

McStas - Mantid

Torben Nielsen

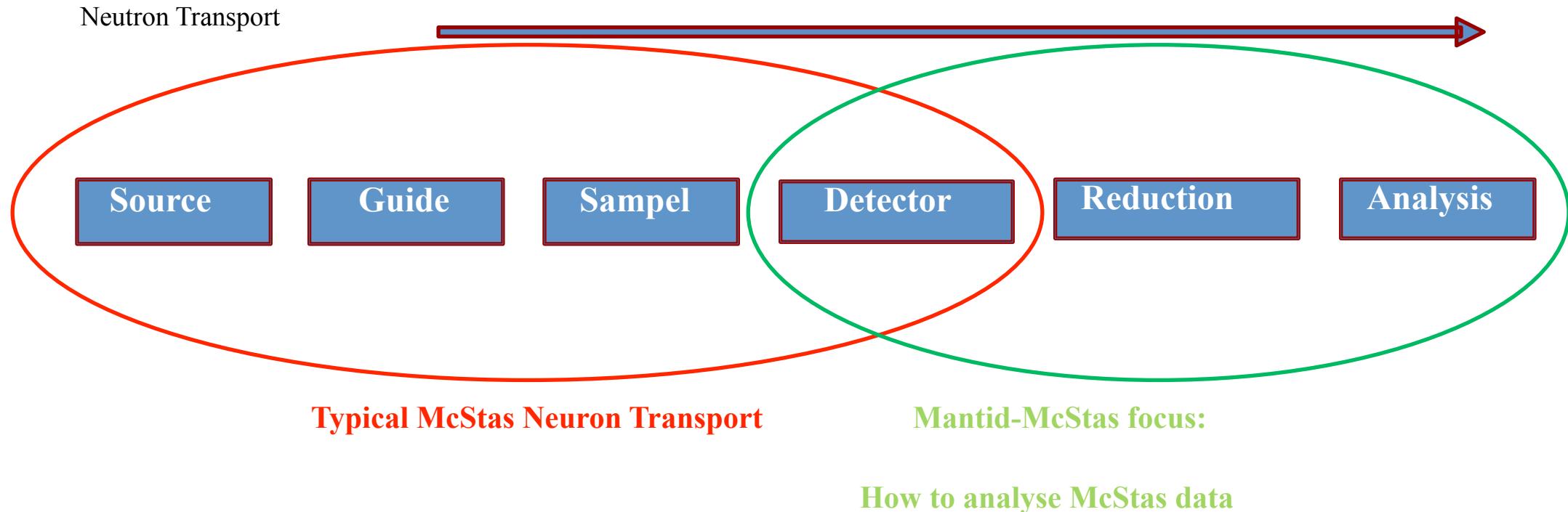
Anders Markvardsen

Peter Willendrup

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Comparison

Classic McStas

Post processing:
iFit/ Matlab/ own code

mcstas - plot



mcstas - transport

Mantid-McStas

Post processing:
Mantid algorithms

mantidplot



mcstas - transport

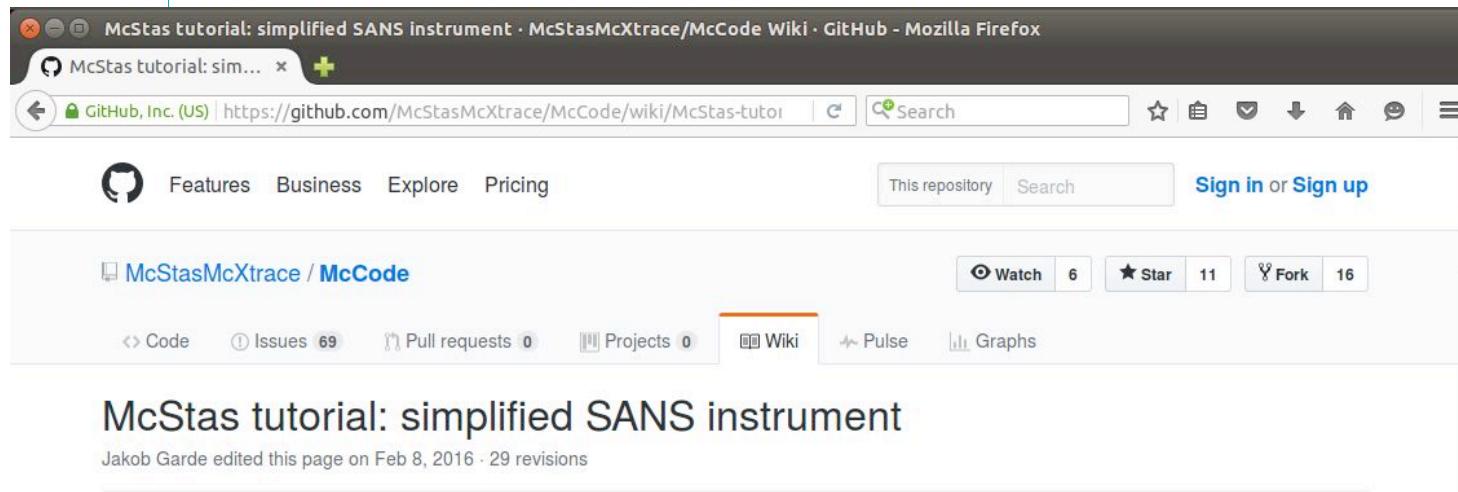
3

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)

4

Illustration: simplified SANS



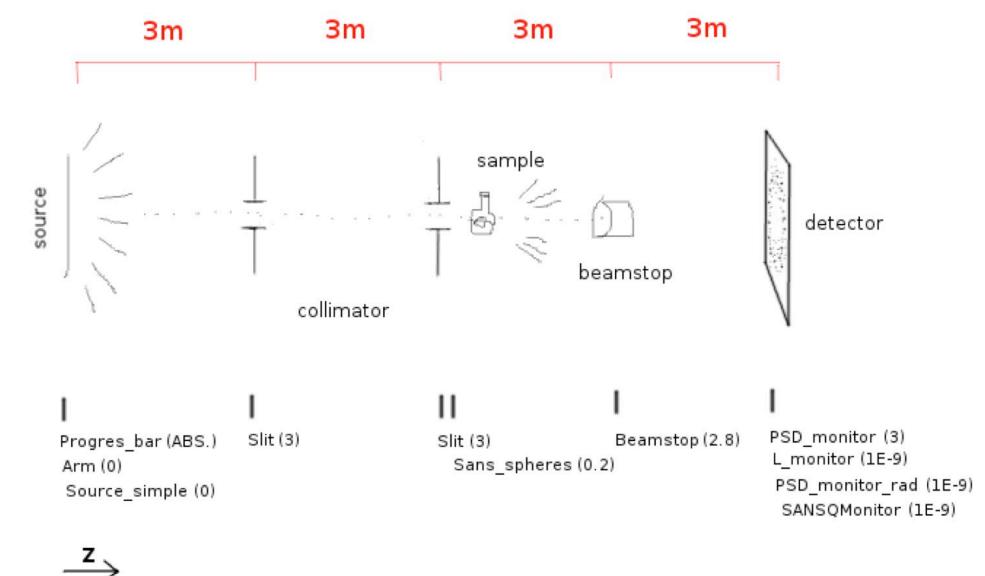
The screenshot shows a GitHub repository page for 'McStas tutorial: simplified SANS instrument'. The repository has 6 watches, 11 stars, and 16 forks. The 'Wiki' tab is selected. The page title is 'McStas tutorial: simplified SANS instrument' and it was last edited by Jakob Garde on Feb 8, 2016.

McStas tutorial: simplified SANS instrument

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

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.

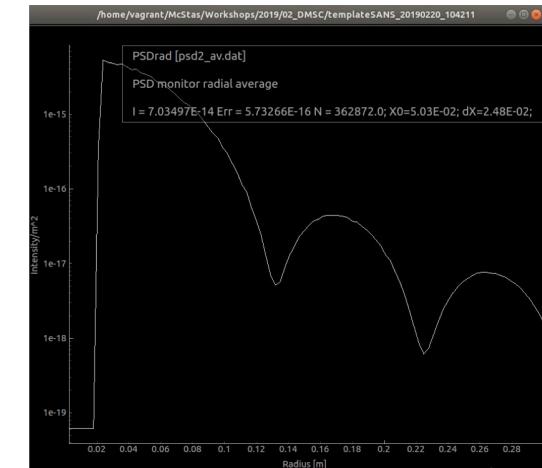
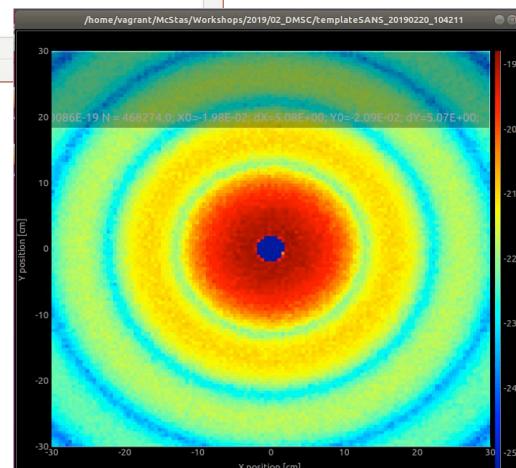
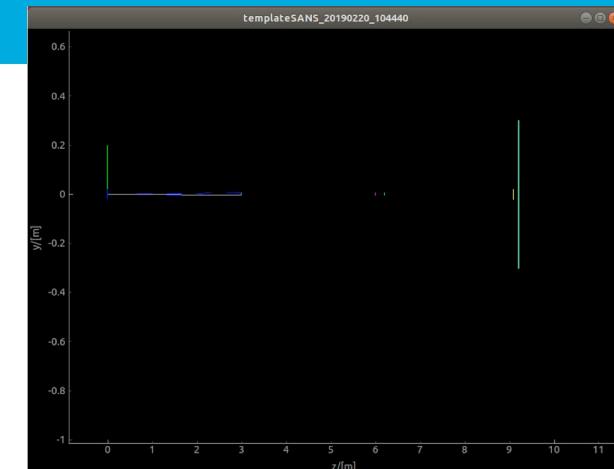
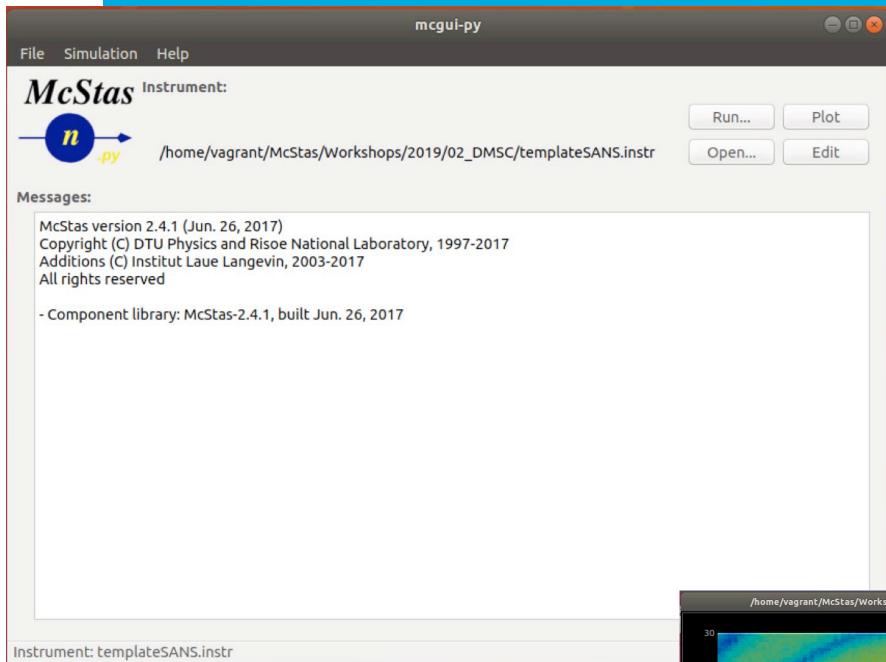


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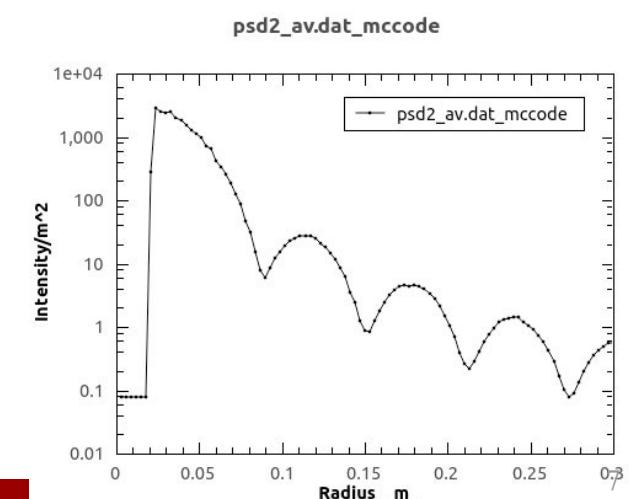
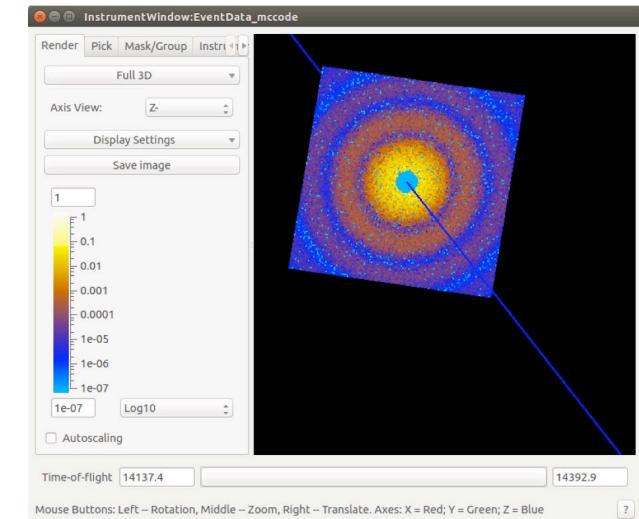
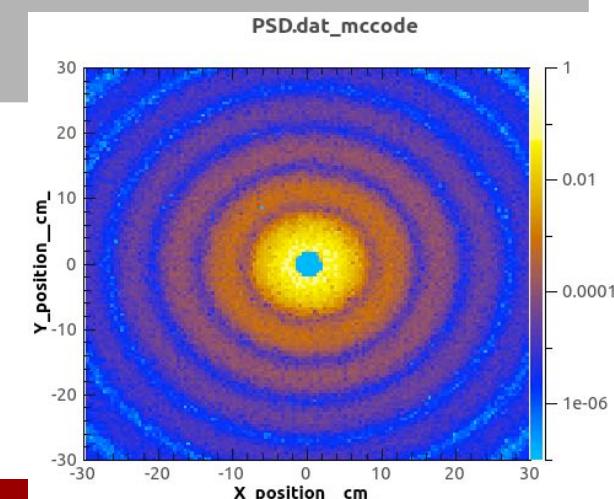
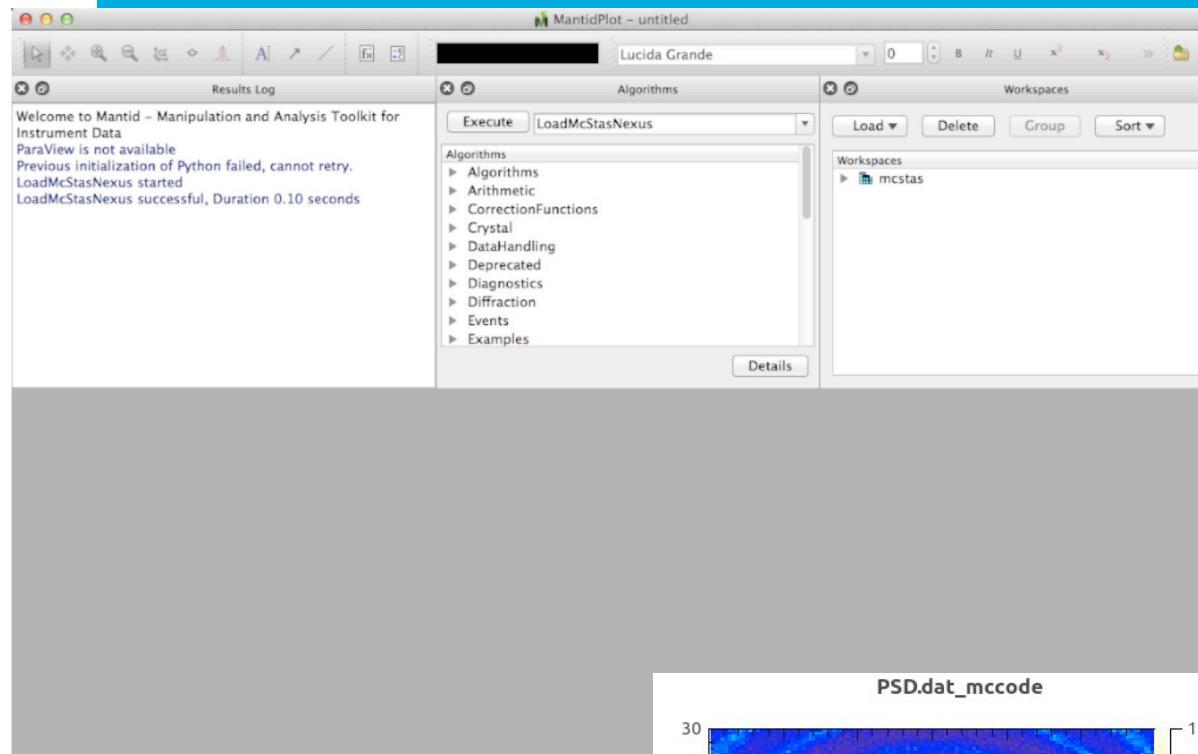
McStas


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

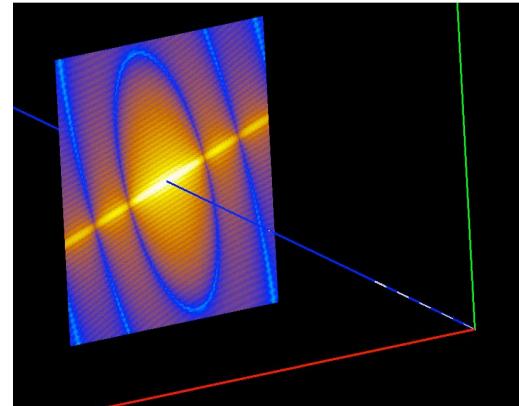
McStas GUI:



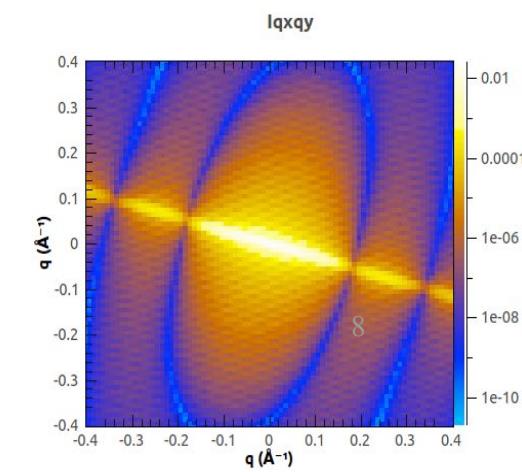
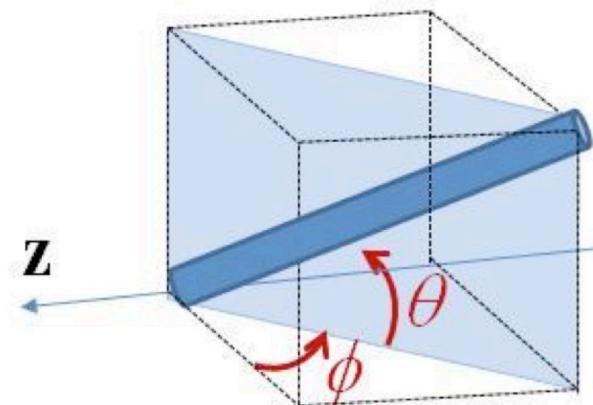
Mantid GUI:



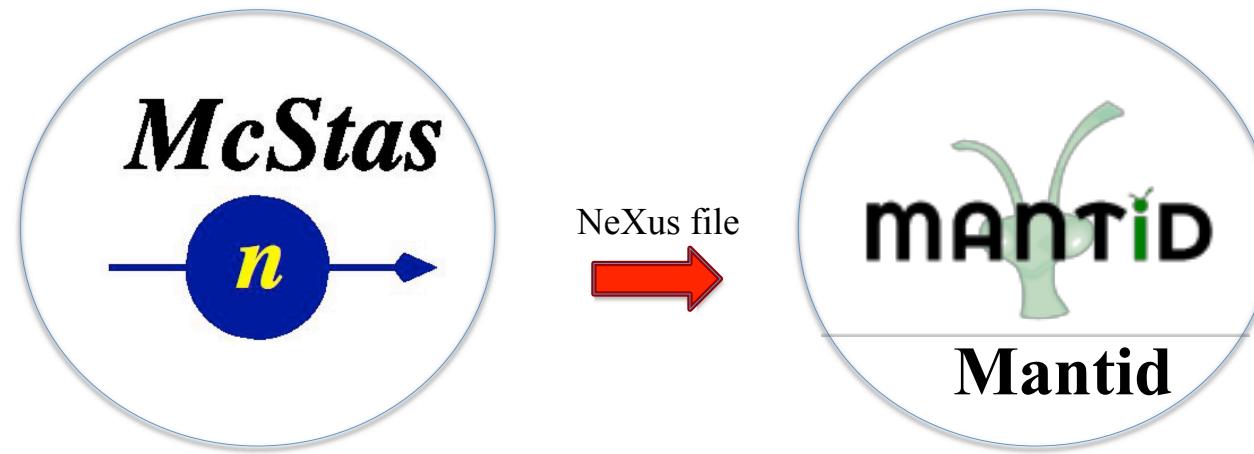
Example: Usage of Mantid



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



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

9

McStas Nexus file

HDFView 2.9

File Window Tools Help

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

TableView - events - /entry1/data/k01_events_dat_list_p_x_y_n_id_t/ - /home/ub/tmp/McStas_Event/McStas/Exp_Data/mccode.h5

Table

events

Event 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	0.021276...
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...	0.006773...	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	

Text

IDF 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)

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

Log Info Metadata

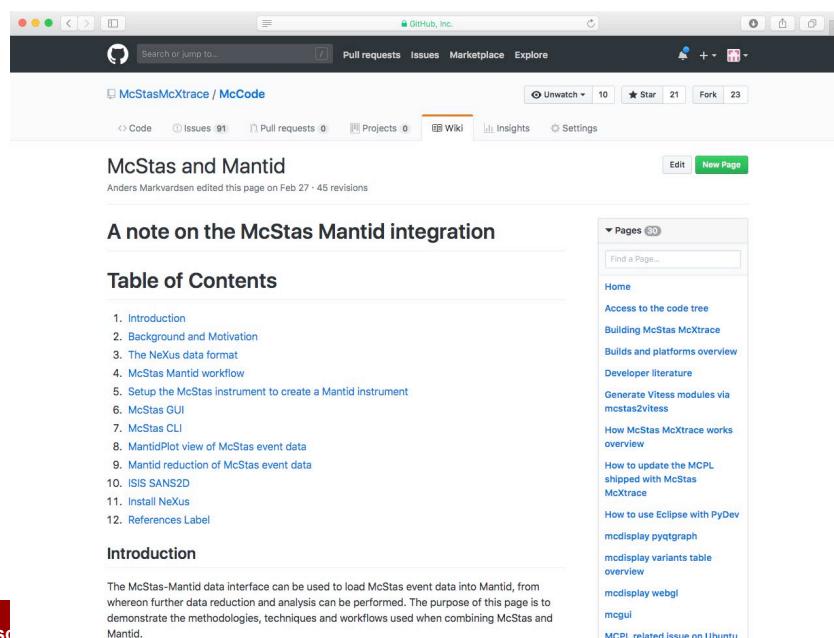
IDF xml data, TOF and pixel ID's

- Mantid's IDF store geometry information used 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.

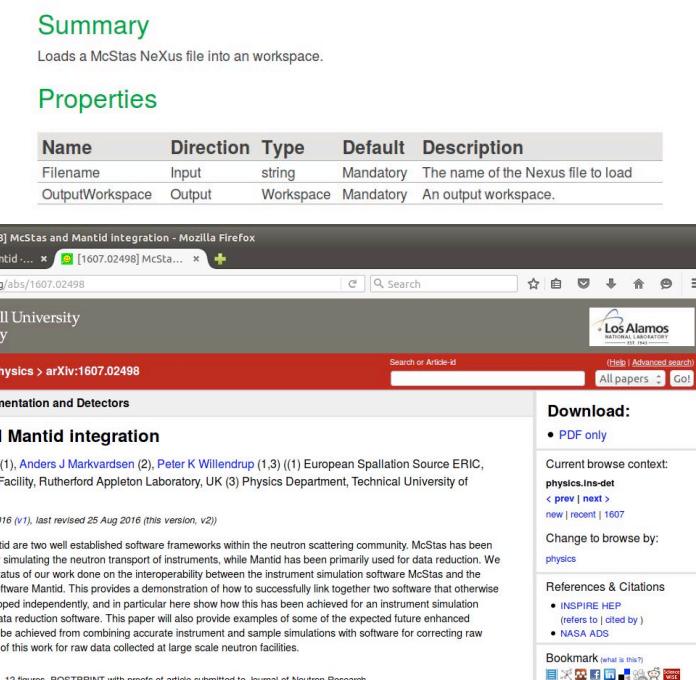
In other words:
Establishing k_i and k_f

How to use: Online documentation

- Github McStas wiki pages
<https://github.com/McStasMcXtrace/McCode/wiki/McStas-and-Mantid#setup-the-mcstas-instrument-to-create-a-mantid-instrument>)
- Archive - lanl.arXiv.org
- Built-into Mantid



The screenshot shows a GitHub repository page for 'McStasMcXtrace / McCode'. The main content is titled 'McStas and Mantid' and discusses the integration between the two software packages. It includes a 'Table of Contents' section with links to various documentation pages.

The screenshot shows a screenshot of a web browser displaying an arXiv.org page. The title is 'McStas and Mantid integration' by Torben R Nielsen, Anders J Markvardsen, Peter K Willendrup. The page includes a 'Download' section with PDF options, a 'References & Citations' section, and a 'Bookmark' section.

McStas instrument 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(....)**”

templateSANS.instr vs templateSANS_Mantid.instr

templateSANS.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, 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_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, 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

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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
12

```

Line 10, Column 3 Tab Size: 4 Plain Text

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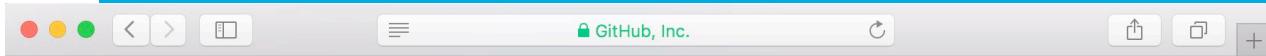


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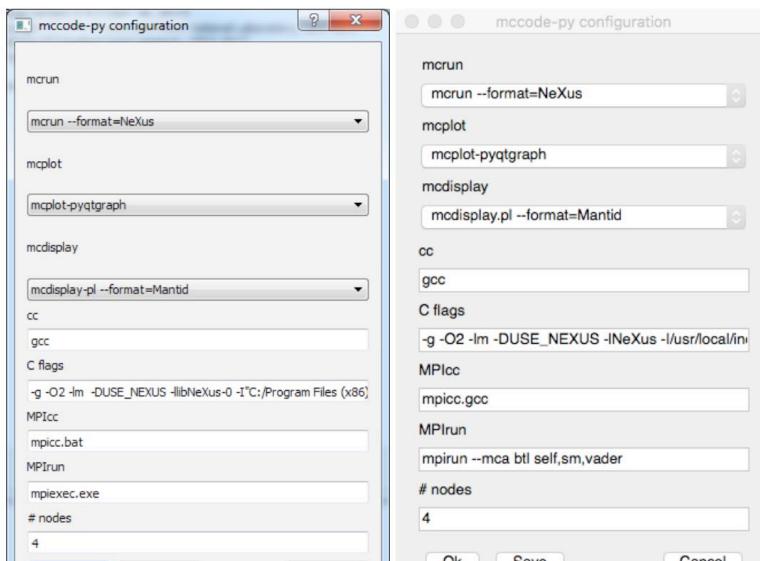
How to run the simulation



McStas GUI

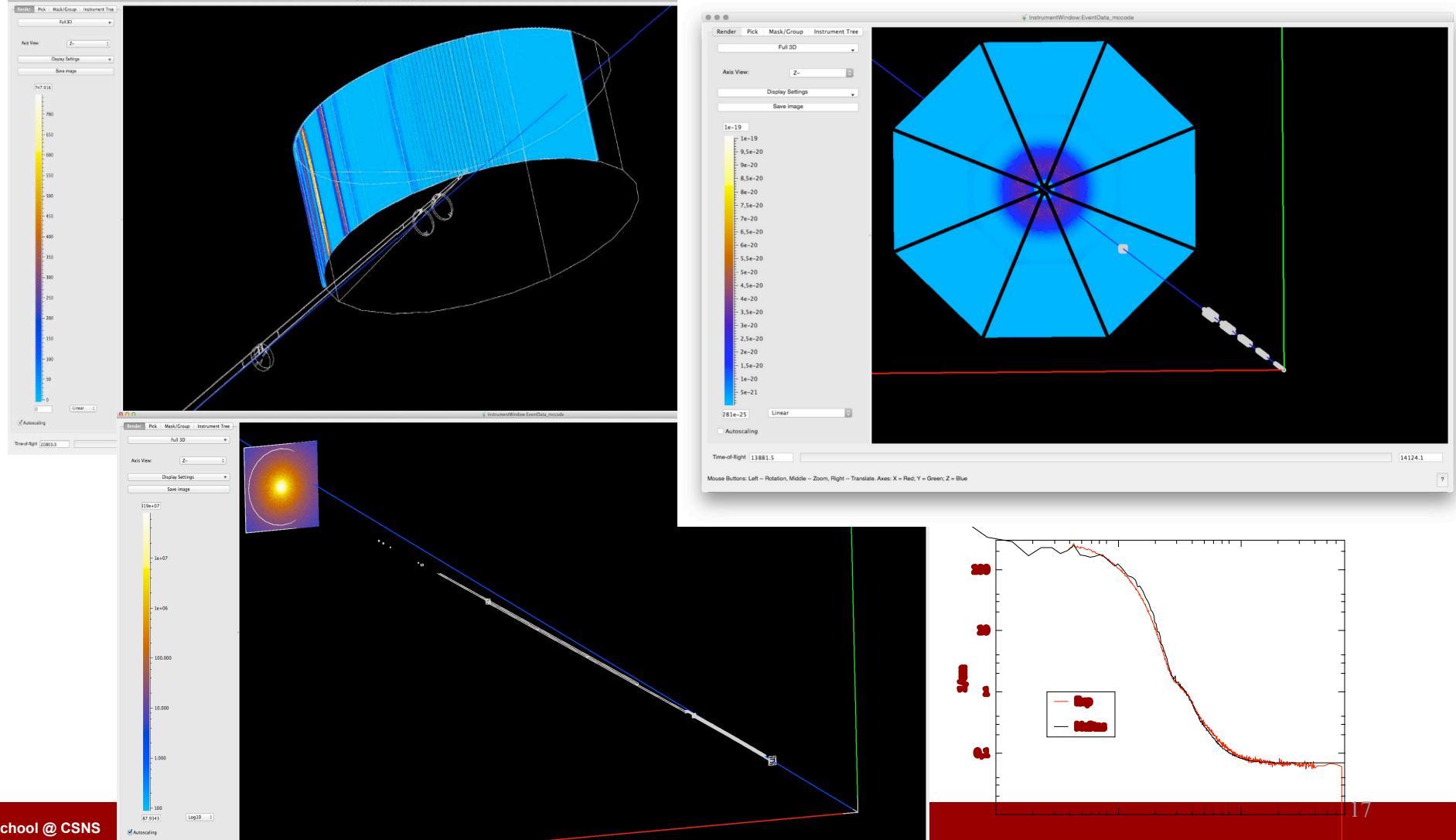
Generating McStas event data for Mantid can be achieved from the McStas GUI `mogui`. Below we show how to setup the simulation on Windows 7, OSX 10.12, and Ubuntu 16.04. For `McStas` we use version 2.4.1. For `Mantid` use version 3.4 or later.

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 -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`

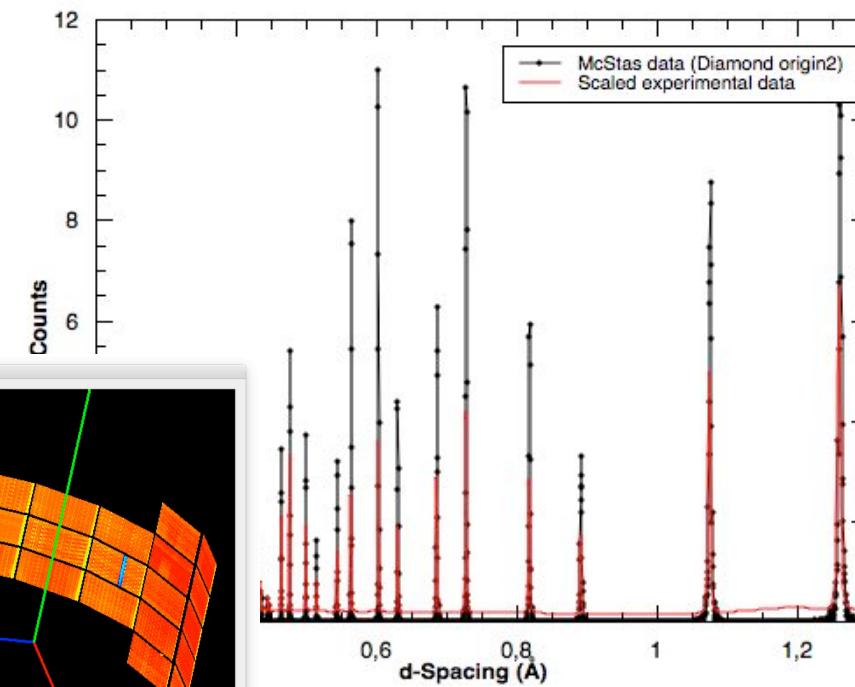
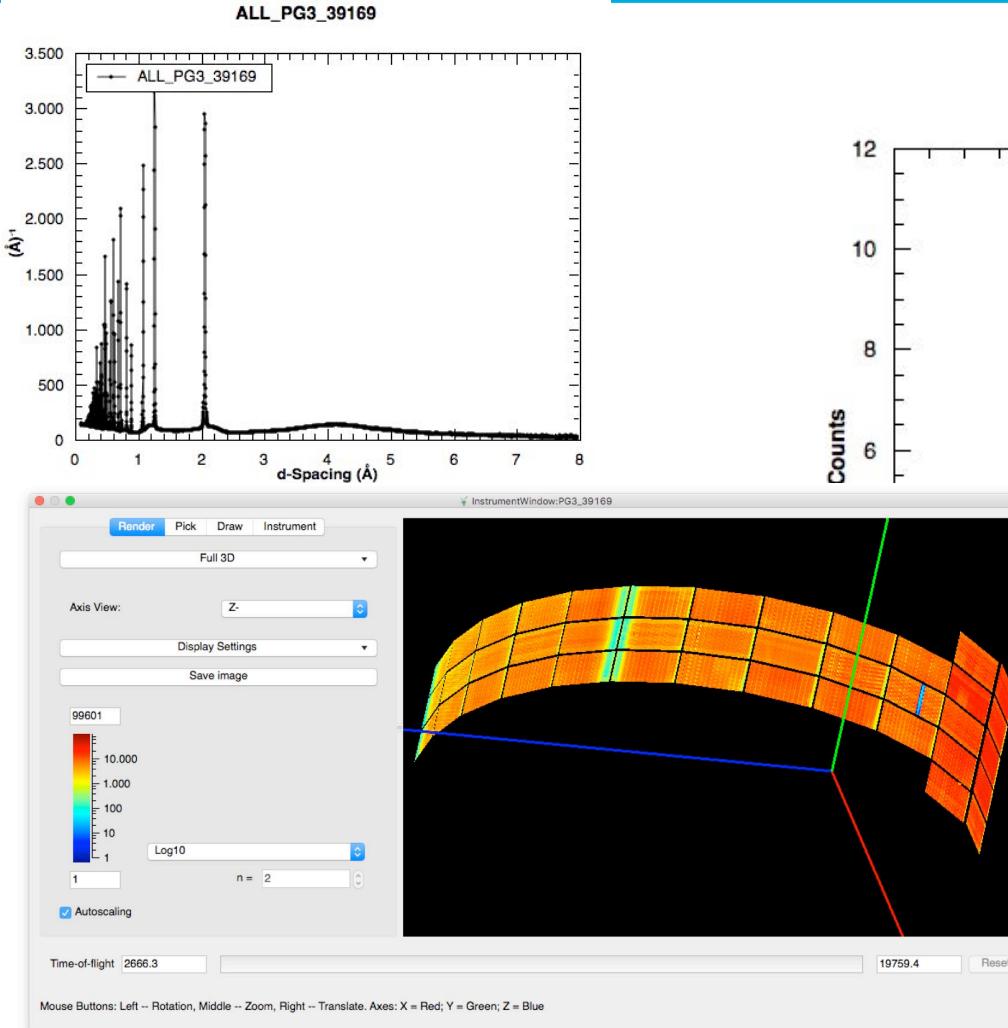


Wikipedia on GitHub

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



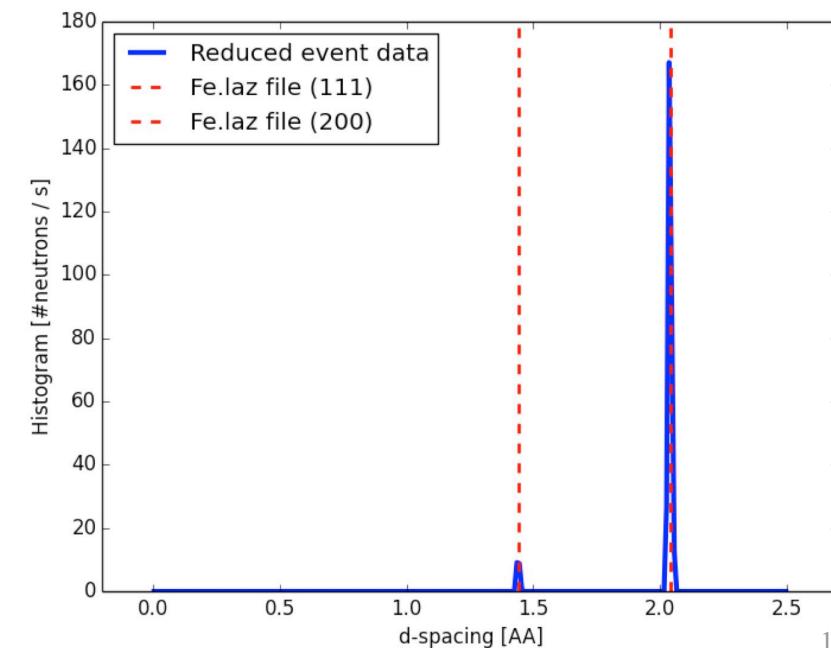
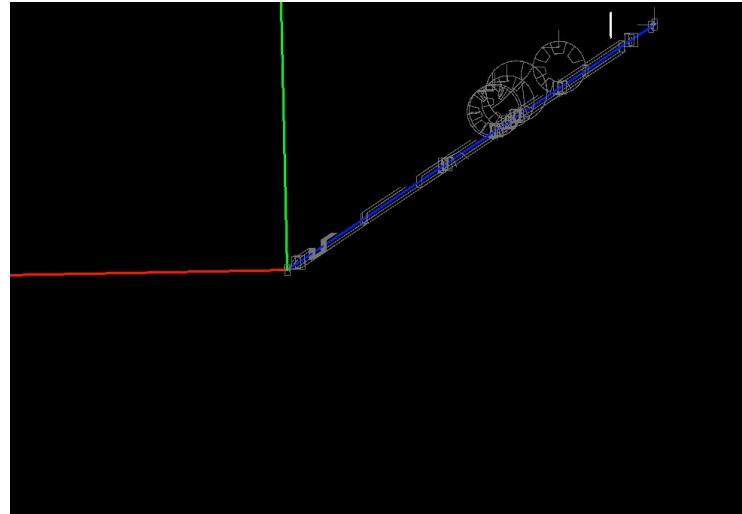
McStas and experimental data: POWGEN



18

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 is 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

20