

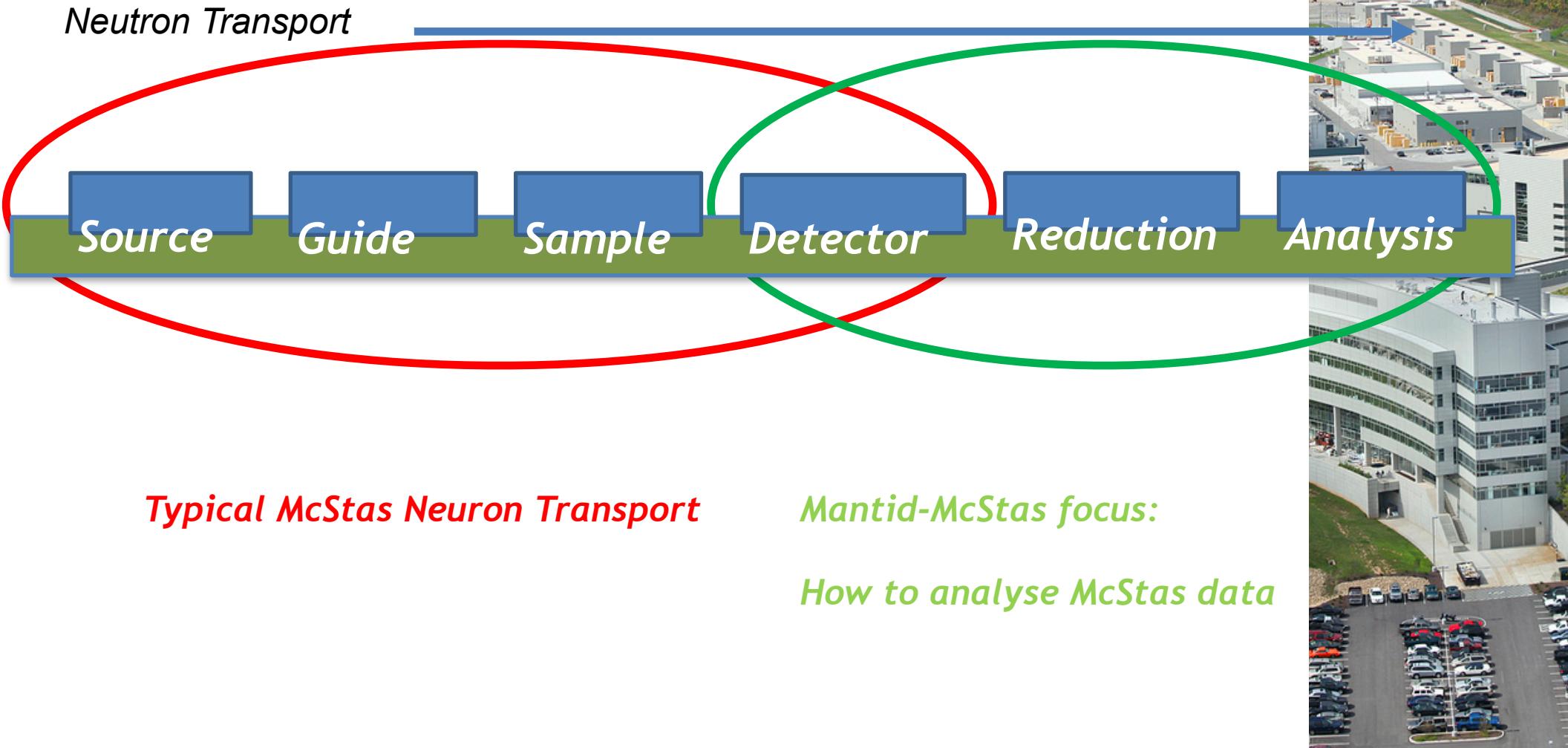
Friday before lunch



Using the McStas + Mantid interface

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

McStas-Mantid and the neutron pipeline



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***

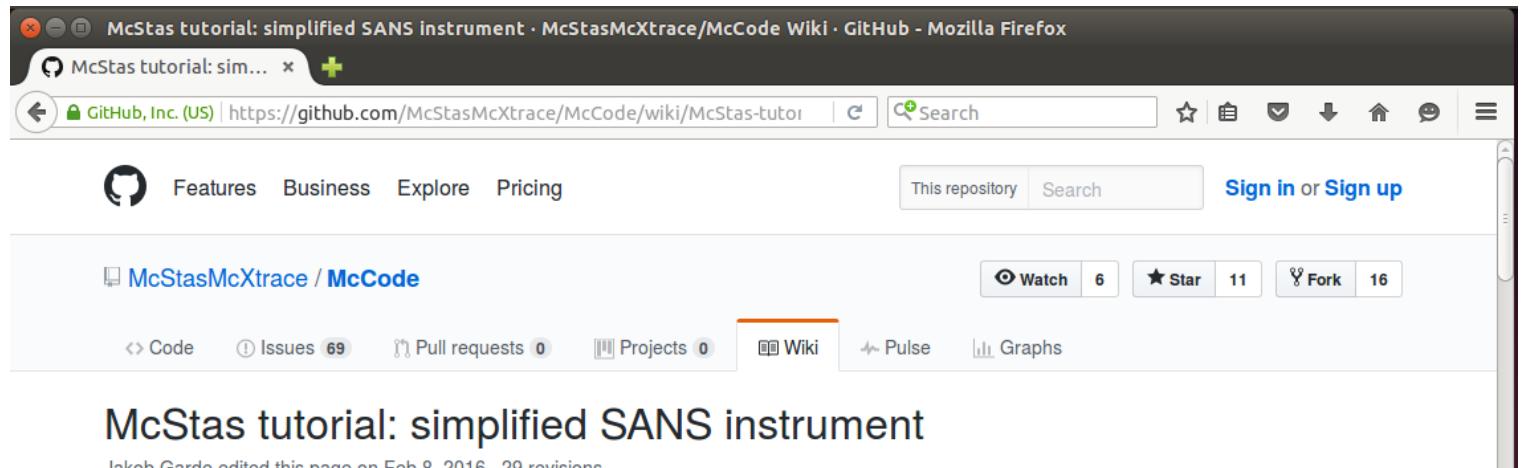


Motivation: II - Benefits for users

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 tutorial: simplified SANS instrument · McStasMcXtrace/McCode Wiki · GitHub - Mozilla Firefox

GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode/wiki/McStas-tutor | Search | Sign in or Sign up

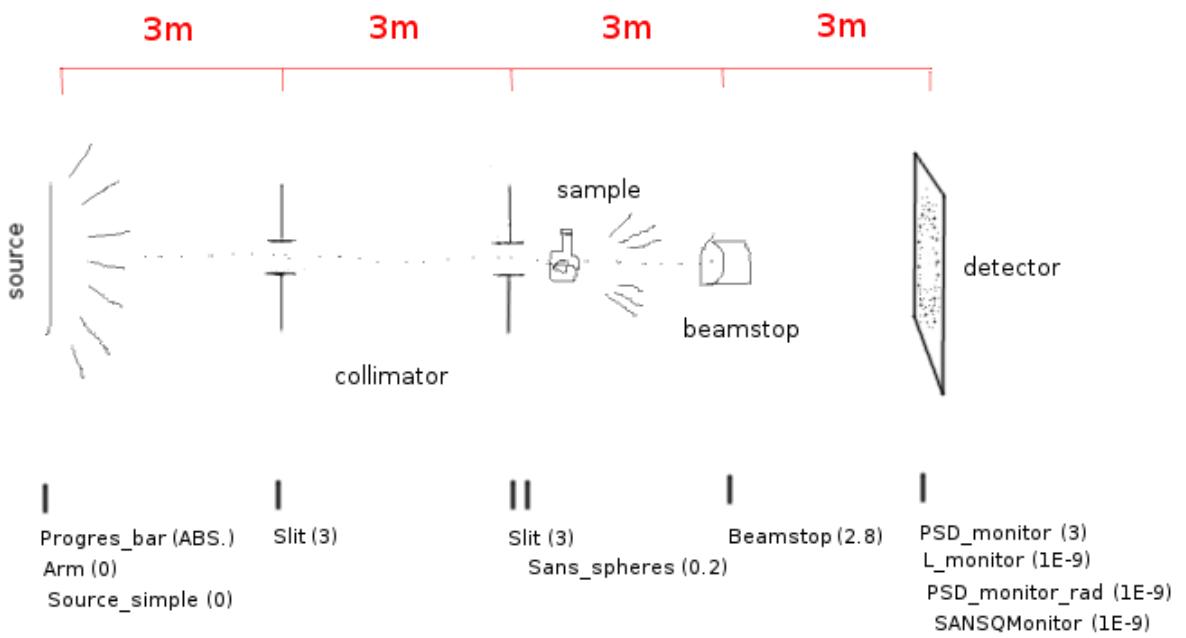
Features Business Explore Pricing This repository Search

McStasMcXtrace / McCode Watch 6 Star 11 Fork 16

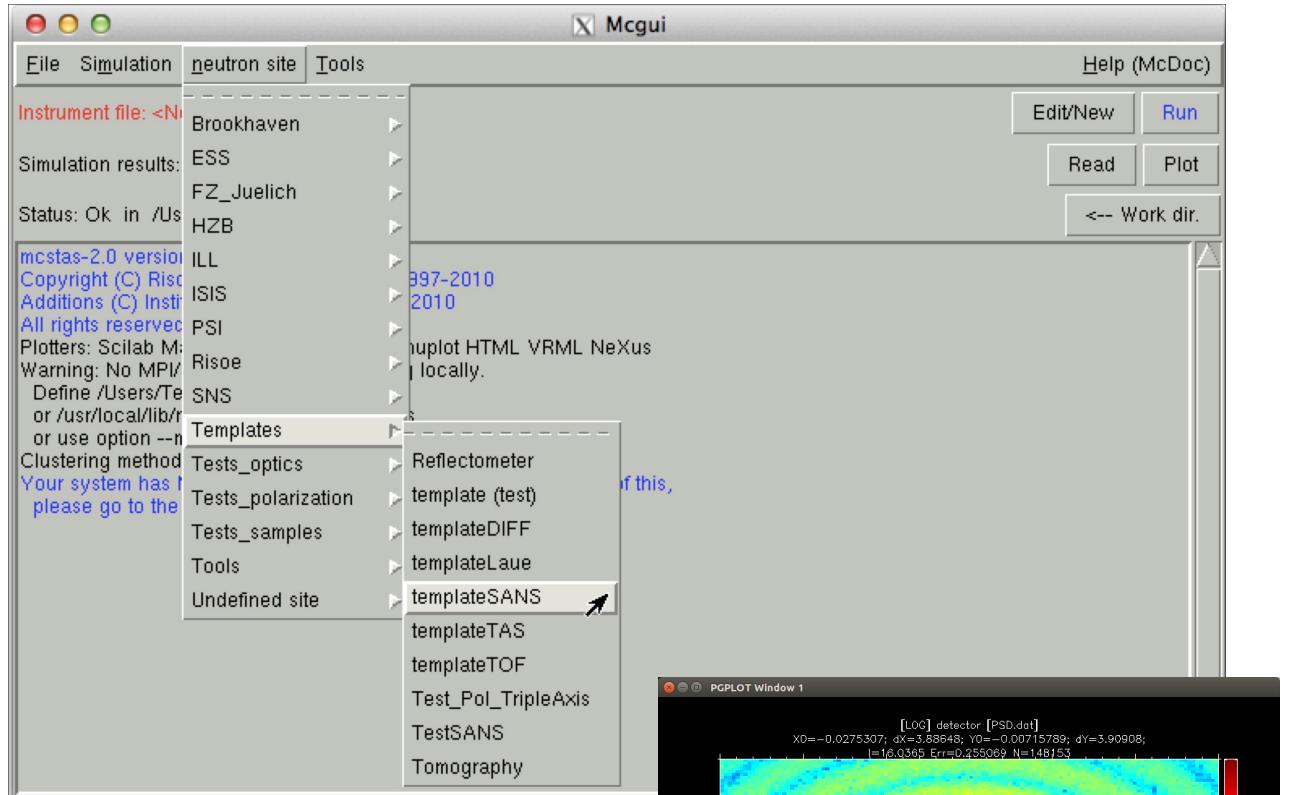
Code Issues 69 Pull requests 0 Projects 0 Wiki Pulse Graphs

McStas tutorial: simplified SANS instrument

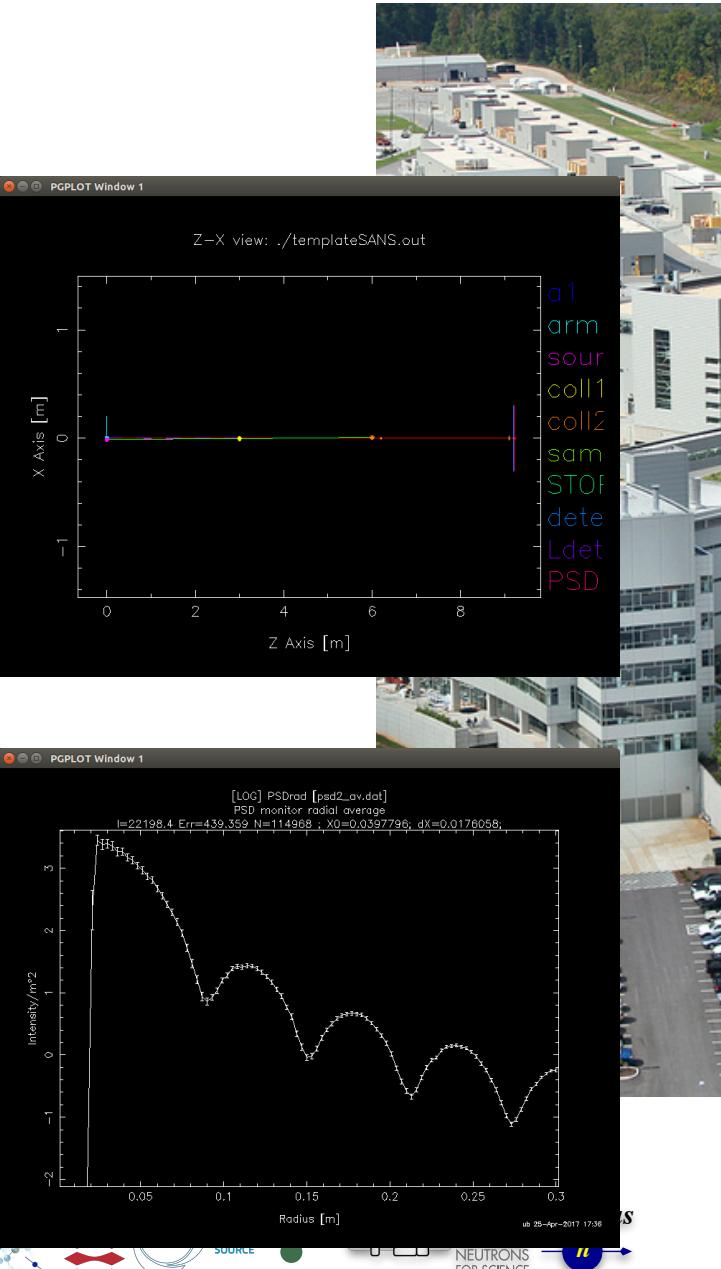
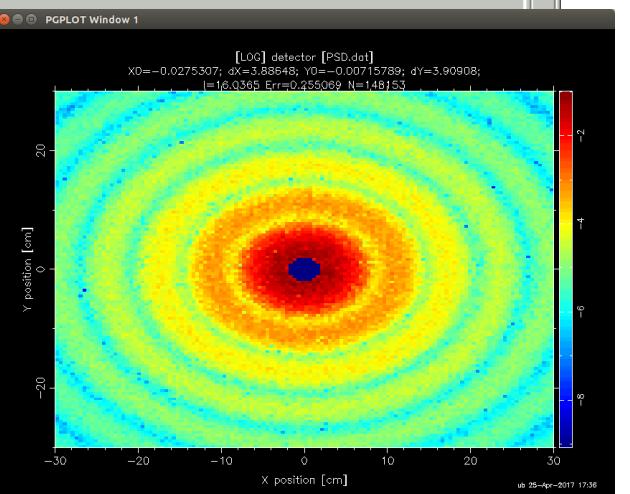
Jakob Garde edited this page on Feb 8, 2016 · 29 revisions



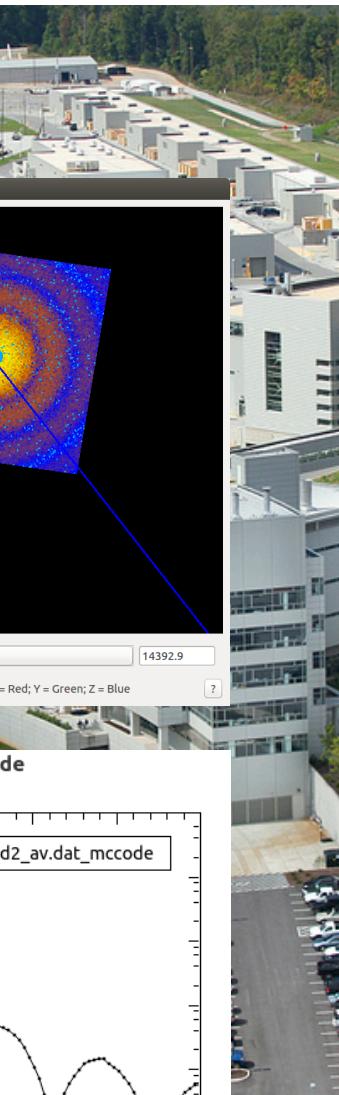
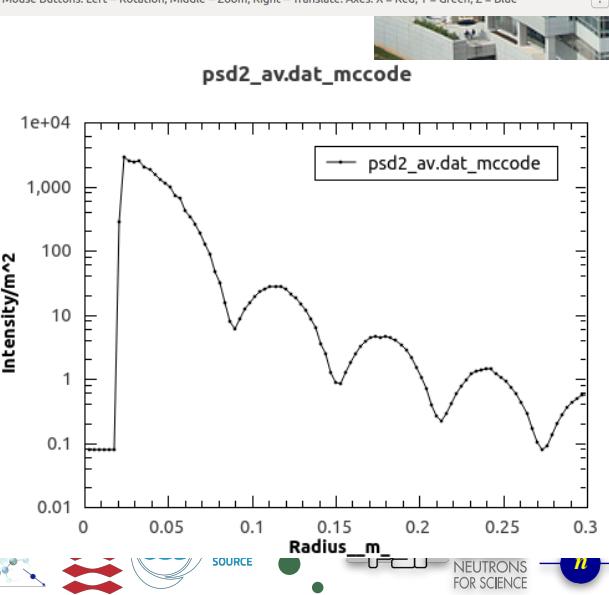
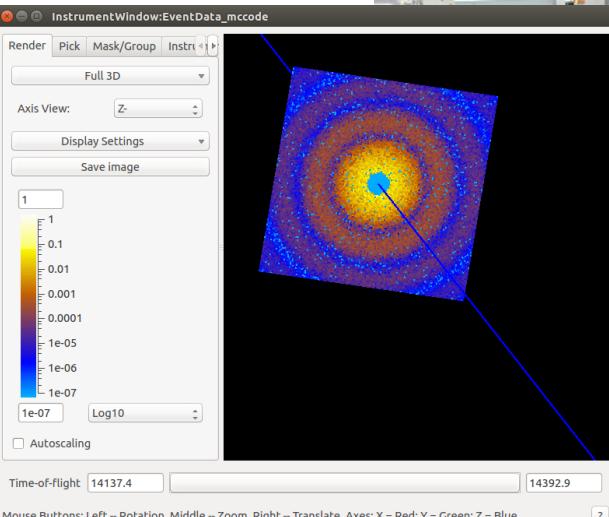
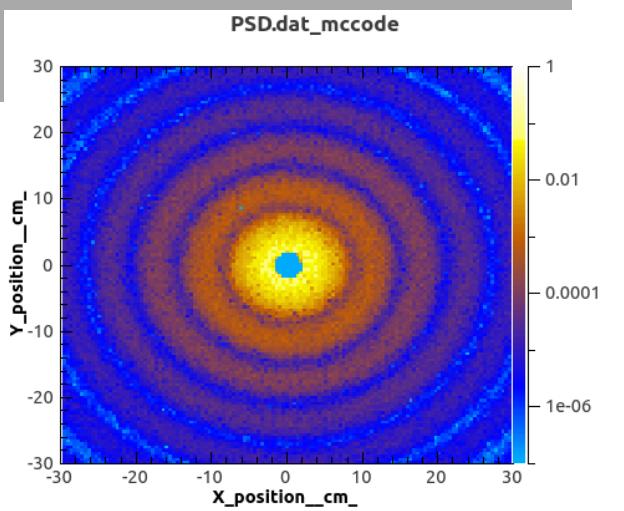
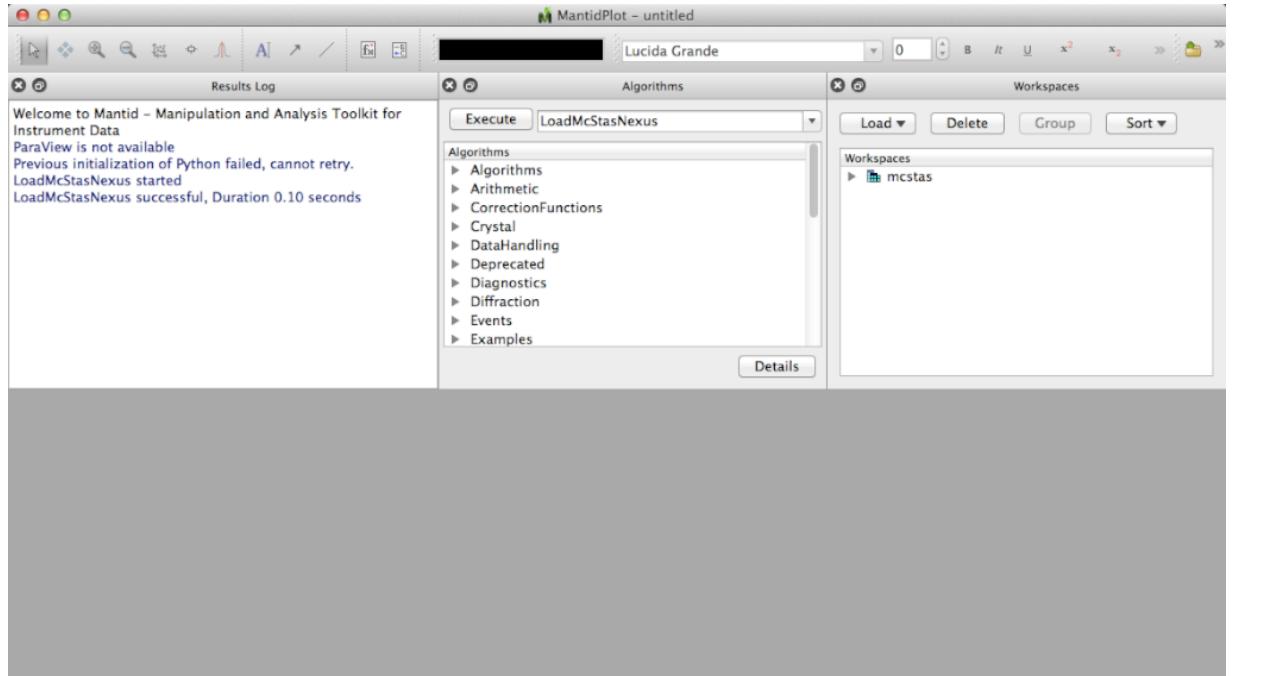
McStas GUI: templateSANS



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

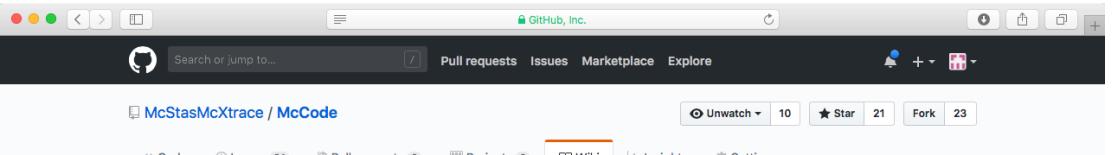


Mantid GUI: templateSANS McStas data



How to use: Online documentation

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



The screenshot shows the GitHub interface for the McStasMcXtrace / McCode repository. It displays the repository's main page with options like 'Code', 'Issues', 'Pull requests', 'Marketplace', and 'Explore'. Below this, there's a summary of activity: 91 issues, 0 pull requests, 0 projects, and a 'Wiki' tab which is currently selected. Other tabs include 'Insights' and 'Settings'. The 'Wiki' tab contains a section titled 'McStas and Mantid'.

McStas and Mantid

Anders Markvardsen edited this page on Feb 27 · 45 revisions

A note on the McStas Mantid integration

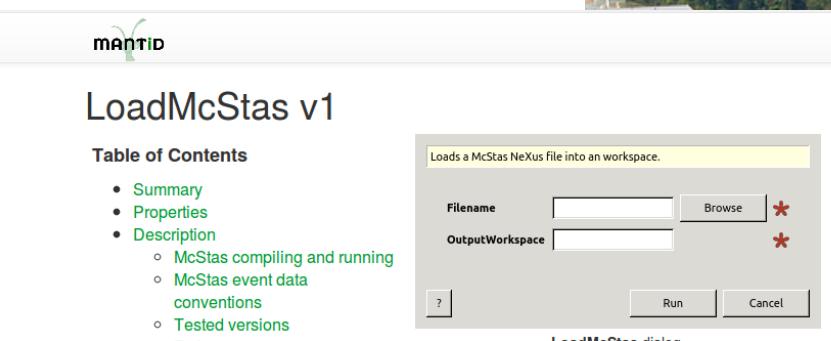
Table of Contents

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 whereon 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.

- Home
- Access to the code tree
- Building McStas McXtrace
- Builds and platforms overview
- Developer literature
- Generate Vitess modules via mctas2vitess
- How McStas McXtrace works overview
- How to update the MCPL shipped with McStas McXtrace
- How to use Eclipse with PyDev
- mcdisplay pyqtgraph
- mcdisplay variants table overview
- mcdisplay webgl
- mcgui
- MCPL related issue on Ubuntu



The screenshot shows the 'LoadMcStas v1' dialog box. It has fields for 'Filename' and 'OutputWorkspace', both with red asterisks indicating they are required. There are 'Run' and 'Cancel' buttons at the bottom. The dialog is overlaid on a background image of a building and trees.

LoadMcStas v1

Table of Contents

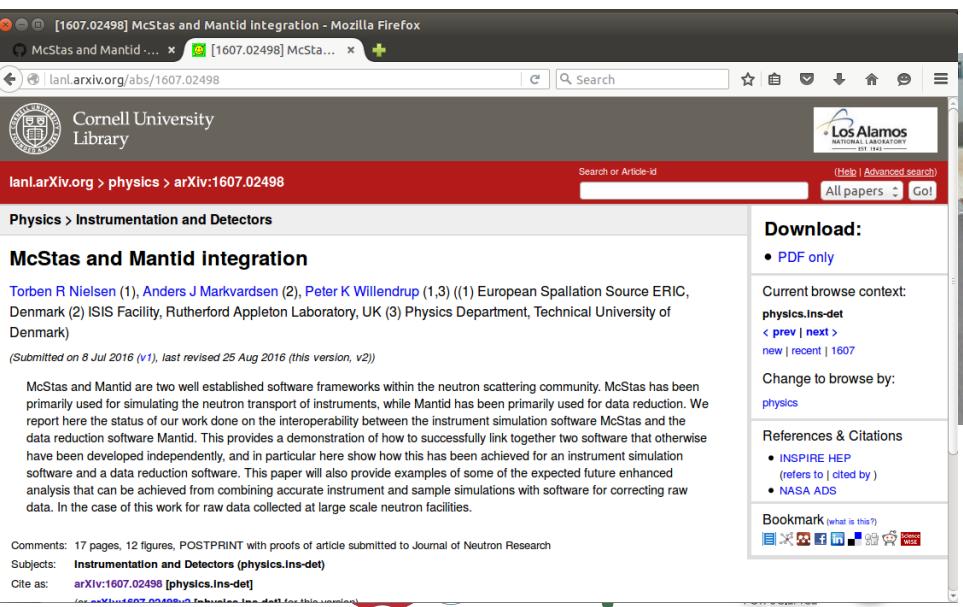
- Summary
- Properties
- Description
 - McStas compiling and running
 - McStas event data conventions
 - Tested versions
 - References

Summary

Loads a McStas Nexus file into an 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.



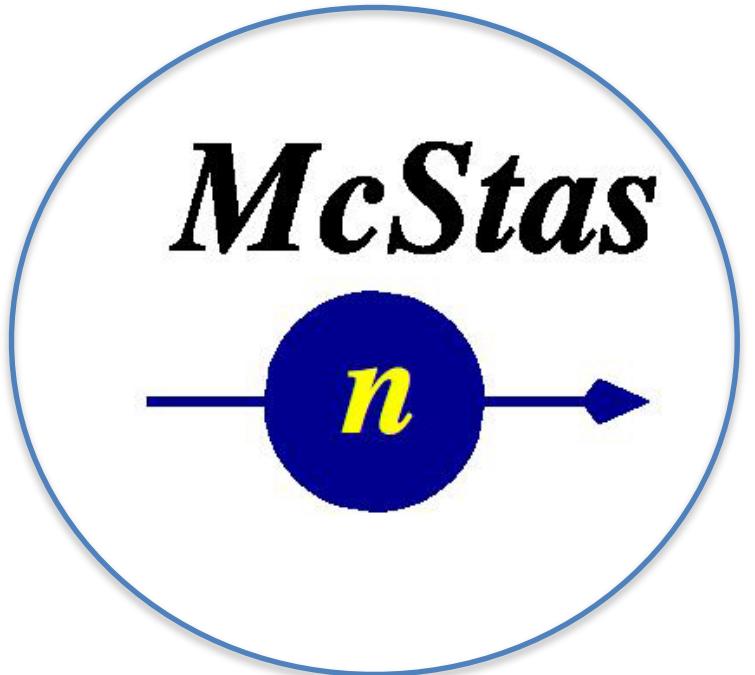
The screenshot shows a browser window displaying the arXiv paper 'McStas and Mantid Integration'. The URL is [lancarxiv.org/abs/1607.02498](https://arxiv.org/abs/1607.02498). The page title is 'Physics > Instrumentation and Detectors'. The abstract discusses the interoperability between McStas and Mantid. The right sidebar includes sections for 'Download', 'Current browse context', 'Change to browse by', 'References & Citations', and 'Bookmark'.

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

Mantid



- 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 pixel id & time for each event
- mcdisplay can auto-generate an IDF

McStas Nexus file

HDFView 2.9

File Window Tools Help

Recent Files /home/ub/tmp/McStas_Event/McStas/Exp_Data/mccode.h5

Clear Text

Event data

IDF xml data

Instrument XML Data:

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- IDF generated using McStas McDisplay and the Mantid backend -->
<!-- For help on the notation used to specify an Instrument Definition File see
http://www.mantidproject.org/IDF -->
<instrument name="ISIS_SANS2d_Mantid.out" valid-from = "1900-01-31 23:59:59"
valid-to = "2100-01-31 23:59:59" last-modified="Tue Apr 4 14:17:50 2017">
<defaults>
    <length unit="meter"/>
    <angle unit="degree"/>
    <reference-frame>
        <!-- The z-axis is set parallel to and in the direction of the beam. The
y-axis points up and the coordinate system is right handed. -->
        <along-beam axis="z"/>
        <pointing-up axis="y"/>
        <handedness val="right"/>
    </reference-frame>
    <default-view axis-view="z"/>
</defaults>
```

LIST OF PHYSICAL COMPONENTS (which the instrument consists of) >

Table View Data:

	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	18720.0	0.041270...
7	0.022012...	0.058801...	-0.08114...	7.0	15	
8	8.530934...	0.012643...	-0.03070...	8.0	17	
9	6.984646...	-0.00867...	0.012712...	9.0	18	
10	0.009140...	-0.07853...	-0.07291...	10.0	15	
11	7.150334...	-0.01082...	0.005151...	11.0	18	
12	0.001010...	0.457856...	0.087702...	12.0	21	
13	0.004965...	0.003146...	-0.04262...	13.0	16	
14	8.629457...	-0.03193...	-0.02392...	14.0	17	
15	7.072494...	0.015294...	-0.01158...	15.0	17	
16	3.898581...	-2.38144...	0.011657...	16.0	18	
17	3.479036...	-0.02370...	-0.00281...	17.0	18	
18	5.870513...	0.006430...	0.00673...	18.0	18	
19	0.010325...	-0.07164...	-0.01926...	19.0	17	
20	3.191063...	-0.00829...	-0.00252...	20.0	18	
21	3.746034...	-0.00570...	0.011053...	21.0	18	
22	0.003724...	0.038904...	0.029156...	22.0	19	
23	3.316878...	-0.00442...	6.097504...	23.0	18	
24	0.023456...	-0.03083...	0.084904...	24.0	21	
25	0.001505...	0.031248...	-0.02562...	25.0	17	

Data View Data:

```
data (22370, 2)
String, length = 7891, 1
Number of attributes = 0
```

Log Info Metadata

templateSANS.instr vs *templateSANS_Mantid.instr*



templateSANS.instr x templateSANS_Mantid.instr x UNREGISTERED

```

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.
33     6, target_index=2)
34 AT (0,0,0.2) RELATIVE coll2
35
36 COMPONENT STOP = Beamstop(
37     radius = 0.02)
38 AT (0, 0, 2.9) RELATIVE sample

```

Line 1, Column 1 Spaces: 2 Plain Text

templateSANS.instr x templateSANS_Mantid.instr x UNREGISTERED

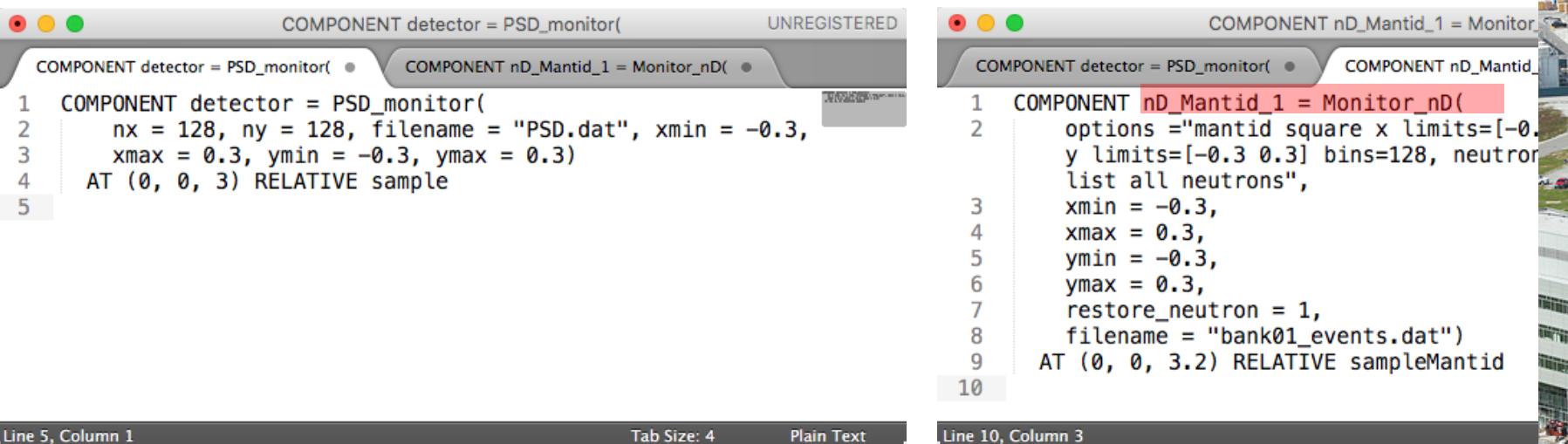
```

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 nD_Mantid_1 = Monitor_nD(      COMPONENT nD_Mantid_1 = Monitor_nD(
1  COMPONENT detector = PSD_monitor(          options ="mantid square x limits=[-0.
2    nx = 128, ny = 128, filename = "PSD.dat", xmin = -0.3,
3    xmax = 0.3, ymin = -0.3, ymax = 0.3)      y limits=[-0.3 0.3] bins=128, neutron
4    AT (0, 0, 3) RELATIVE sample            list all neutrons",
5                                         xmin = -0.3,
                                         xmax = 0.3,
                                         ymin = -0.3,
                                         ymax = 0.3,
                                         restore_neutron = 1,
                                         filename = "bank01_events.dat")
                                         AT (0, 0, 3.2) RELATIVE sampleMantid
                                         10
Line 5, Column 1                                     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**(....)"*

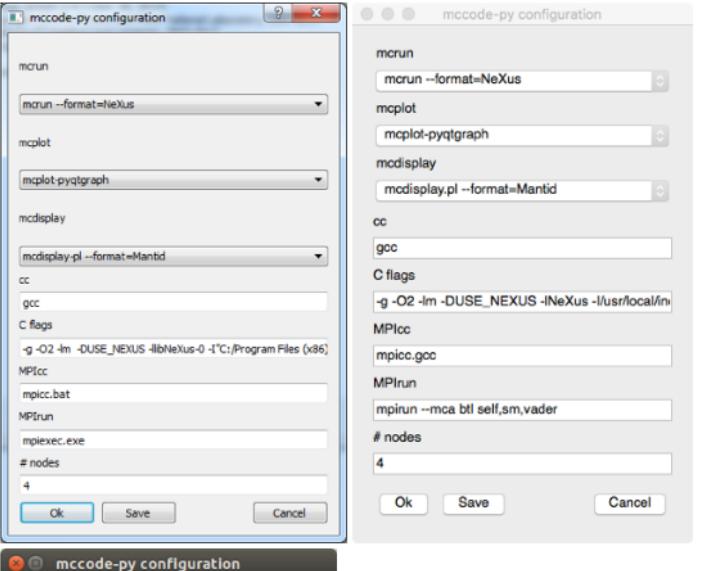
*In the McStas instrument file the sample must be named "**sampleMantid**"*

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

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



How to run simulation


McStas GUI
 Generating McStas event data for Mantid can be achieved from the McStas GUI `mogui`. 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 `mogui` 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 -lNexus -O -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

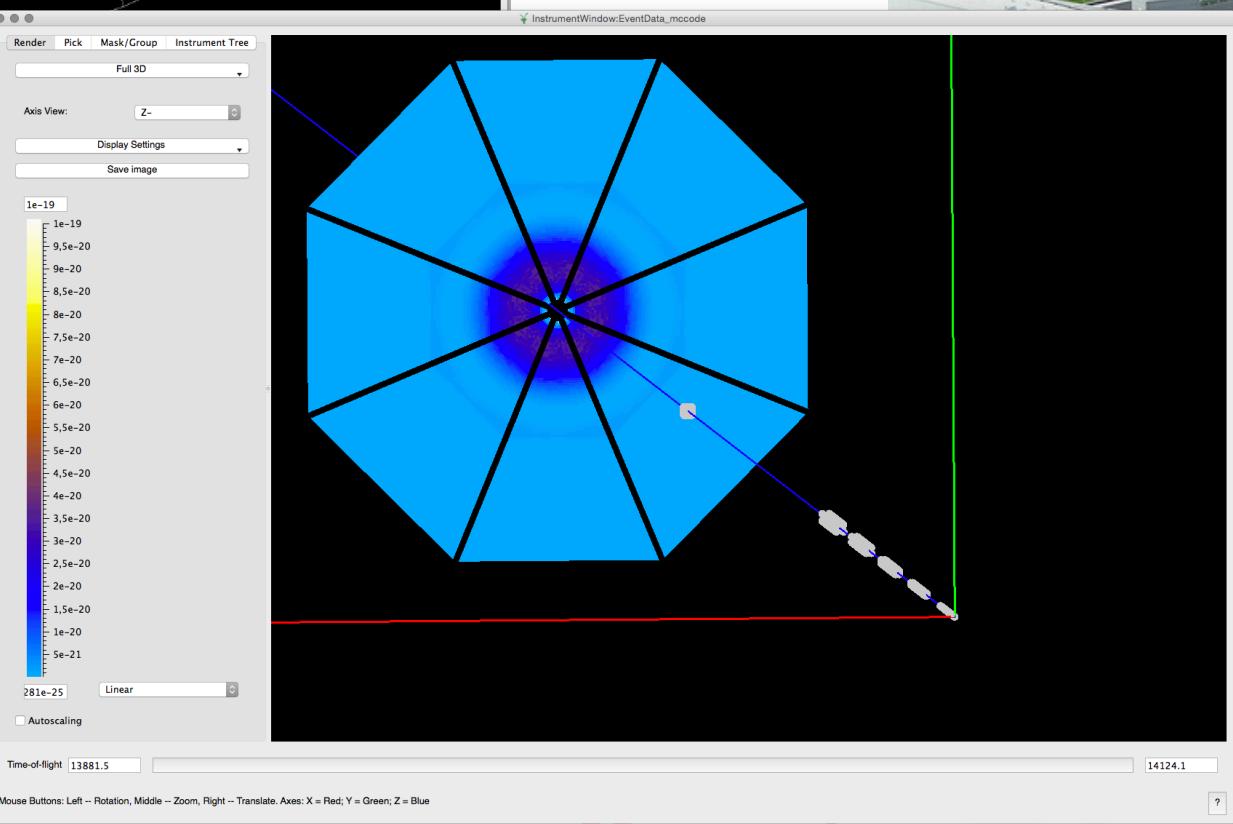
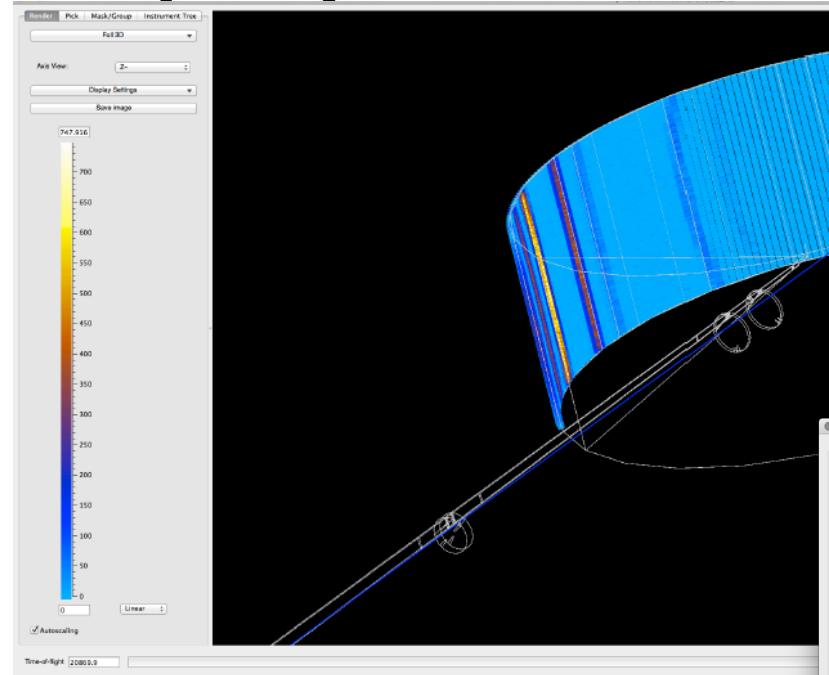


McStas – Mantid: Demo Time

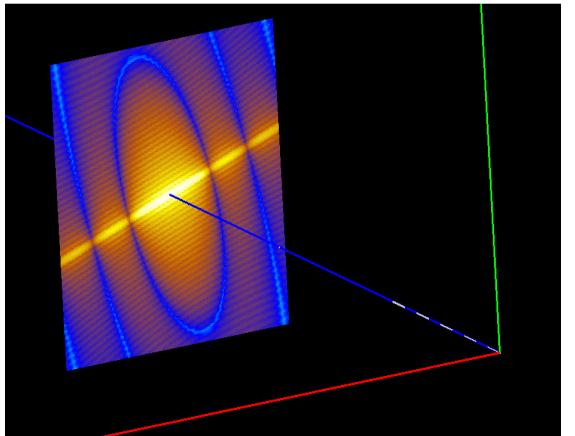
- See how to use Mantid – McStas interface



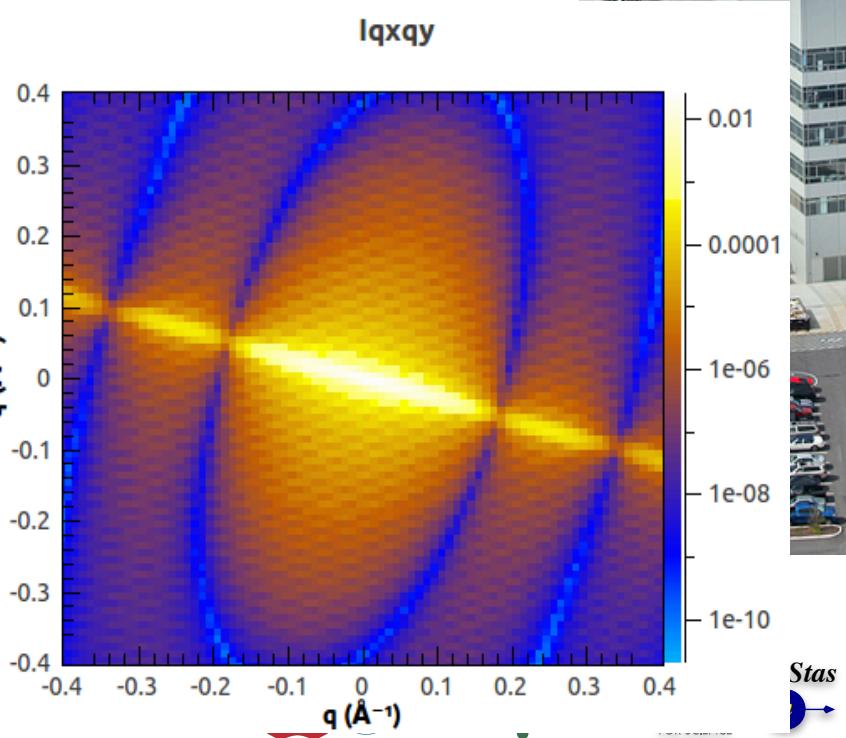
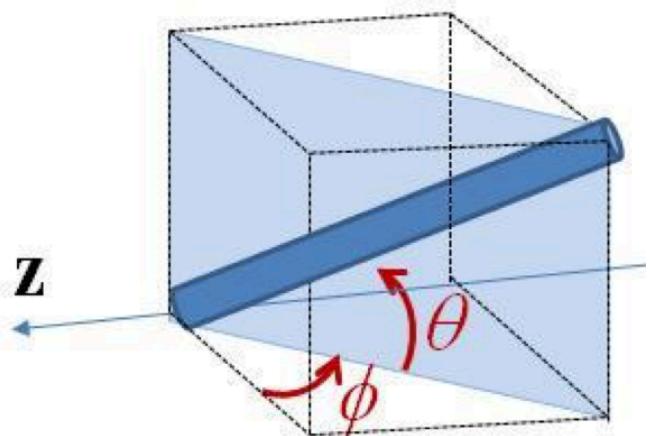
Examples of detectors: IN5 (ILL) and LoKI (ESS)



Example: Usage of Mantid algorithms

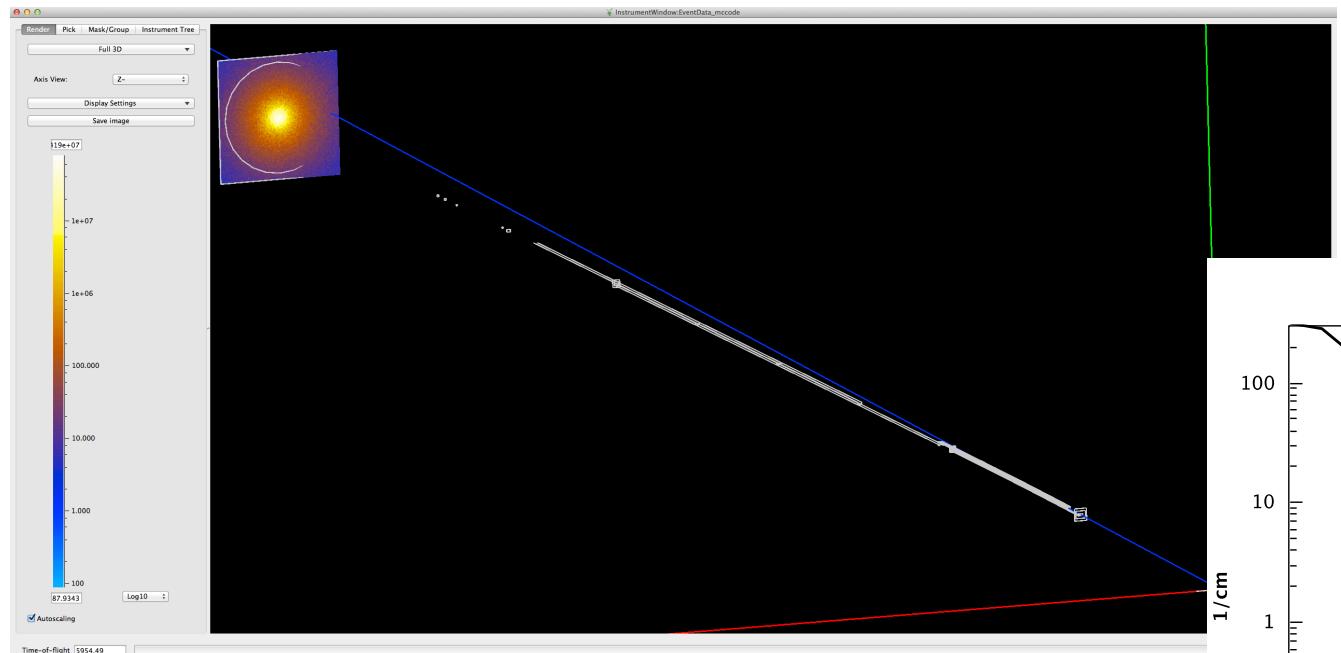


- McStas – Mantid
- 2D scattering kernel from SasView
- 2D reduction in Mantid: Qxy
- Can be send back to SasView fitting

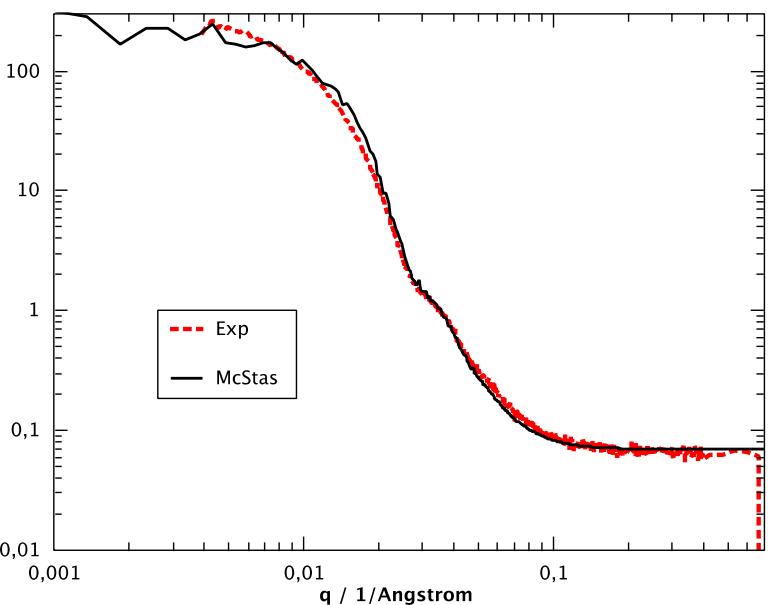


McStas and experimental data: SANS2D

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



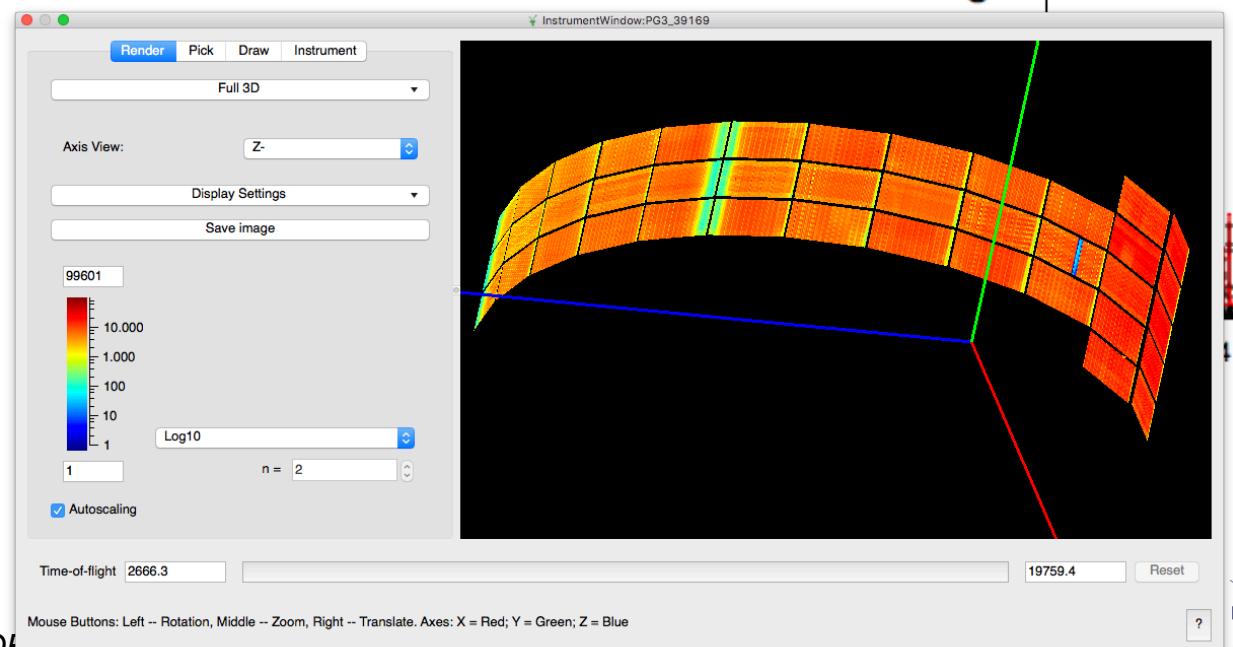
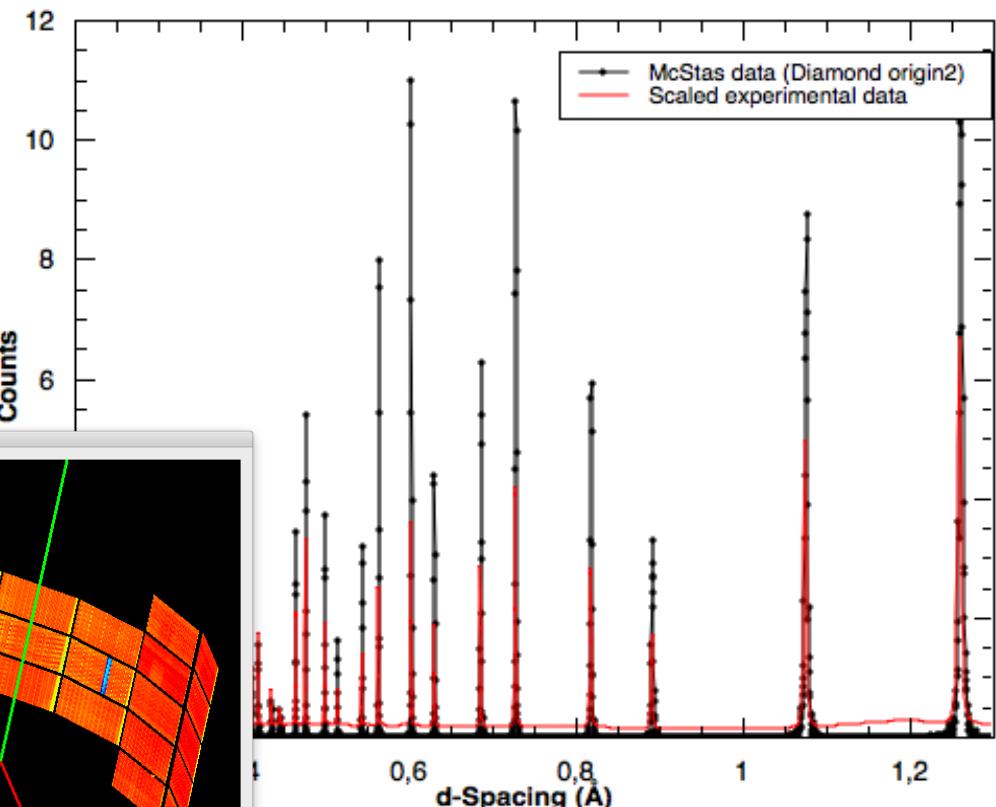
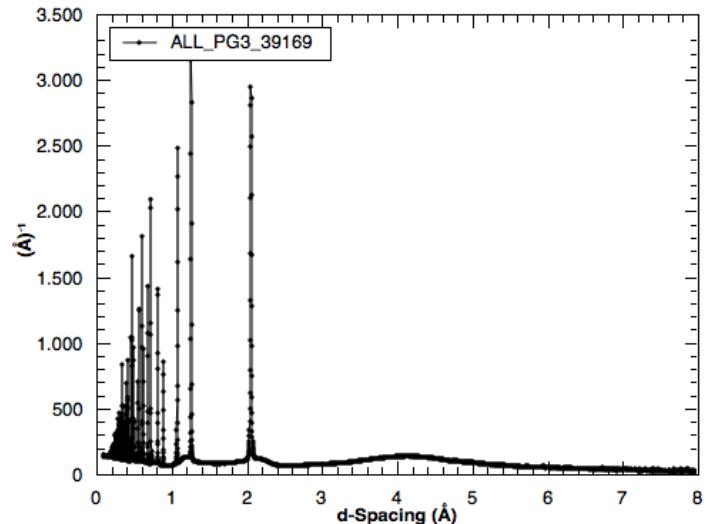
SANS - $r=150 \text{ \AA}$ - $p=0.2$



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

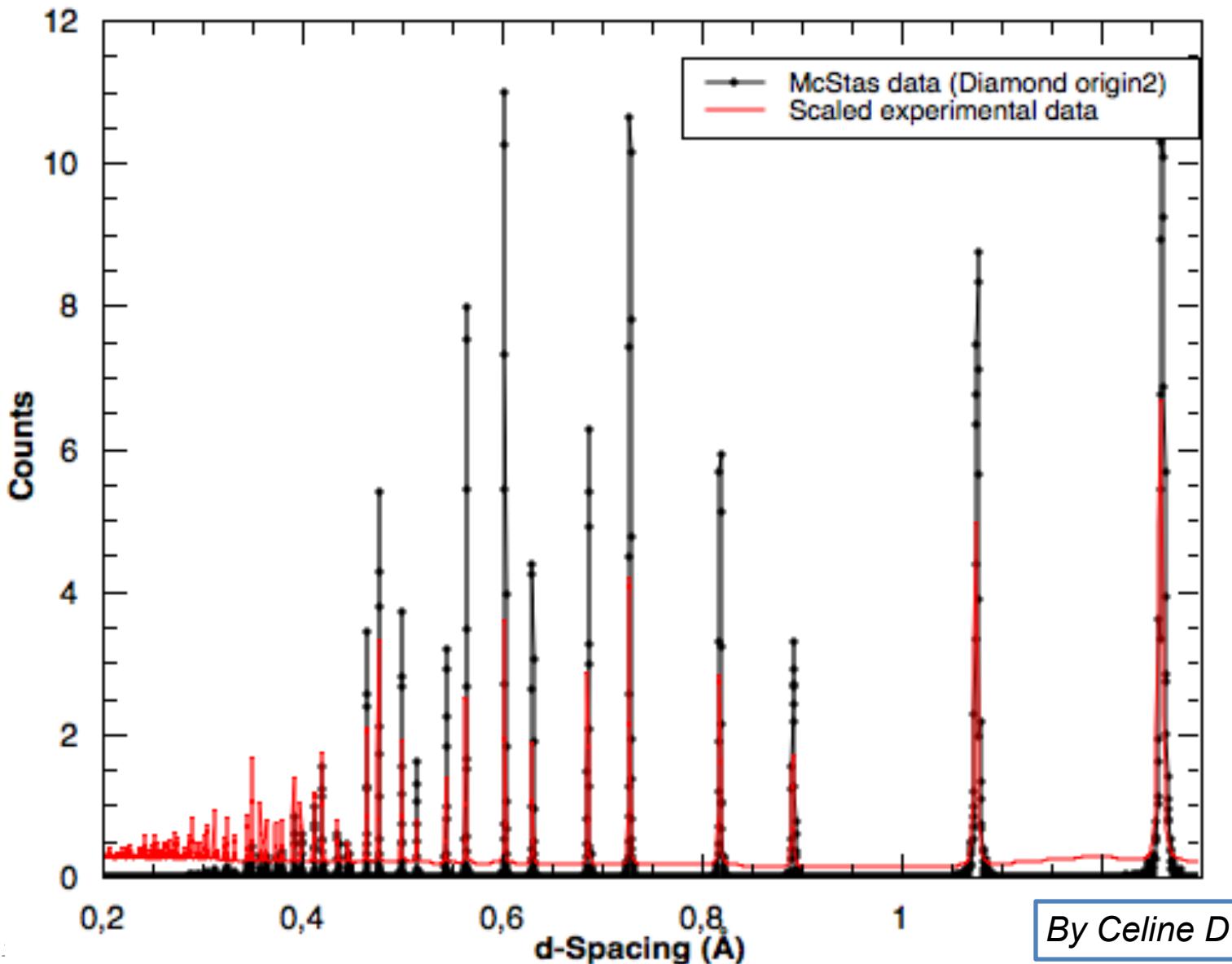
McStas and experimental data: POWGEN

ALL_PG3_39169



By CelineD @ 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.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 -INexus -Im`

Step 2. Run simulation:

- `templateSANS_Mantid.out --format=Nexus`

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



McStas interoperability

