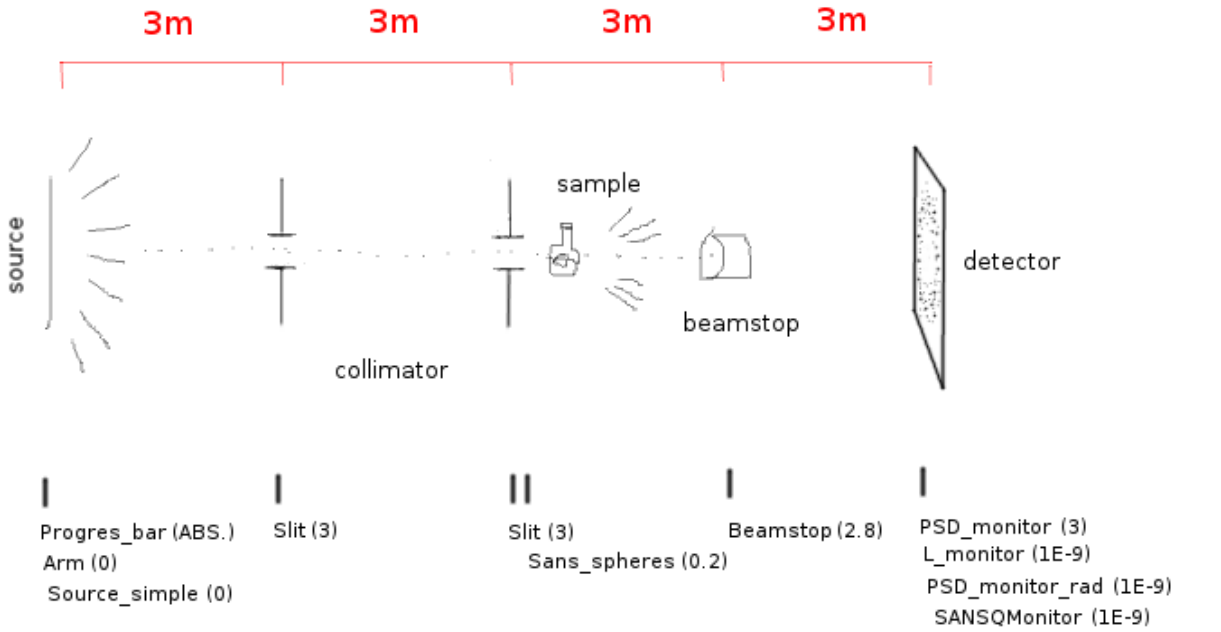
1. *Mantid is well established software – long history*
2. *McStas is well established software – long history*
3. *Wanted to combine the reduction framework and the neutron transport framework*
4. *So users can do transport, reduction and "analysis" in one go*

Motivation: II - Benefits for users

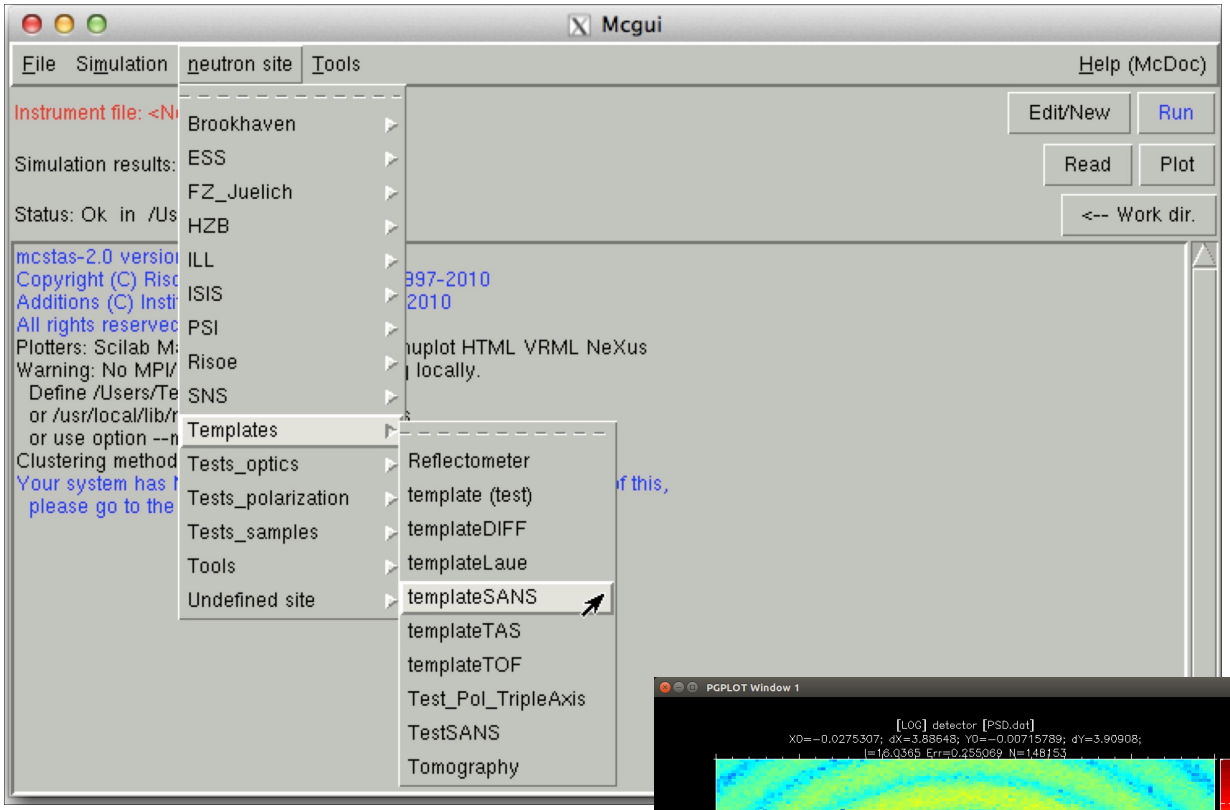
1. *View McStas data in Mantid (simple – but nice to have)*
2. *Import McStas event data to Mantid*
3. *Use already developed and tested algorithms in Mantid to process McStas event data (no need to reinvent stuff!!!)*
4. *Advanced use: Use McStas to quantify (perhaps remove) "spurries" signal on detector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

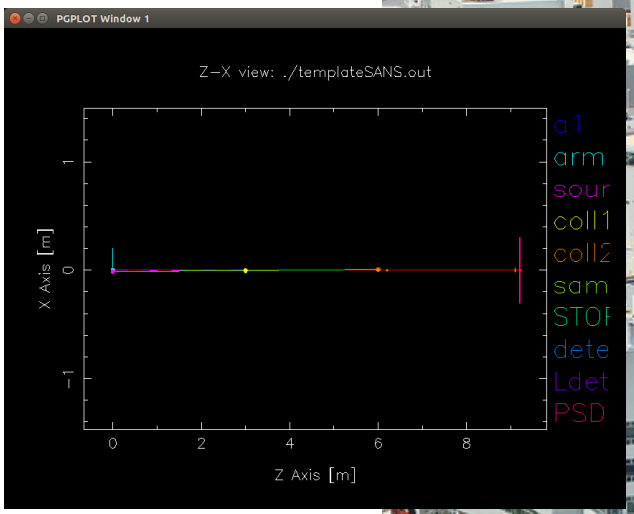
Illustration: simplified SANS instrument

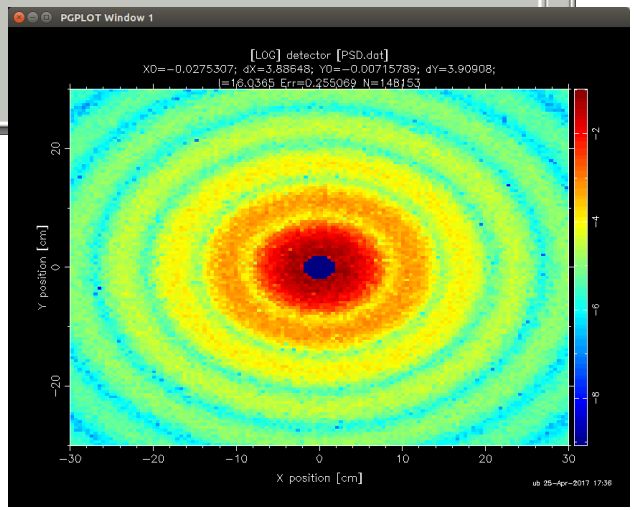


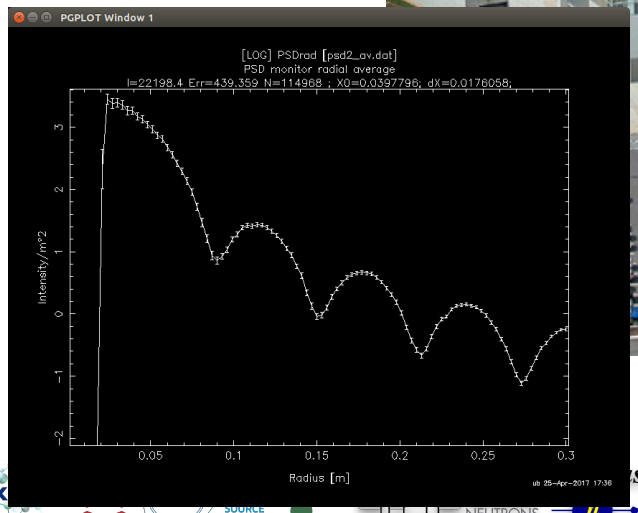


McStas GUI: templateSANS



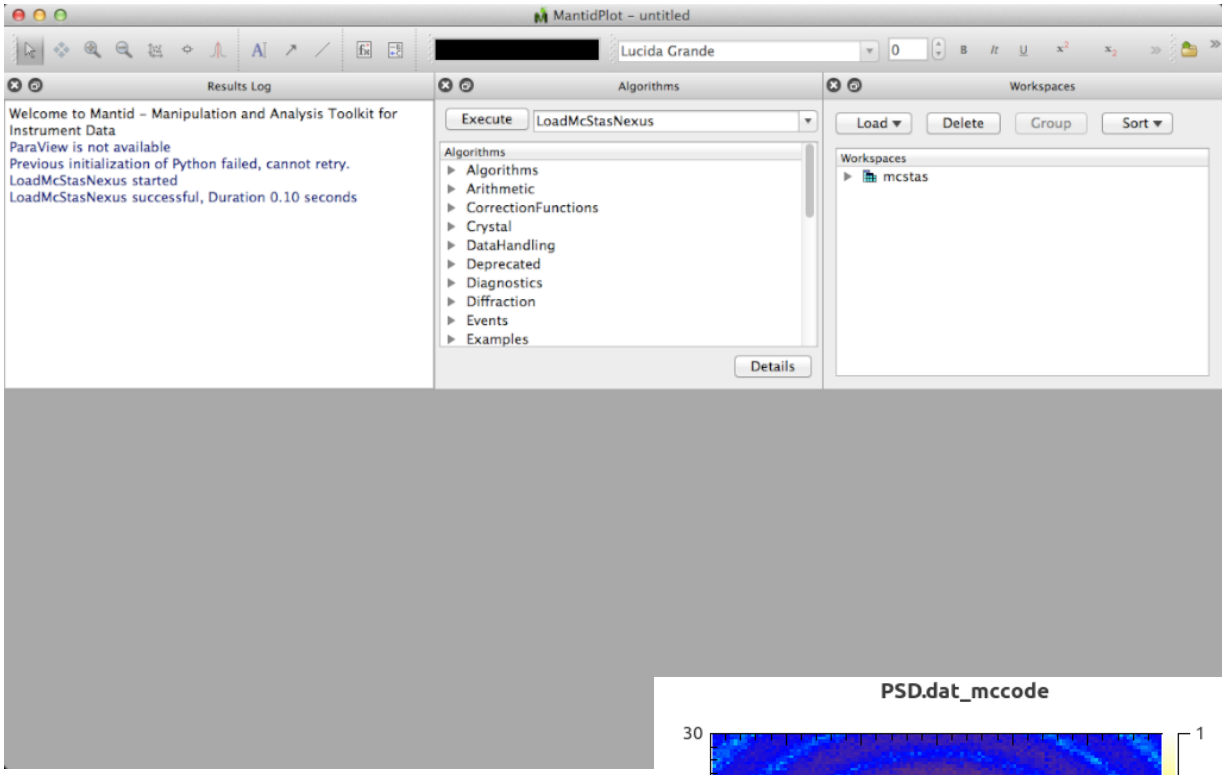


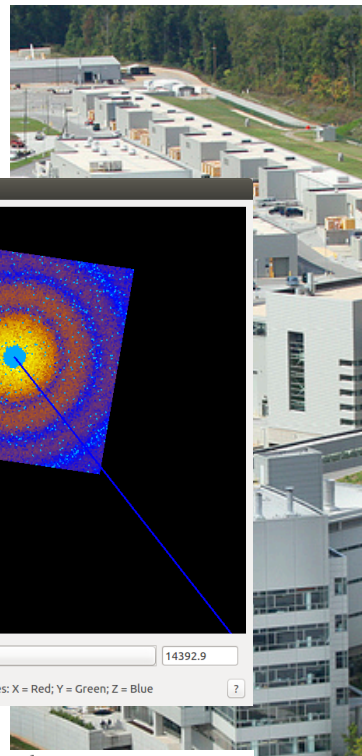


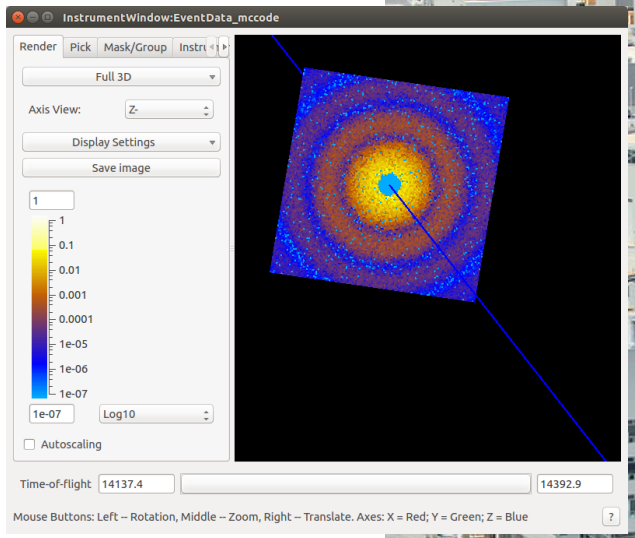


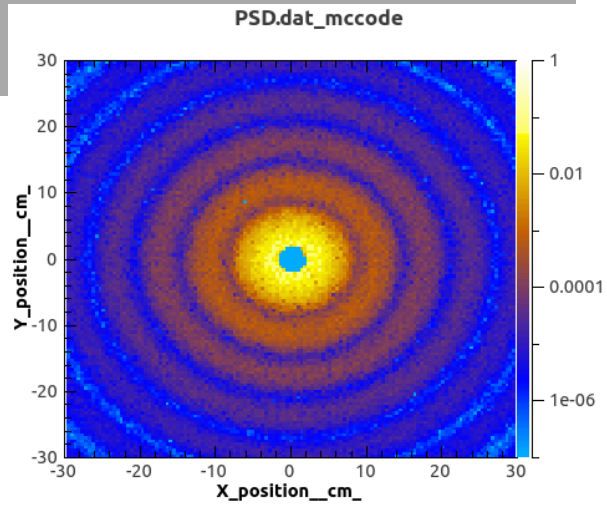
R=150,phi=0.1, d=1,a=0

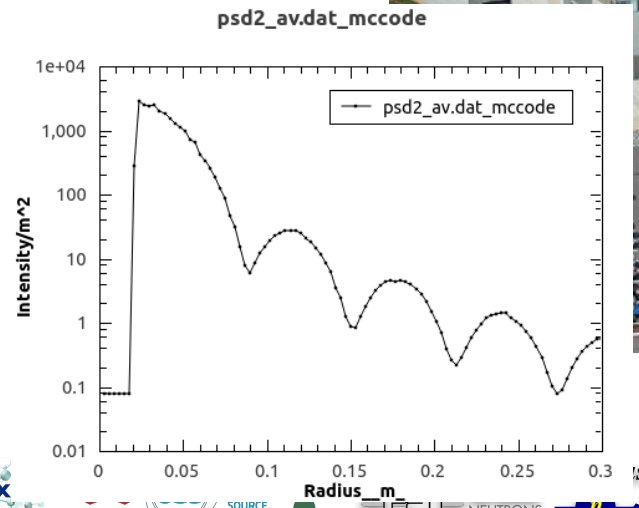
Mantid GUI: templateSANS McStas data











How to use: Online documentation

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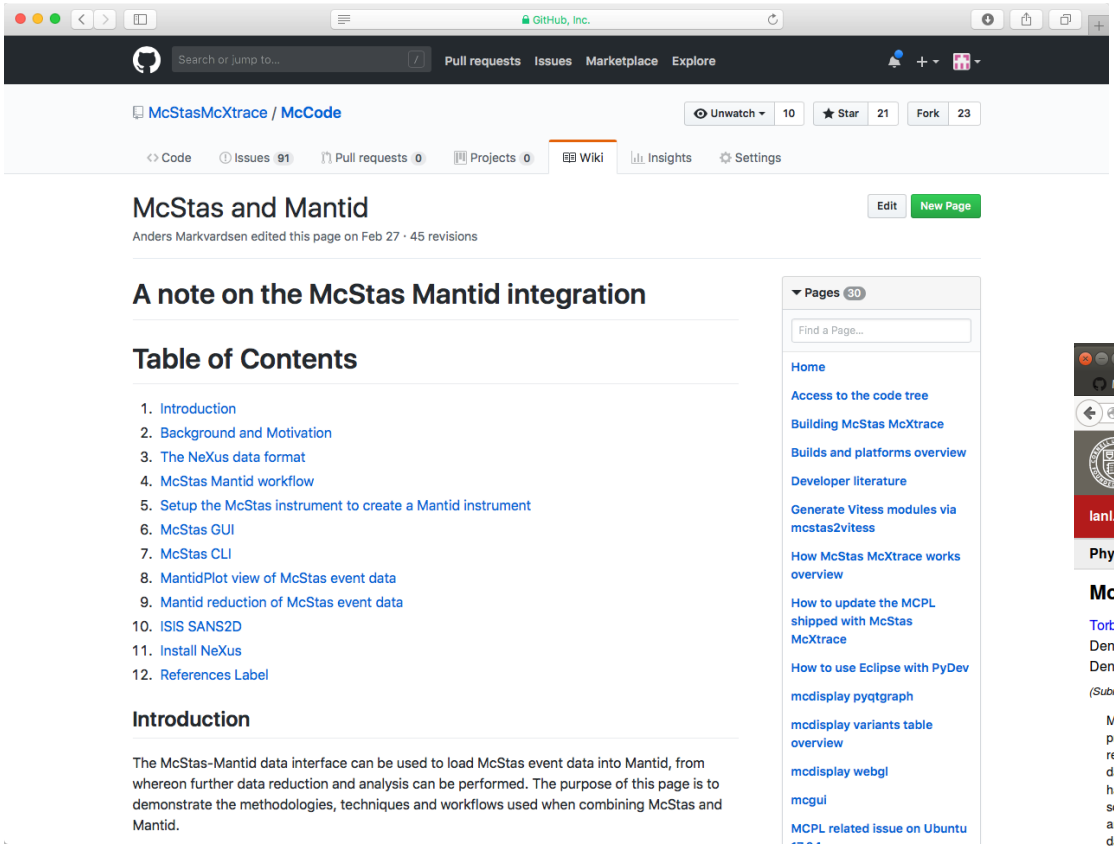
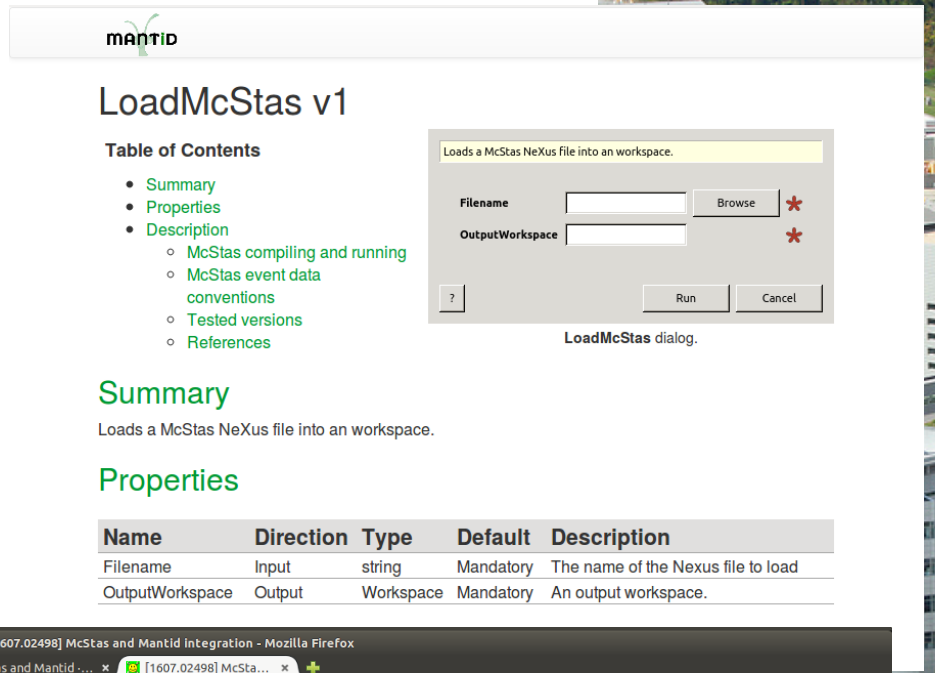
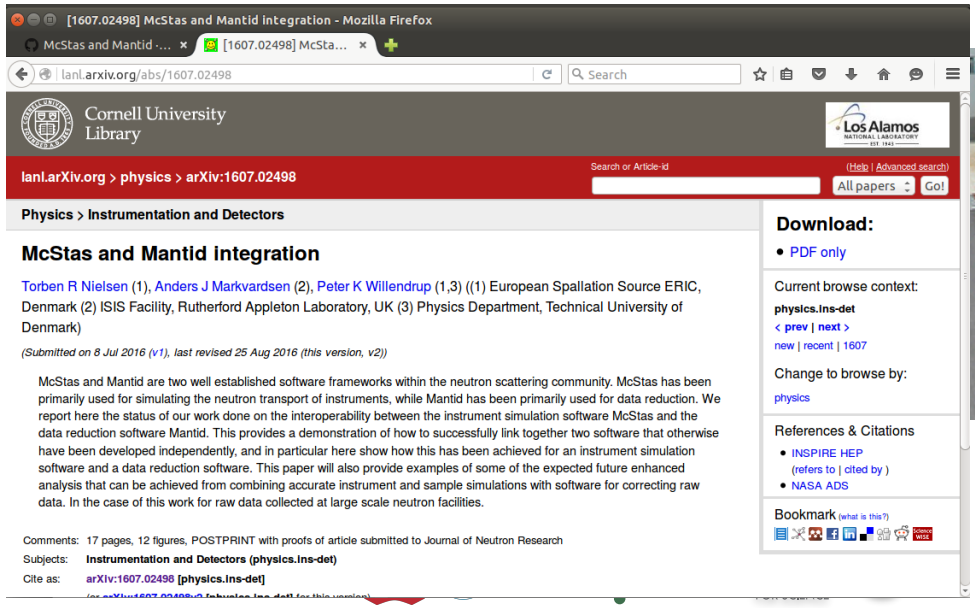
- *Github McStas - Wiki*
- *Nielsen, T. R.; et. al JNR **18** 2015, p. 79-92.*
- *Archive https://arxiv.org/abs/1607.02498*
- *Built-in Mantid*



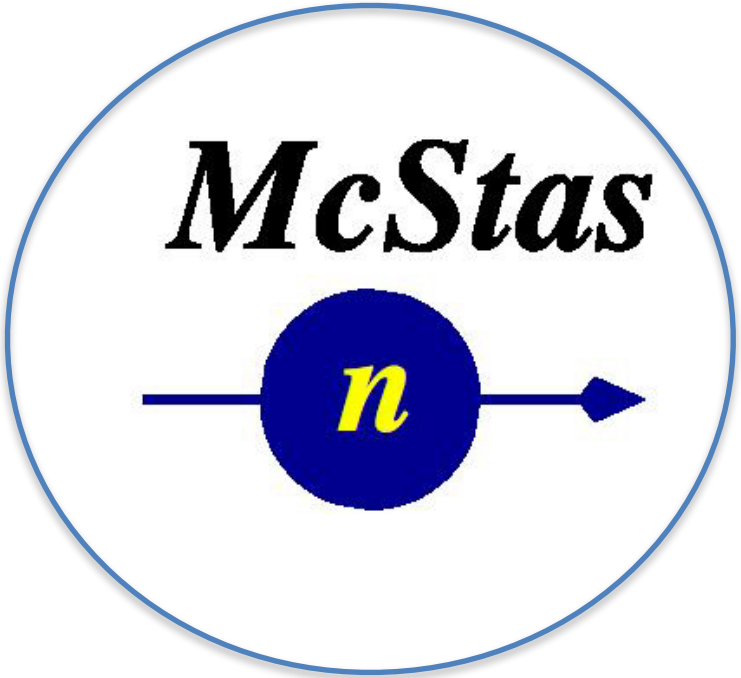




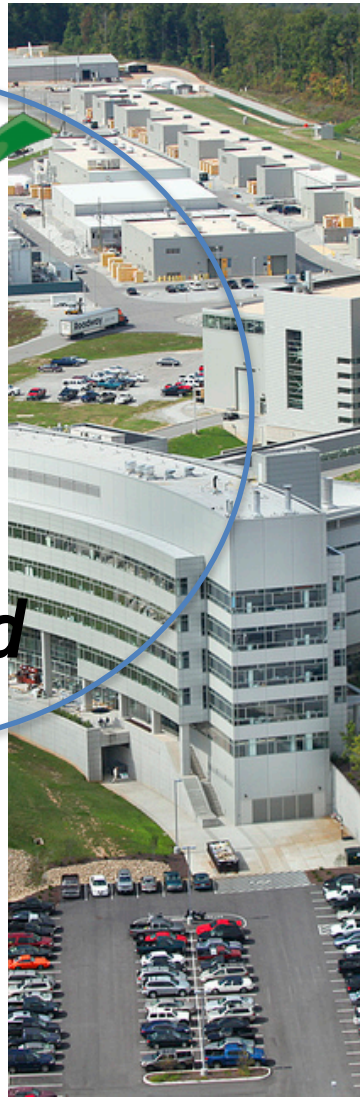
TOF and pixel ID's

- *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

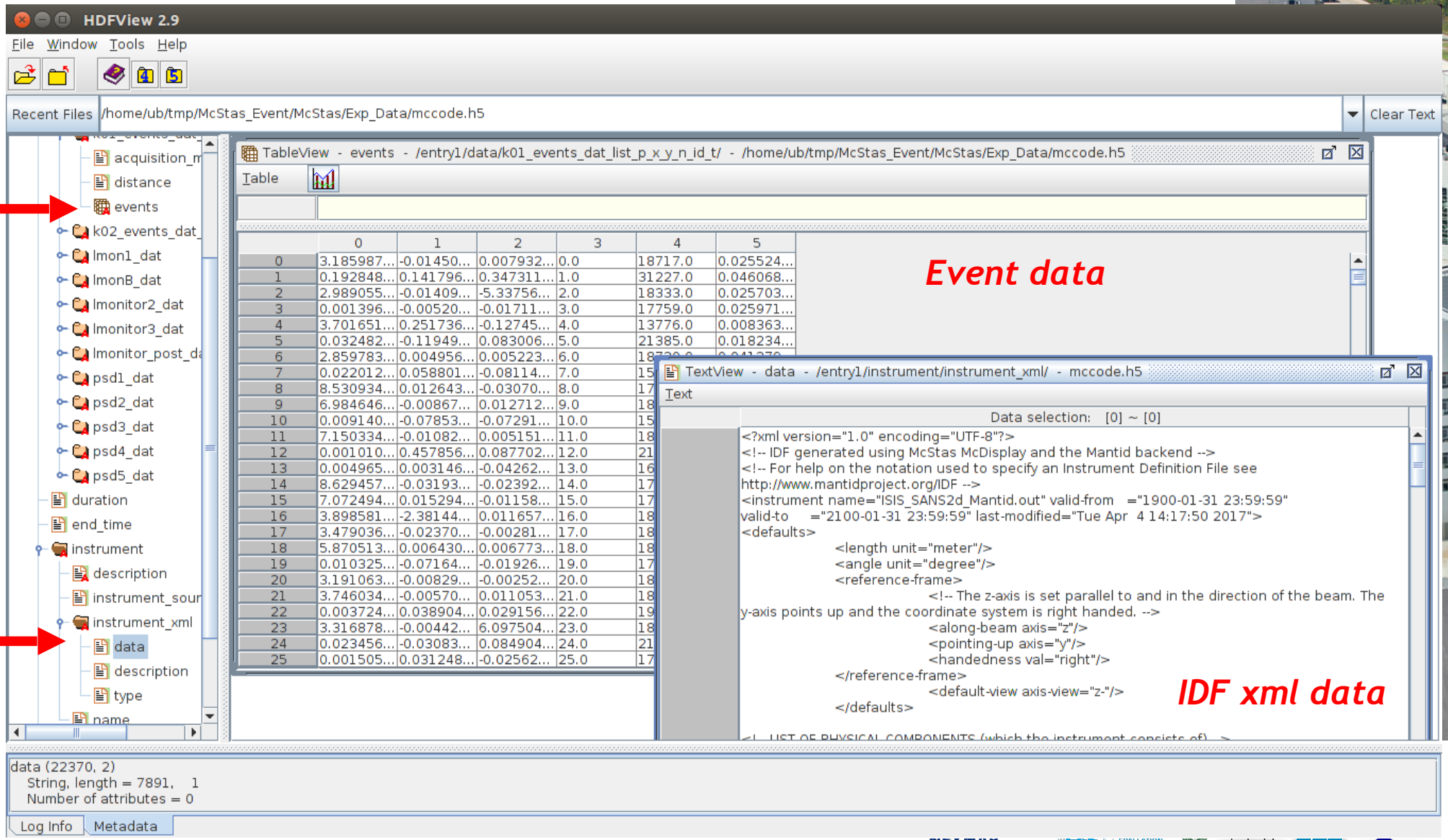


NeXus file



- 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



templateSANS.inst vs templateSANS_Mantid.inst

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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

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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_

COMPONENT detector = PSD_monitor(| COMPONENT nD_Mantid_

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

Line 10, Column 3

McStas event KEYWORDS

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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_#**"*

How to run simulation

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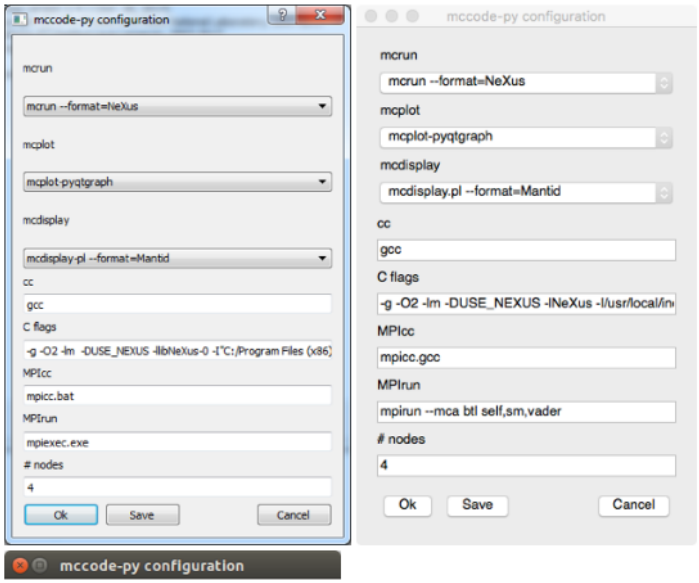
GitHub, Inc.

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:
   - In the section `mcrun` select `mcrun --format=NeXus`
   - In the section `mcplot` select `mcplot-pyqtgraph`
   - In the section `mcdisplay` select `mcdisplay-pl --format=Mantid` (Windows) or `mcdisplay.pl --format=Mantid` (OSX or Ubuntu)
   - 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`

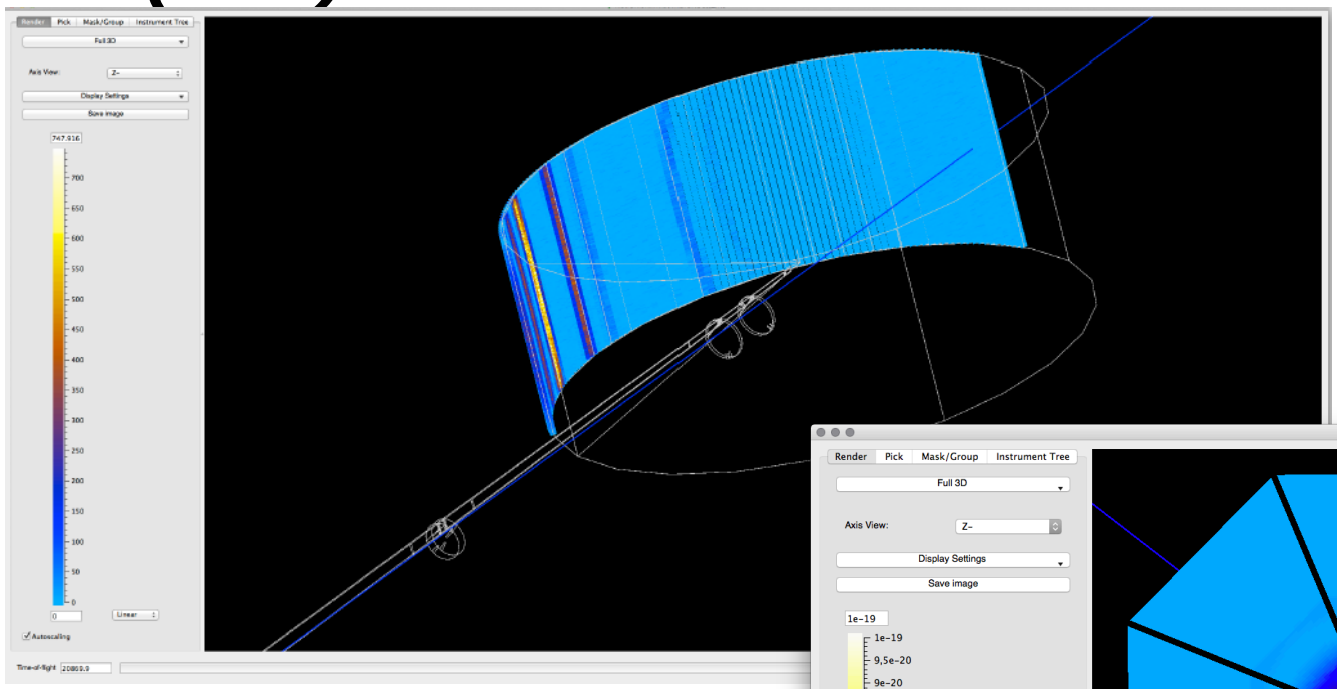


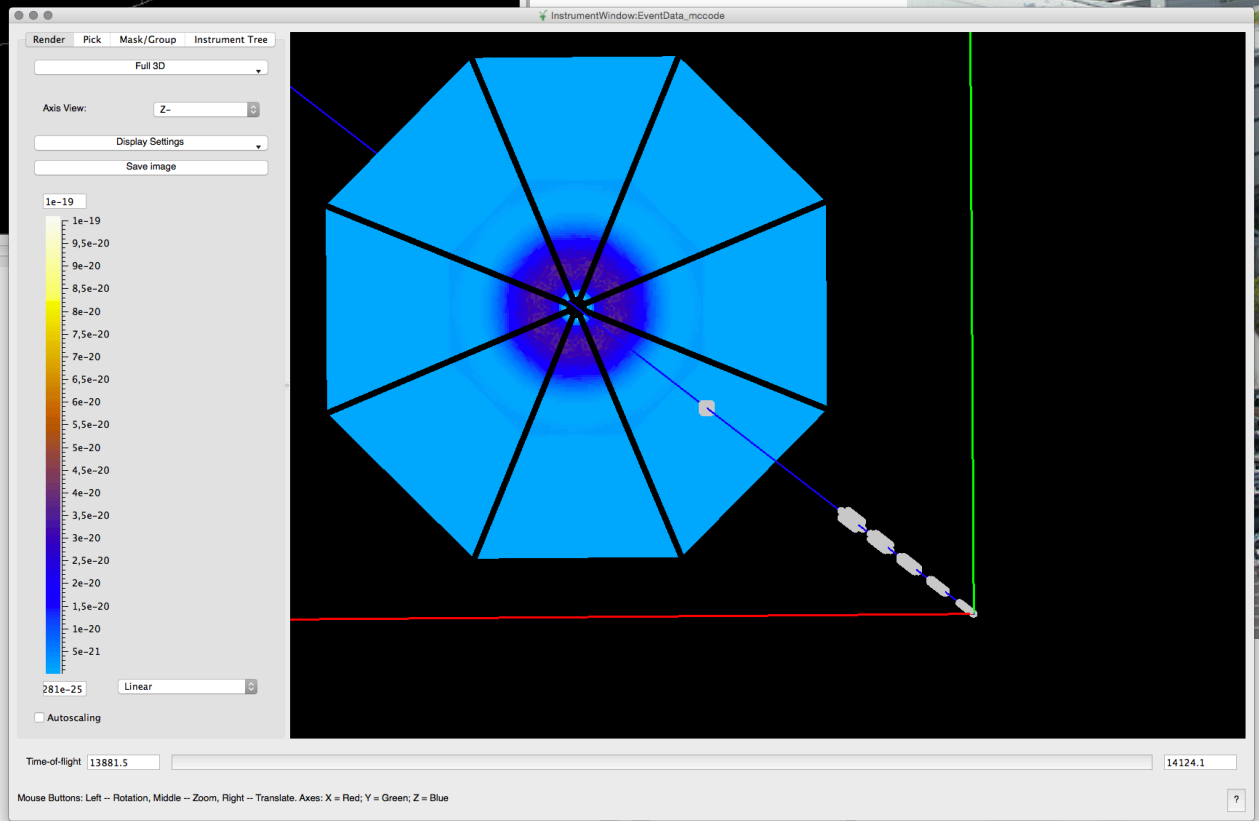
Wiki page on GitHub

McStas – Mantid: Demo Time

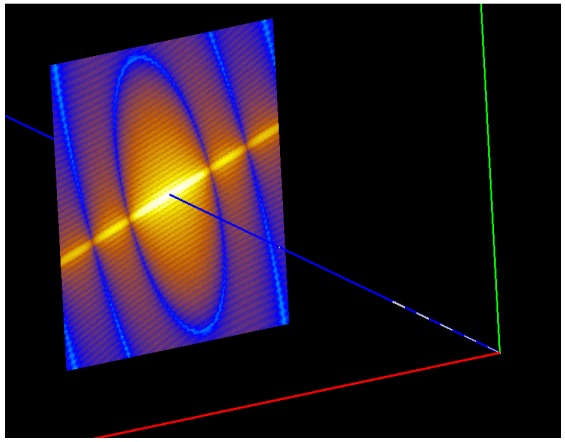
- *See how to use Mantid – McStas interface*

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

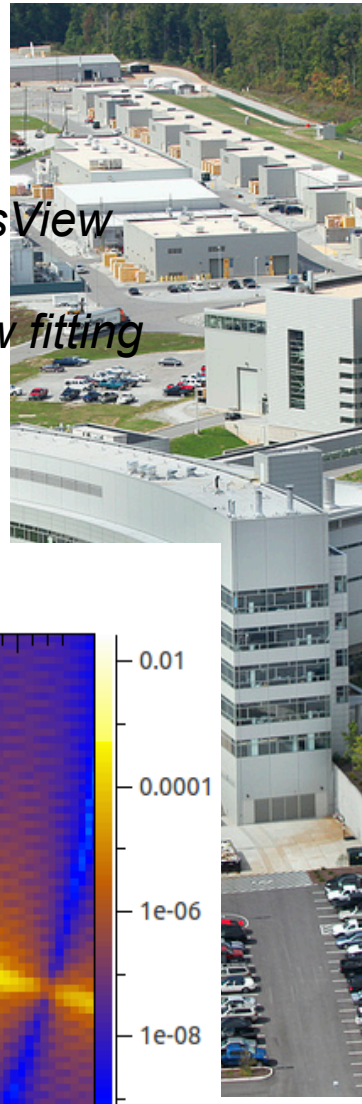


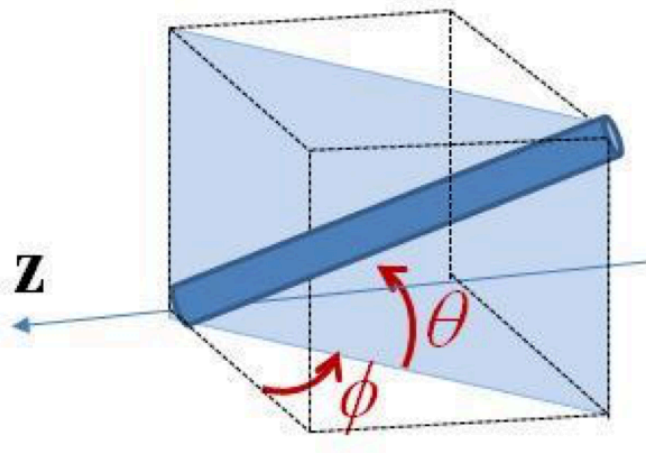


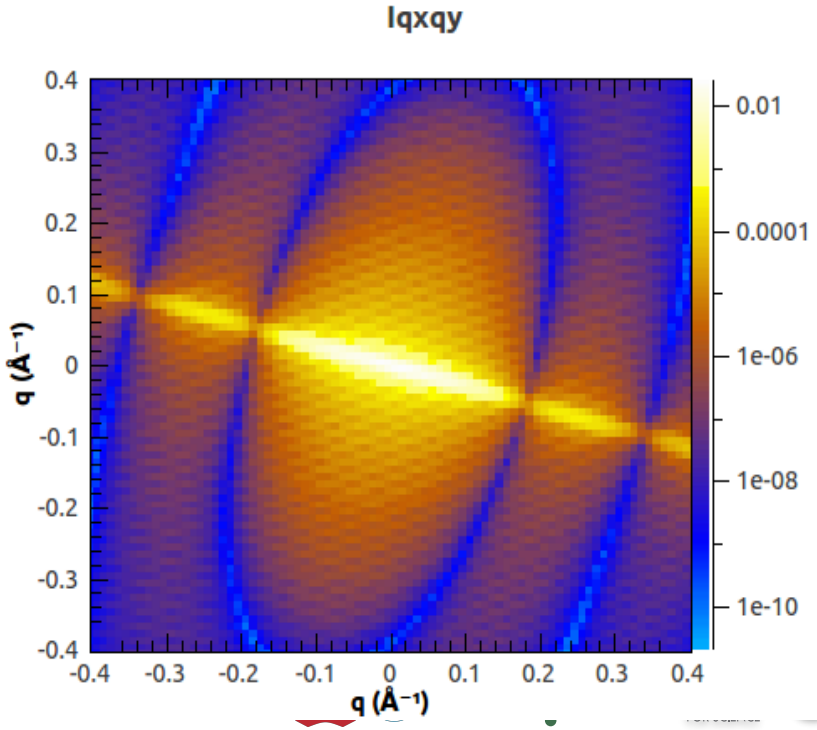
Example: Usage of Mantid algorithms



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

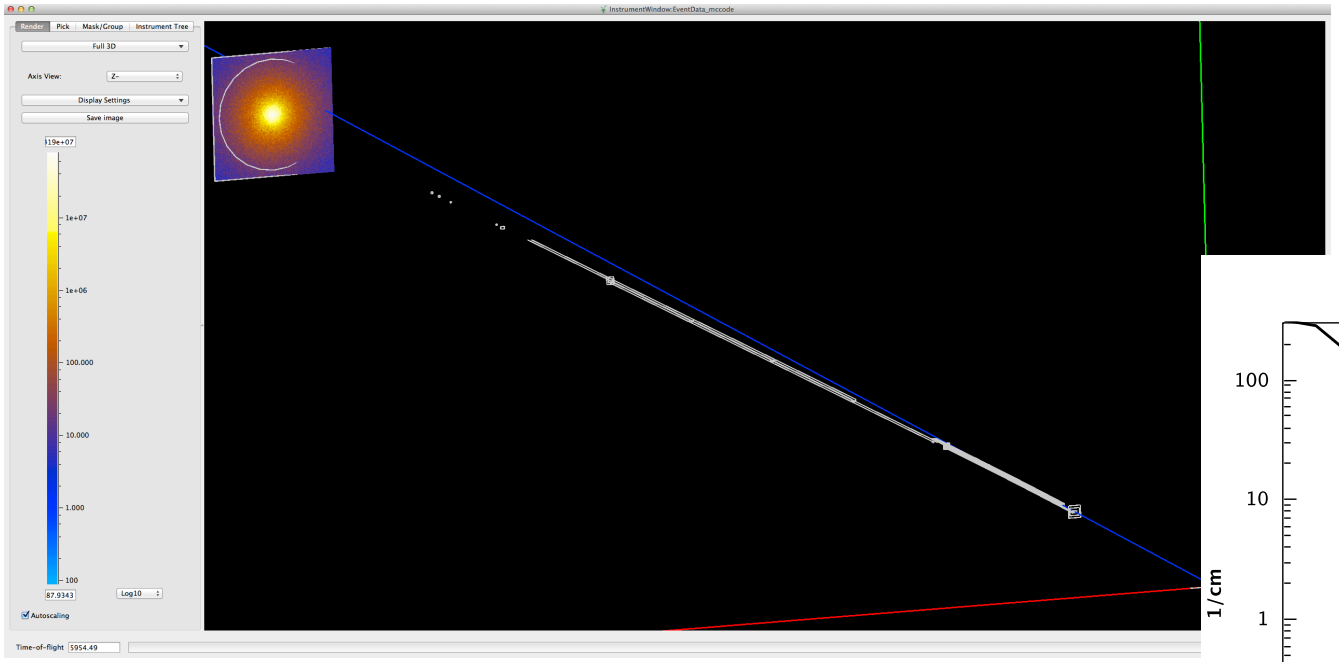


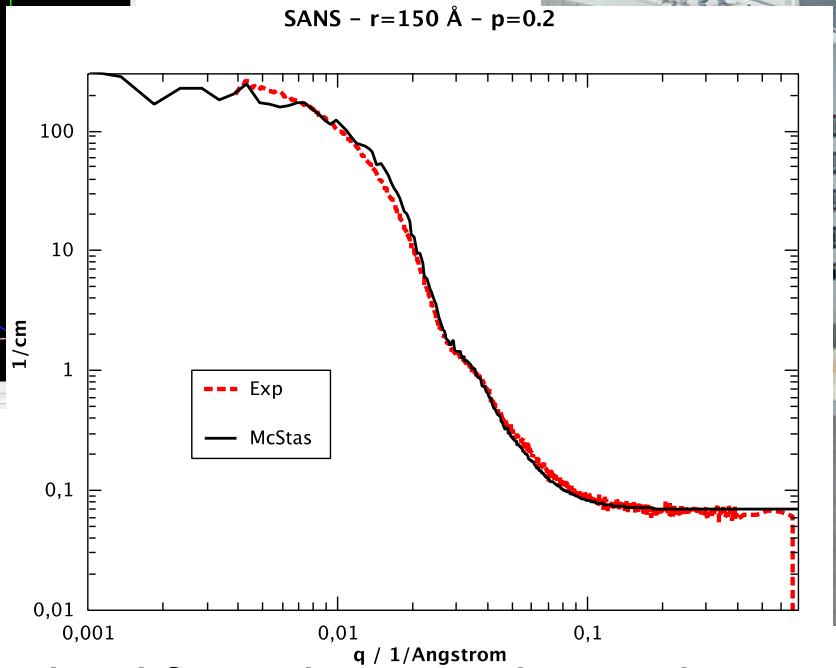




McStas and experimental data: SANS2D

Mantid view of the McStas event data generated for the ISIS_SANS2d.instr file.





Comparison of rescaled scatting intensity I(q) derived from the experimental data and a McStas simulation. Nanospheres of radius 150 Å, polydispersion 0.2.

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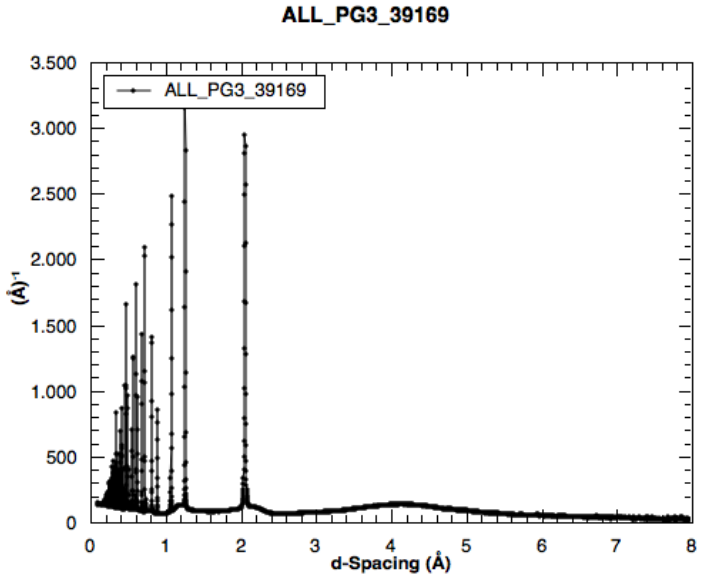
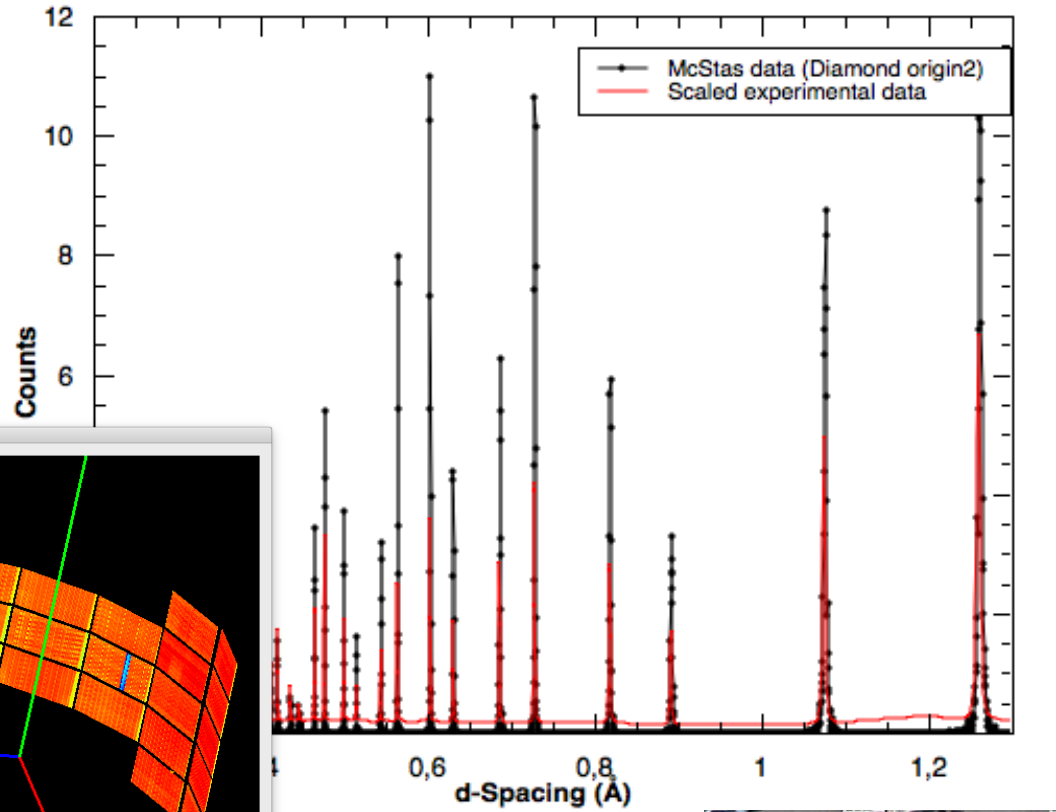
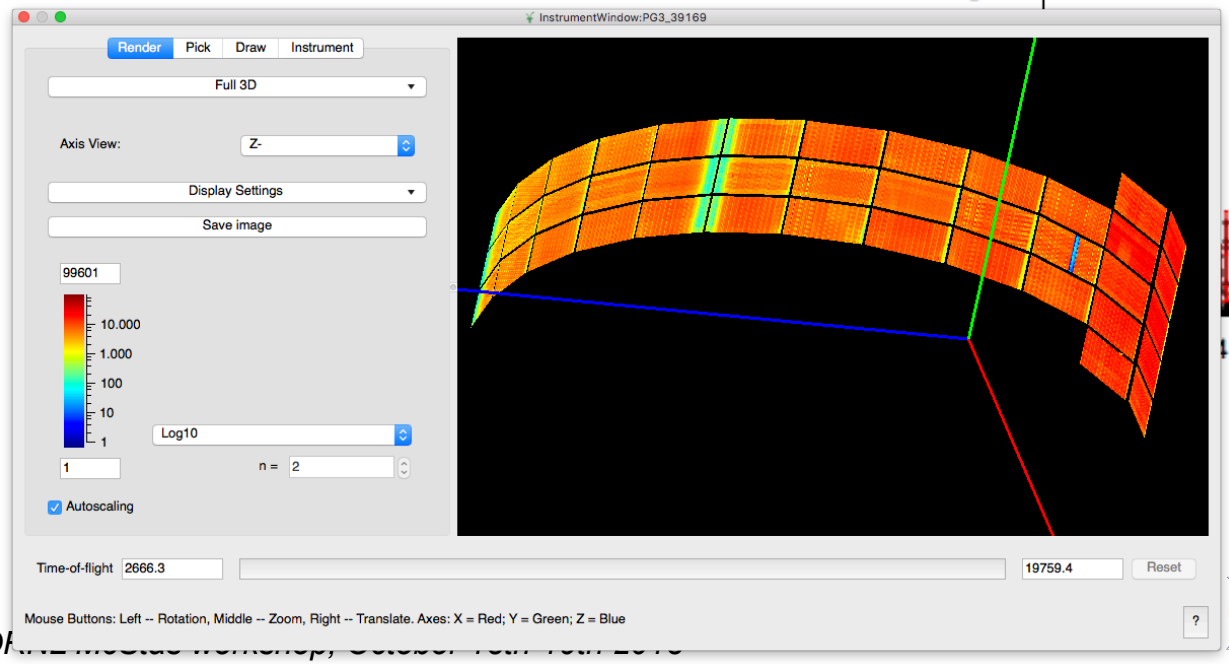
McStas and experimental data: POWGEN







By CelineD @ ESS + SNS collaboration

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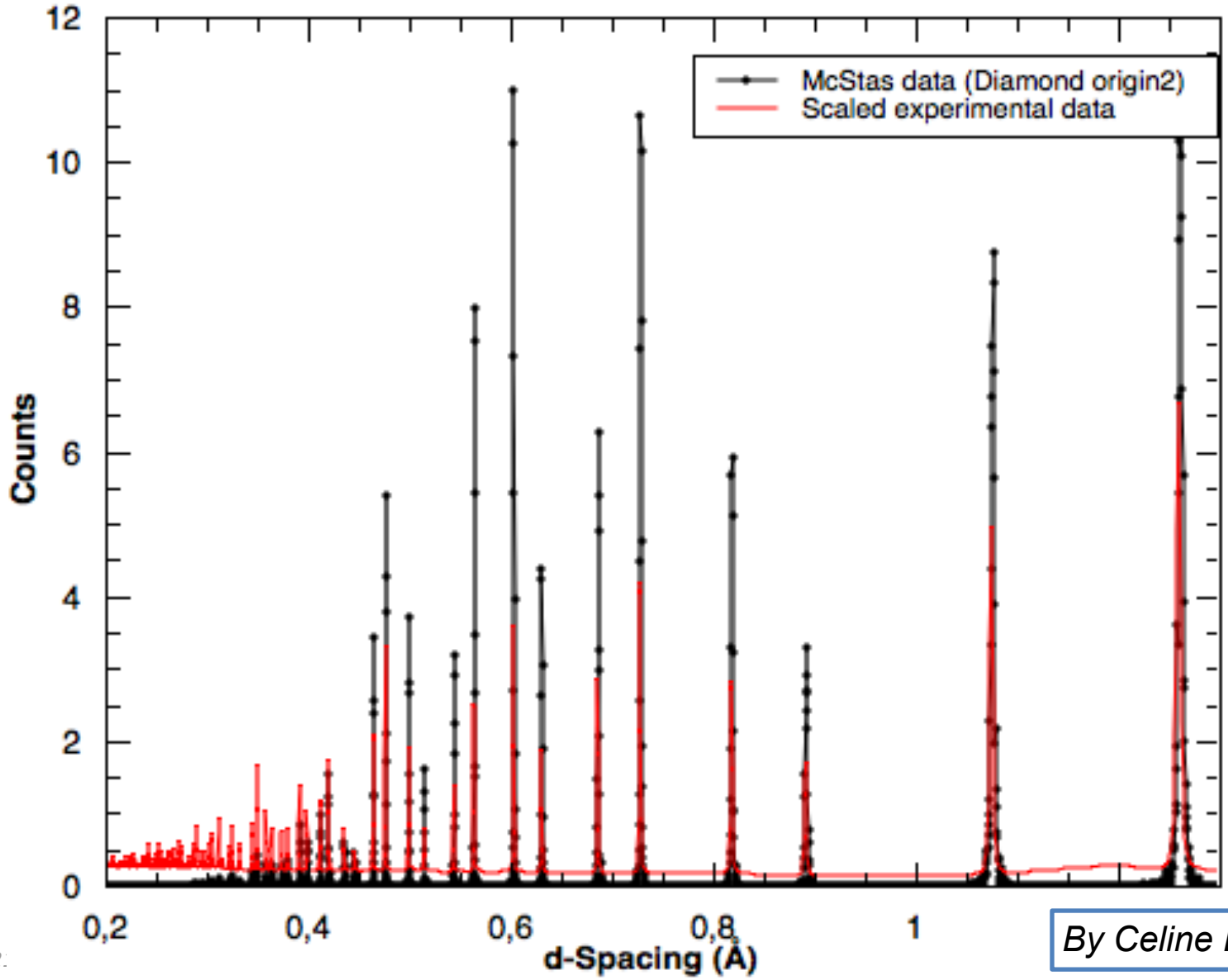
McStas and experimental data: POWGEN



By Celine D @ ESS + SNS collaboration

- *The end …….*

How to use: Generate the IDF

How-to generate McStas event data for Mantid

Step 1. Generate IDF:

- *mcdisplay.pl 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*

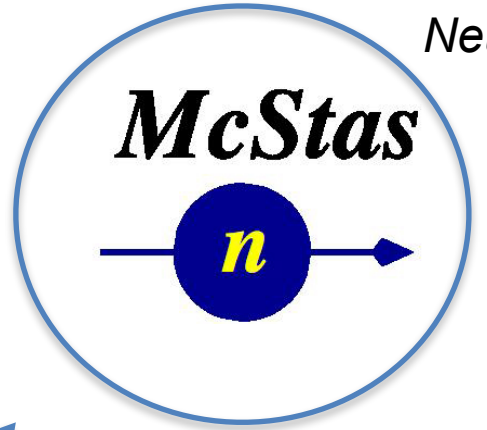
Step 2. Run simulation:

- *templateSANS_Mantid.out --format=Nexus*

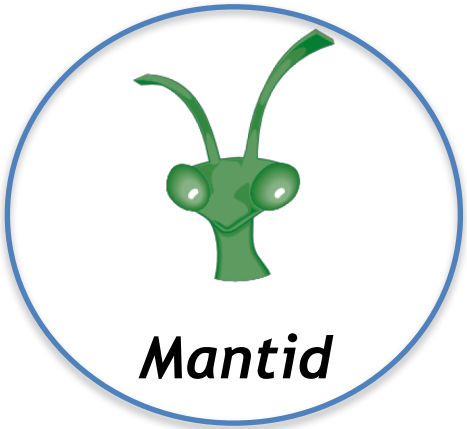
Now IDF is embedded in the NeXus file to be read by Mantid

McStas interoperability

Neutron transport



Reduction



Data analysis