McStas - Mantid

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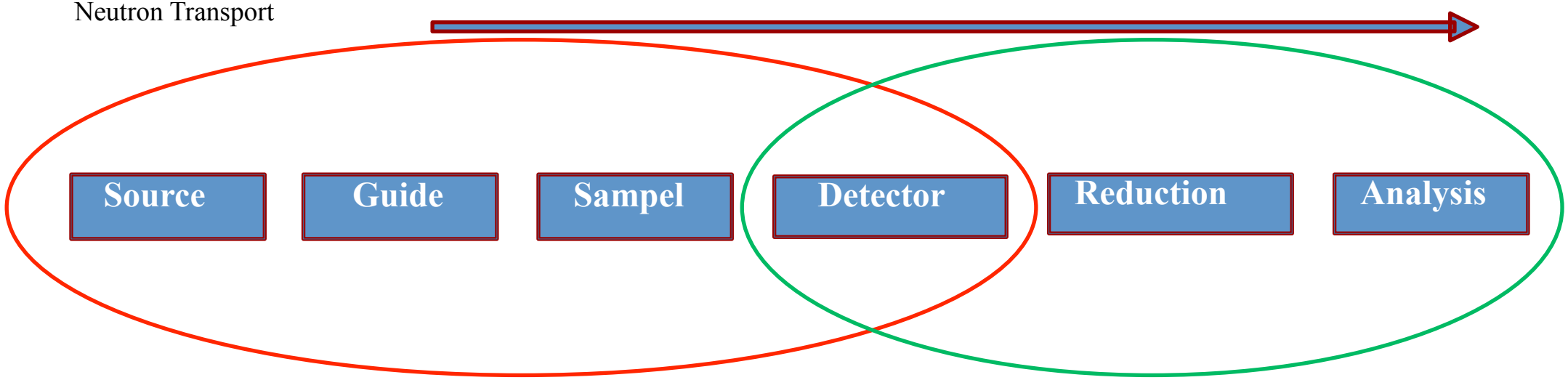
Neutron Transport



Typical McStas Neuron Transport

Mantid-McStas focus:

How to analyse McStas data

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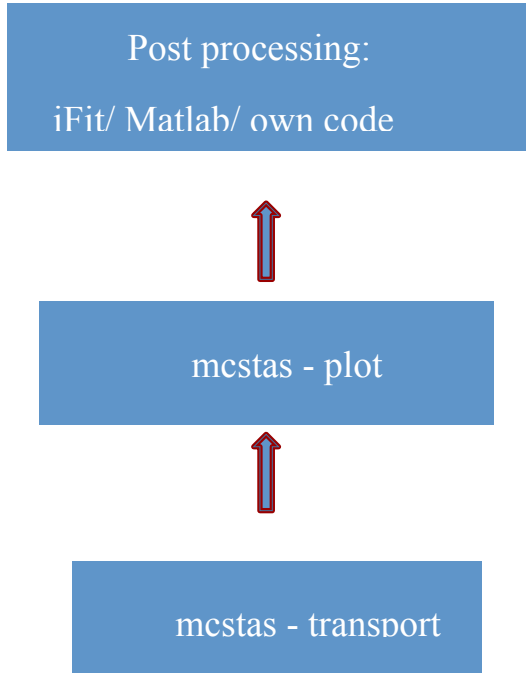
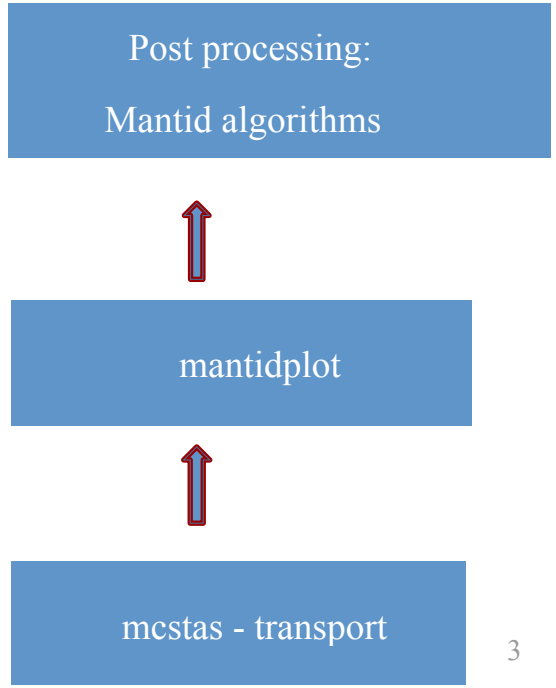
Comparison

Classic McStas



Mantid-McStas



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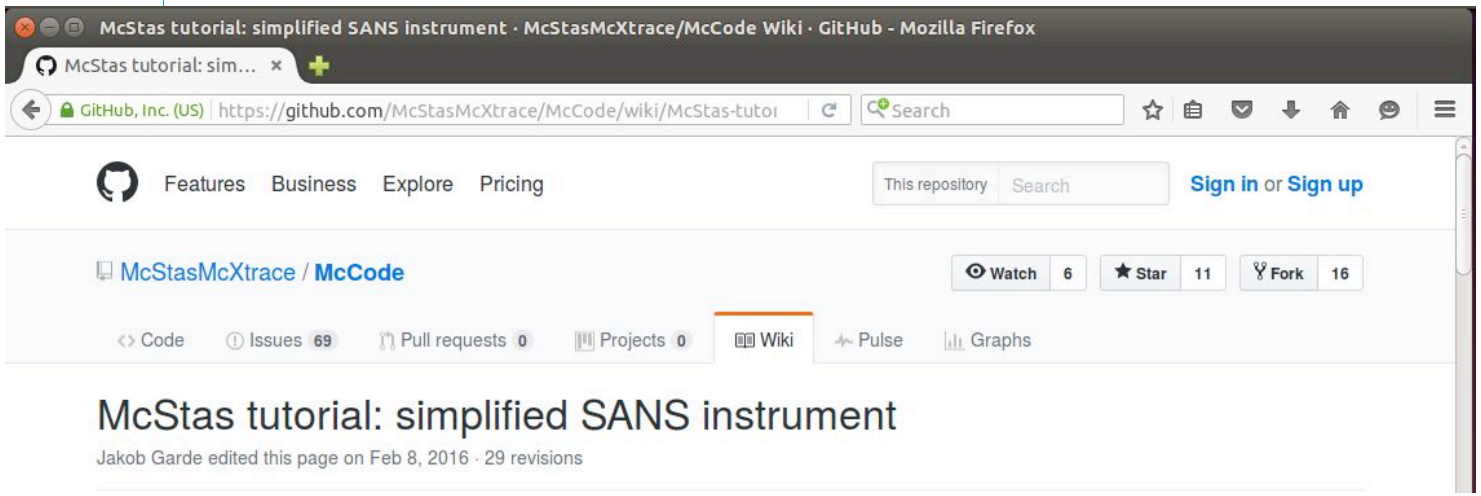
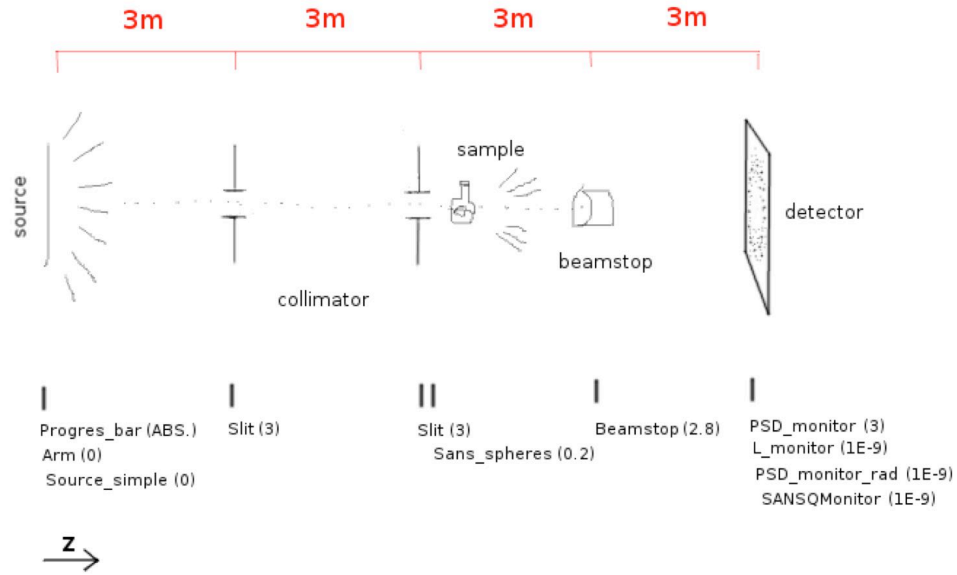
Motivation: new flexible dataflow

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)

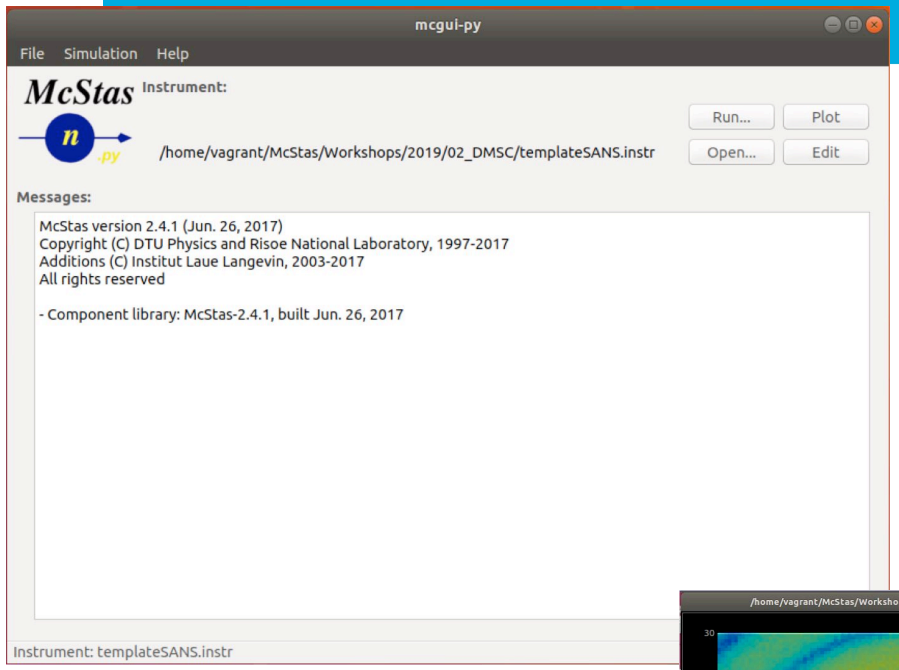
4

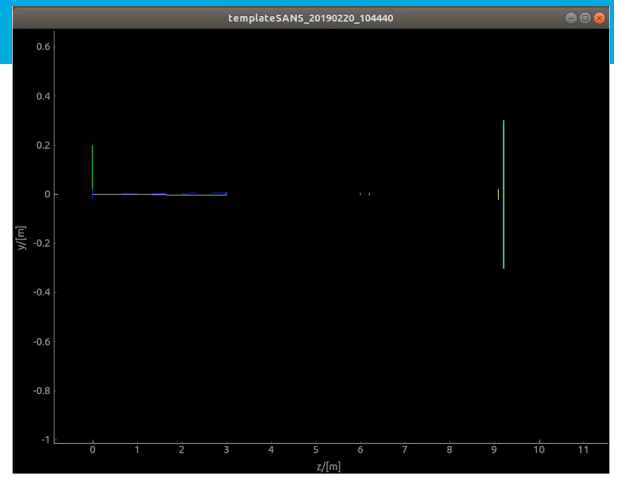
Illustration: simplified SANS

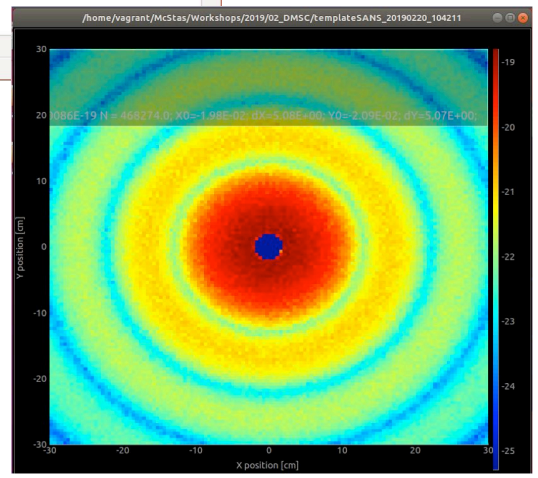


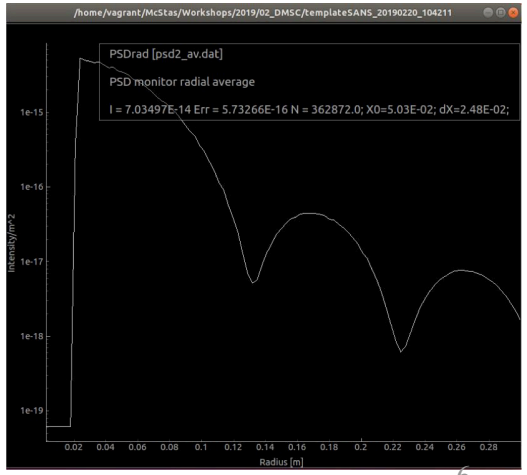


McStas GUI:



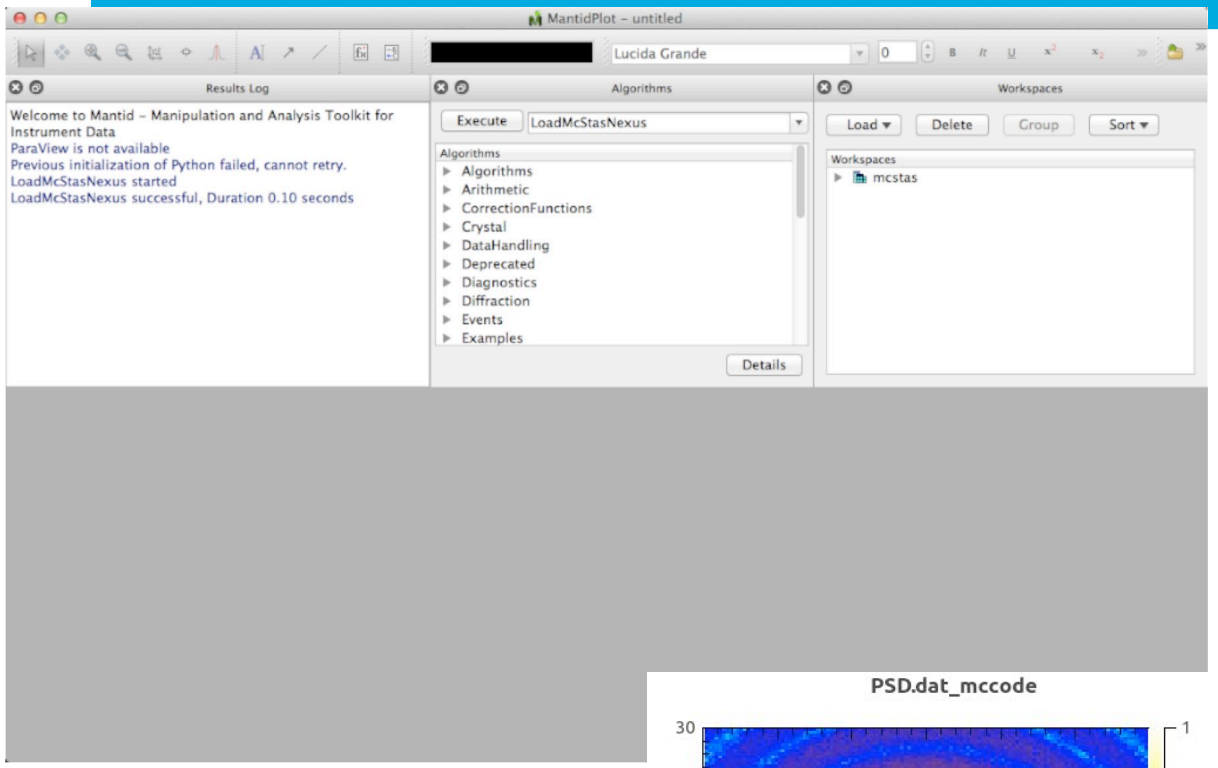


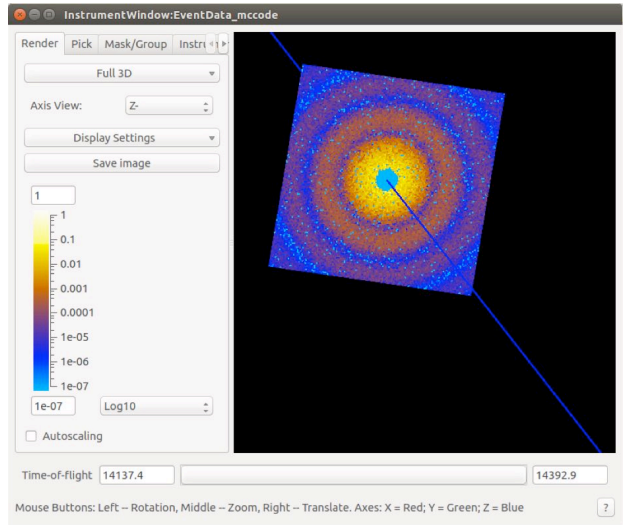


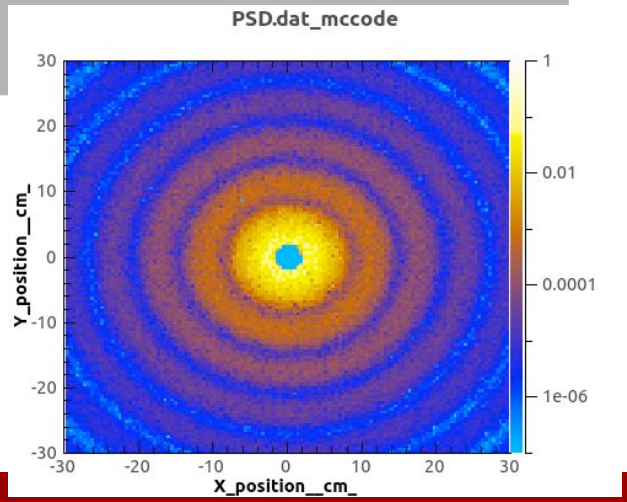


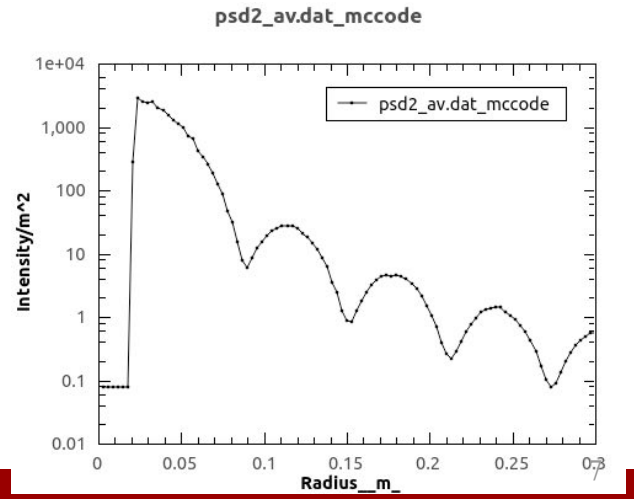
R=150,phi=0.1, d=1,a=0

Mantid GUI:









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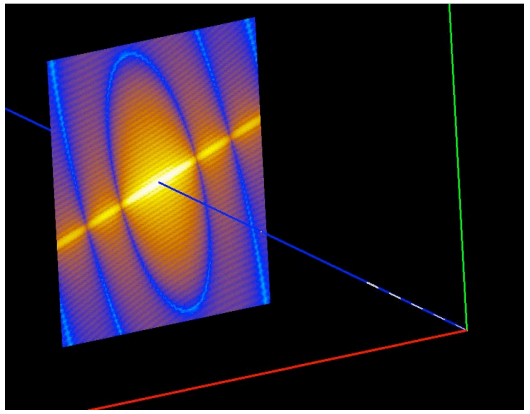
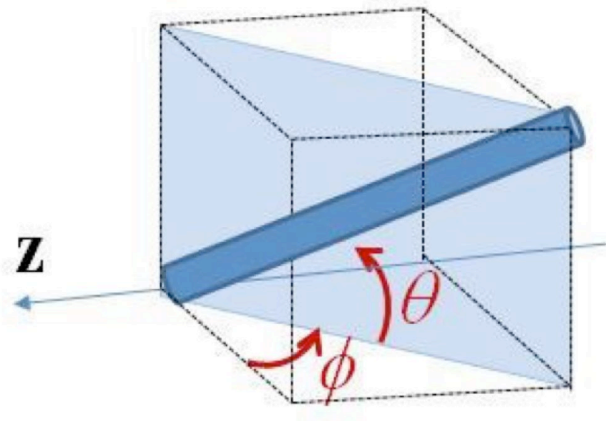
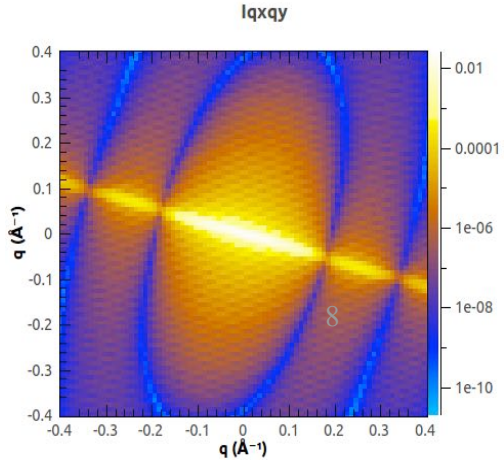
Example: Usage of Mantid



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





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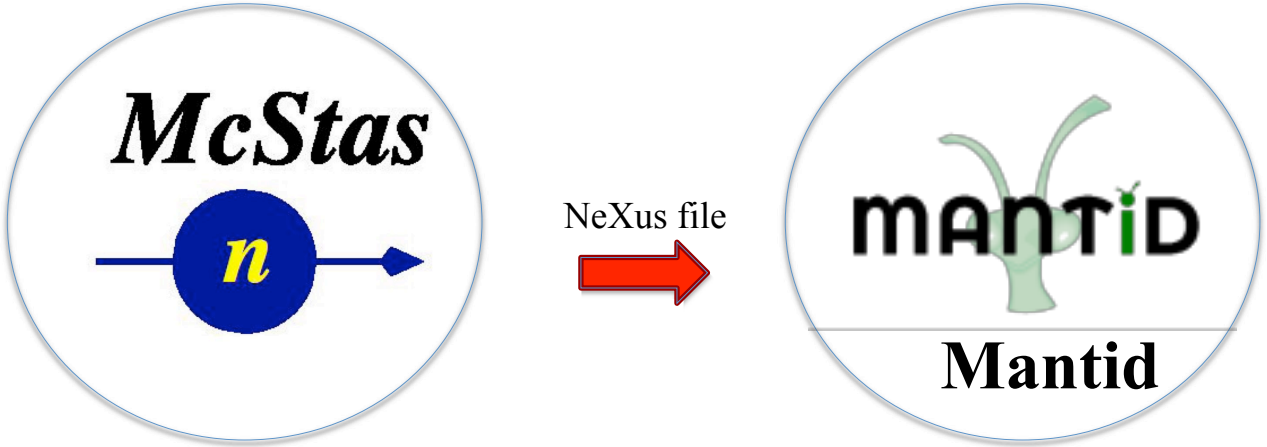
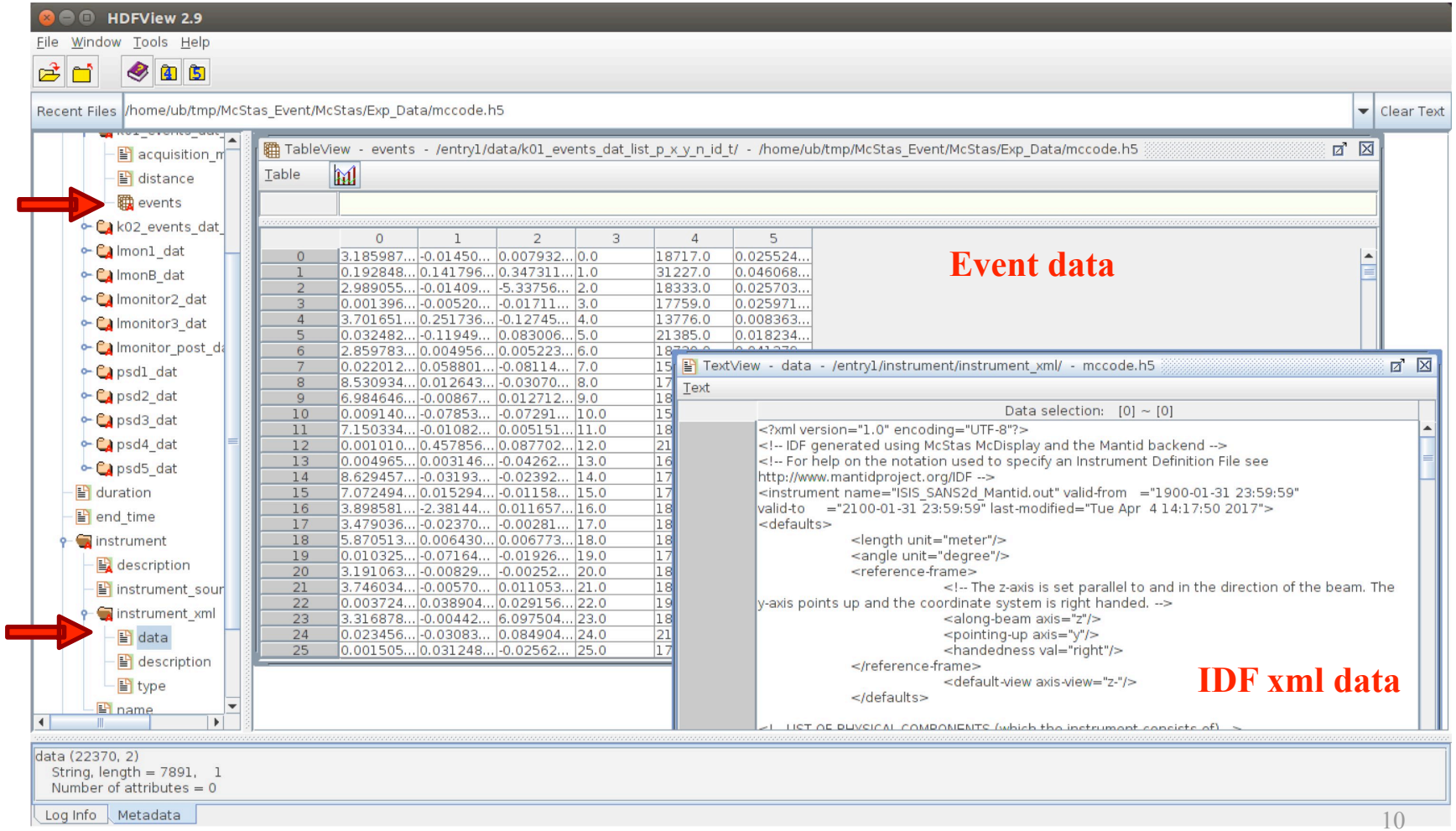
The NeXus file



- 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*

McStas NeXus file



IDF xml data, TOF and pixel ID's

- Mantid's IDF store geometry information use in TOF analysis

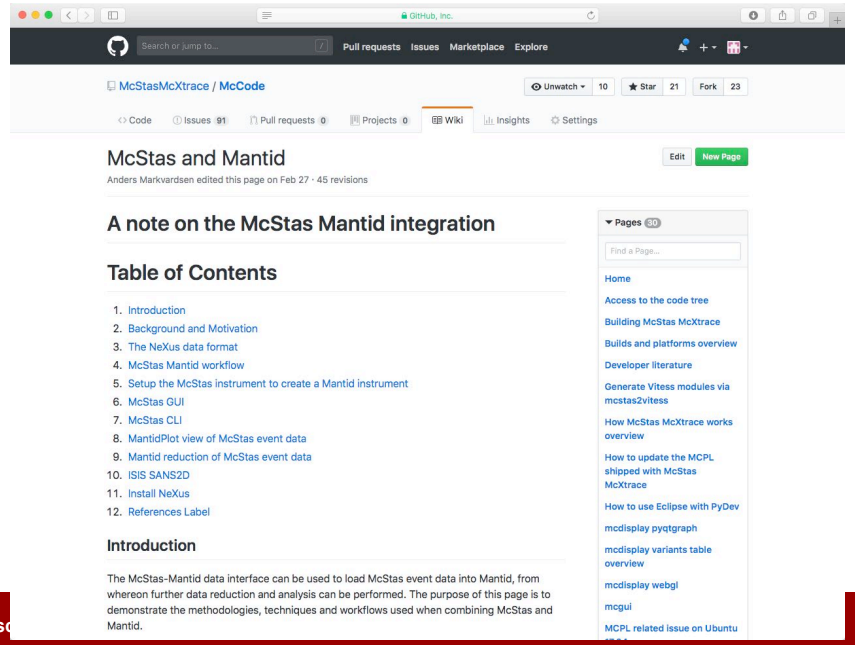
- This implies parsing information about:
  - where the neutron source is located,
  - where the sample is located,
  - where each individual detector pixel is located.

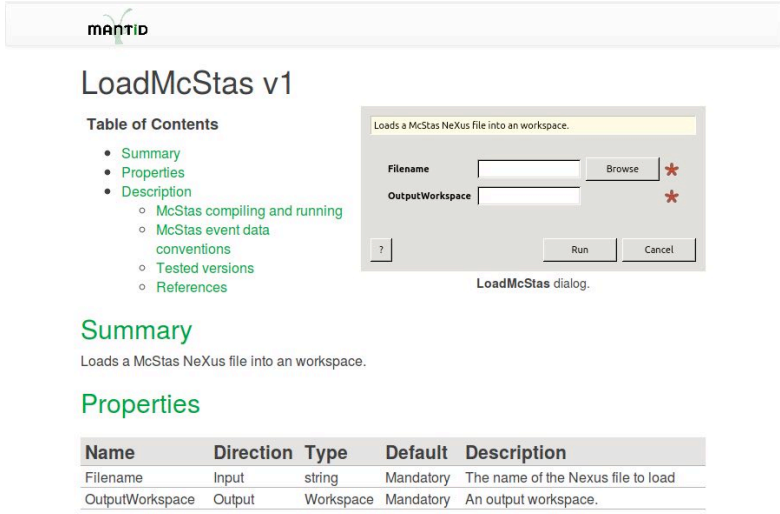
In other words:

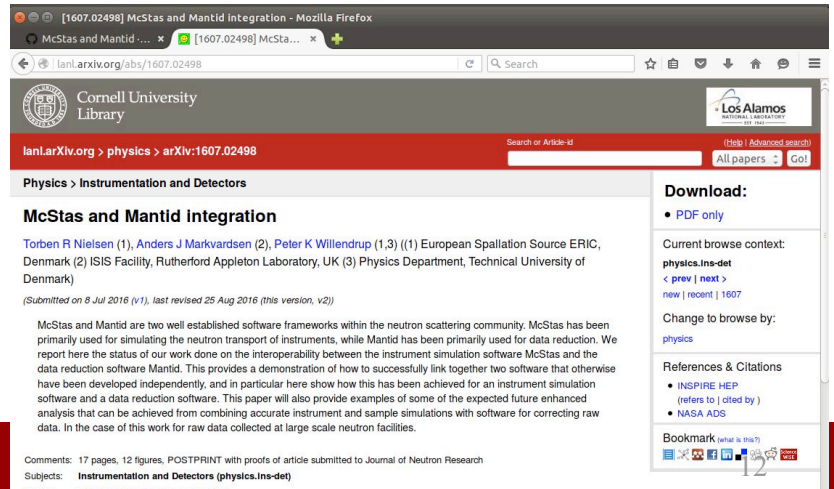
Establishing k_i and k_f

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







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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.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

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
       y limits=[-0.3 0.3] bins=128, neutron pixel min=0 t,
       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 Tab Size: 4 Plain Text

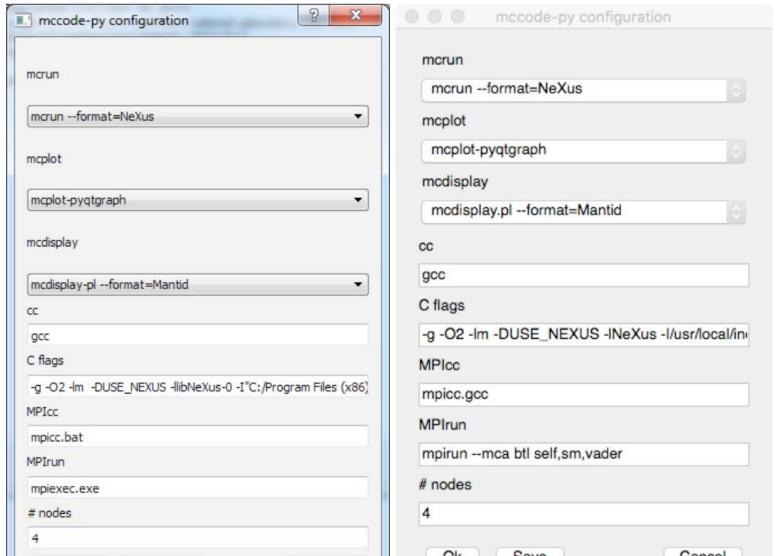
How to run the simulation

GitHub, Inc.

McStas GUI

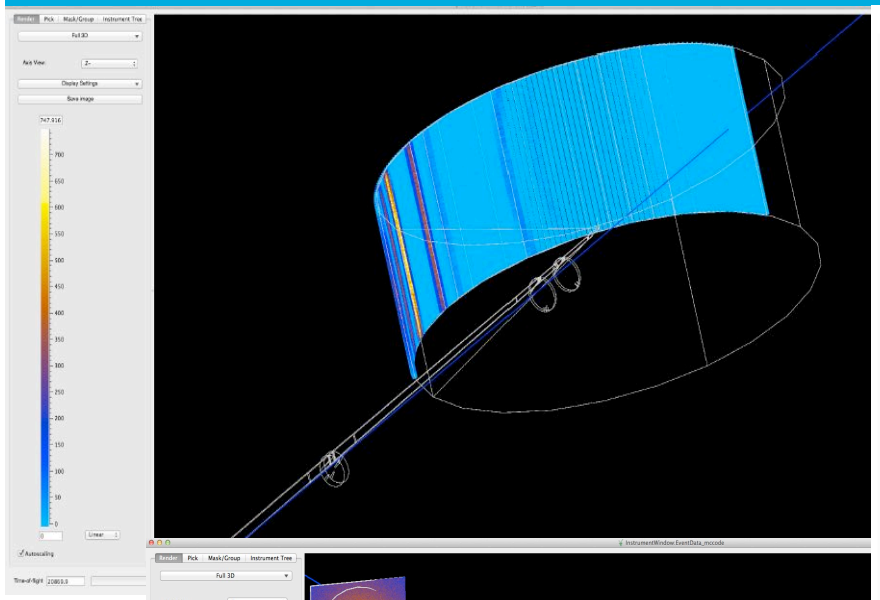
Generating McStas event data for Mantid can be achieved from the McStas GUI `mcgui`. Below we show how to setup the simulation on Windows 7, OSX 10.12, and Ubuntu 16.04. For McStas we use version 2.4.1. For Mantid use version 3.4 or later.

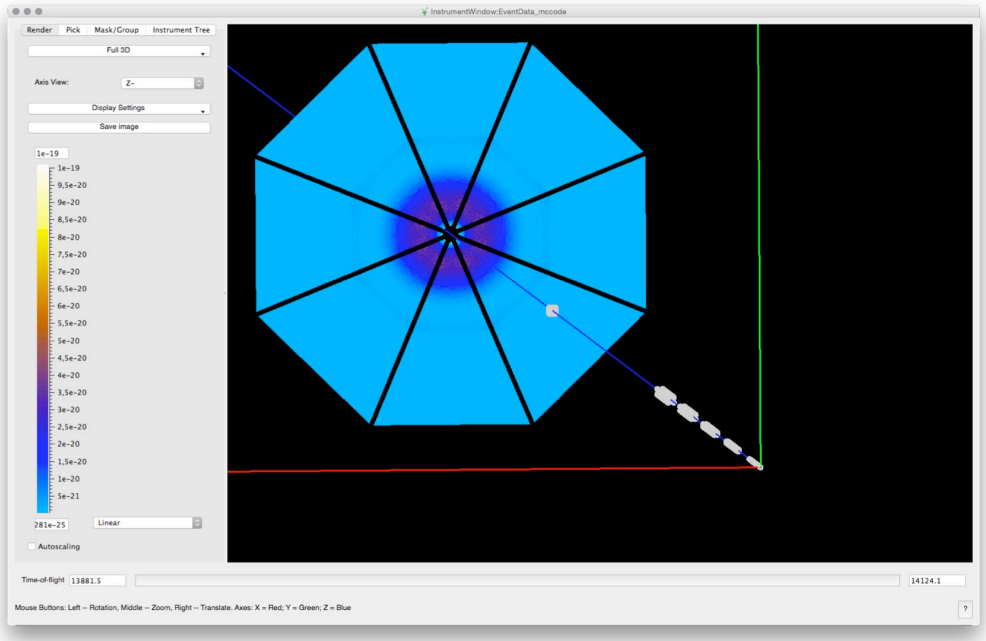
1. Open the McStas configuration file. In `mcgui` go to: File -> Configuration
2. Change the setting as shown in figures below:
   - In the section `mcrun` select `mcrun --format=NeXus`
   - In the section `mcplot` select `mcplot-pyqtgraph`
   - In the section `mcdisplay` select `mcdisplay-pl --format=Mantid` (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`

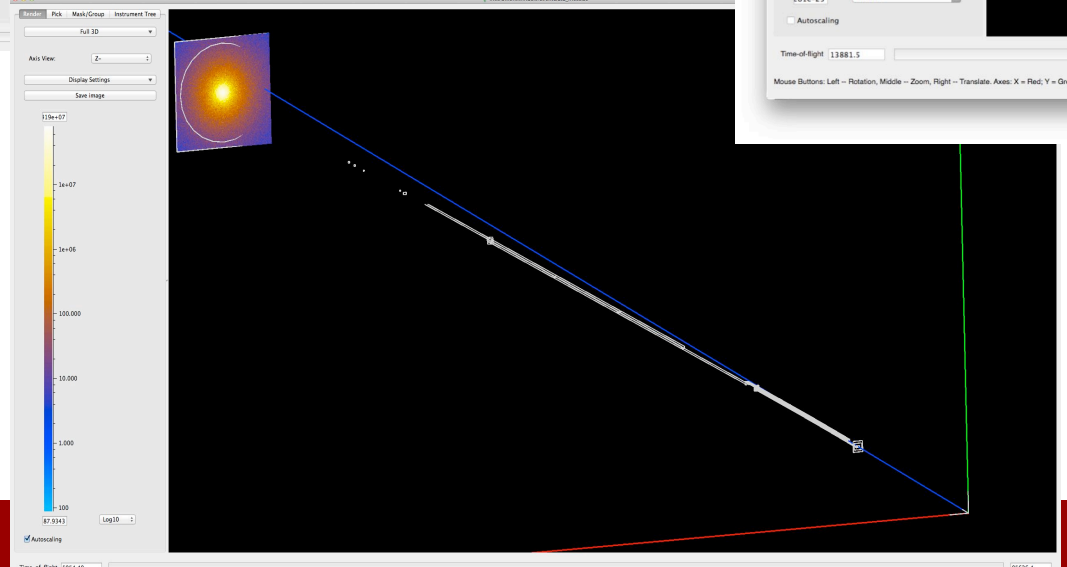


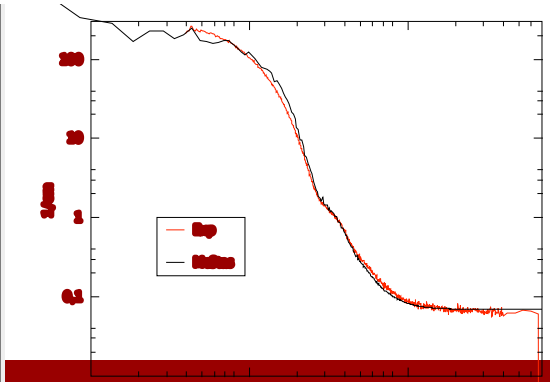
Wikipage on GitHub

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

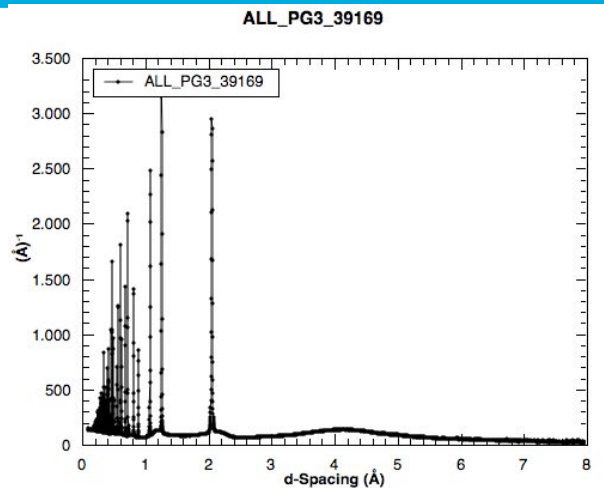


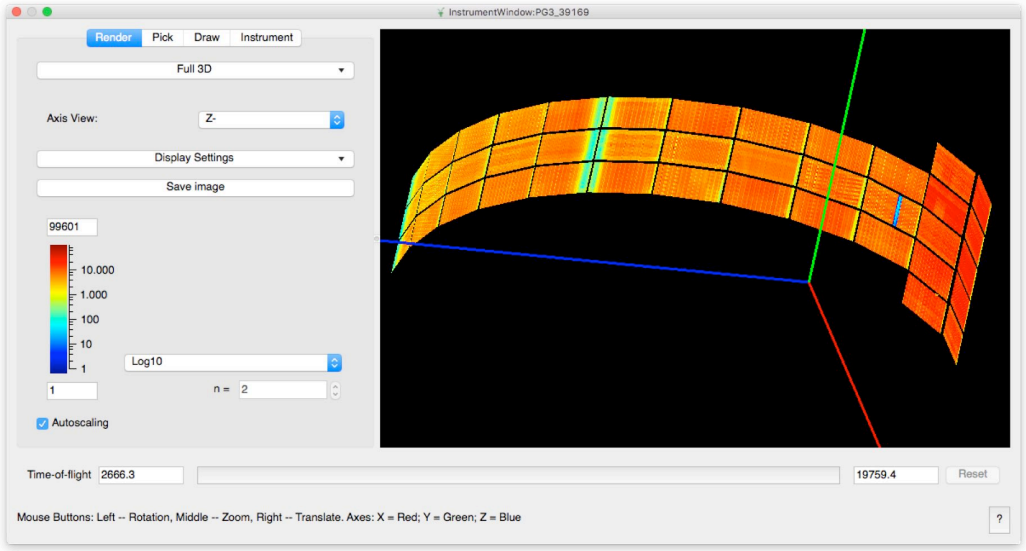


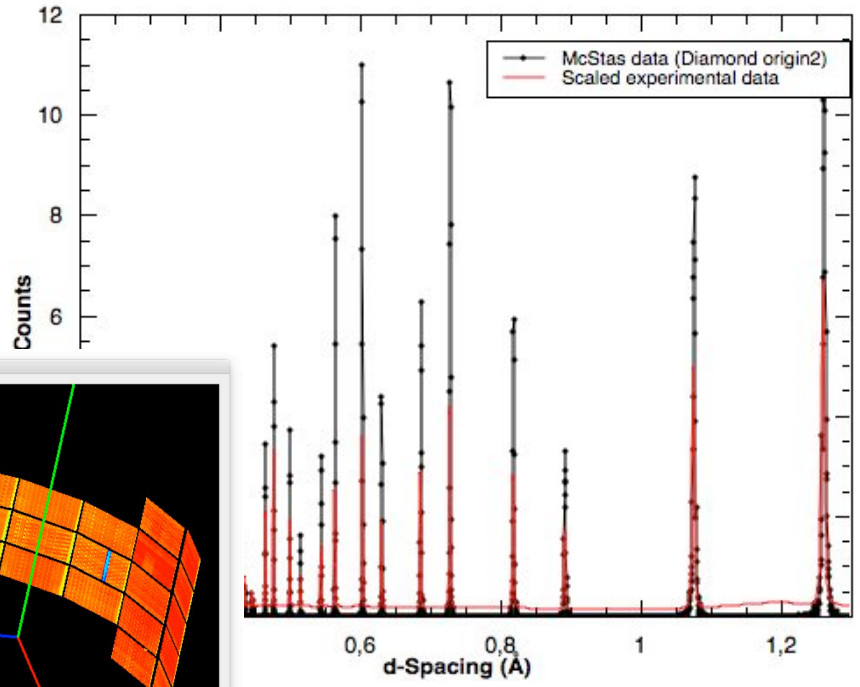




McStas and experimental data: POWGEN

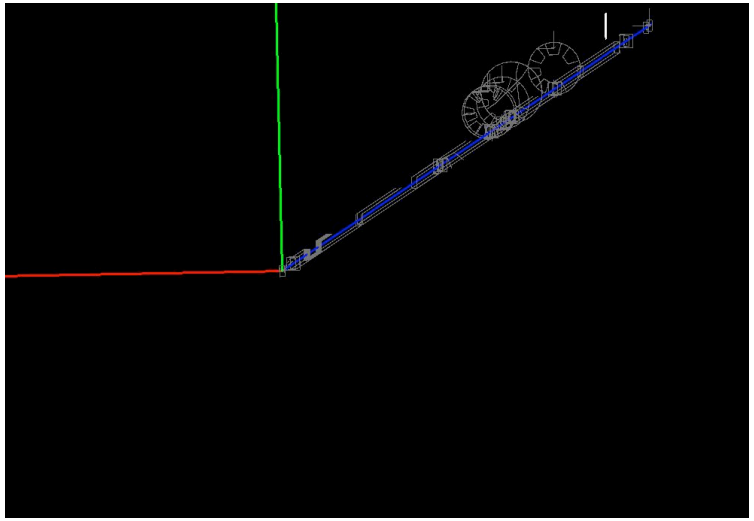


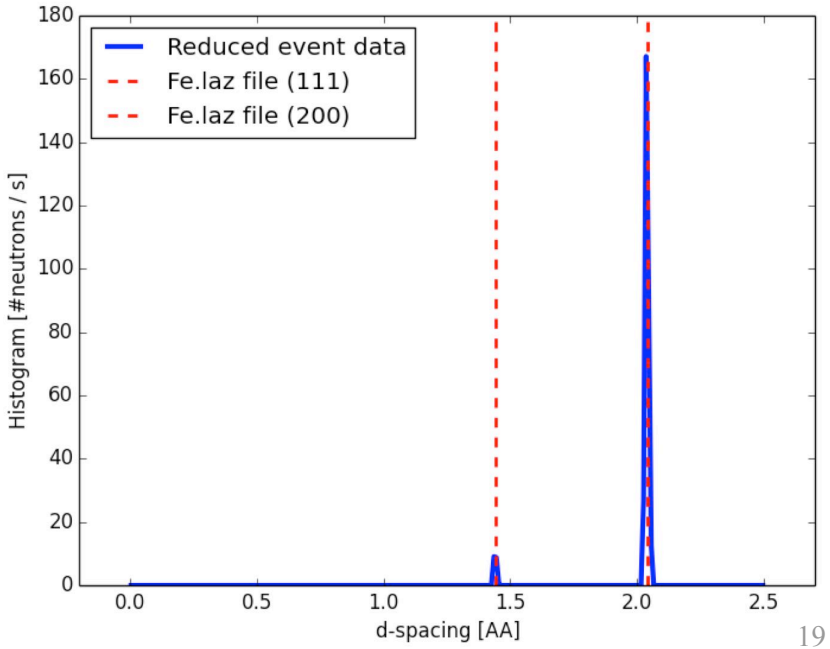




By CelineD@ ESS + SNS collaboration

Example –V20 –Powder diffraction Fe





Summary

1. Easier to post-process (event) data than making a completely new McStas simulation / component
   - E.g.:
   - Rebin 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