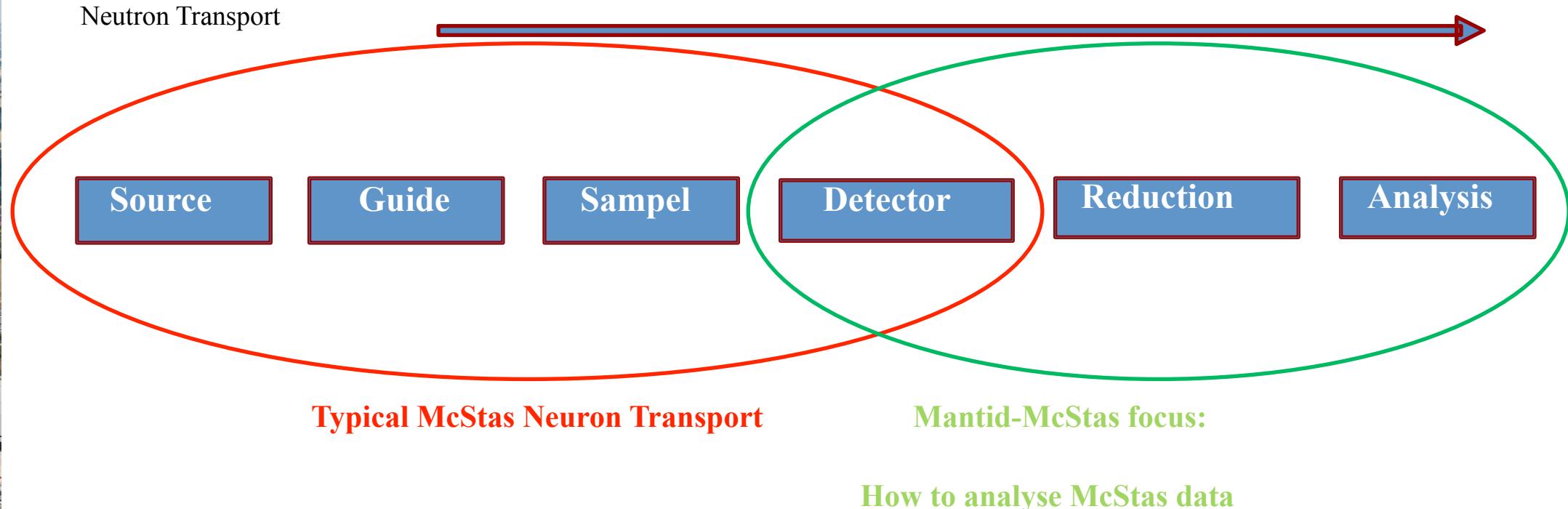


# McStas - Mantid

Torben Nielsen

Anders Markvardsen

Peter Willendrup

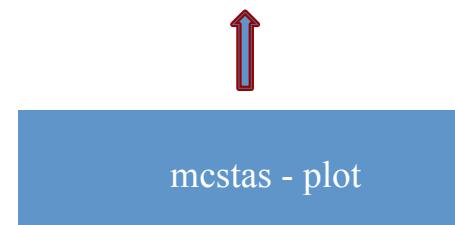




# Comparison

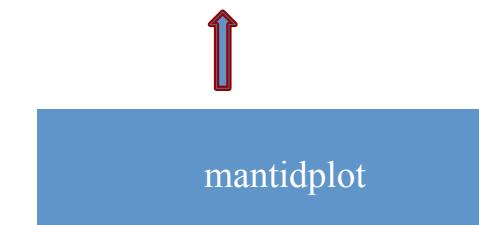
*Classic McStas*

Post processing:  
iFit/ Matlab/ own code



*Mantid-McStas*

Post processing:  
Mantid algorithms





# 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 )



# Illustration: simplified SANS

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

GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode/wiki/McStas-tutor

Features Business Explore Pricing This repository Search Sign in or Sign up

McStasMcXtrace / McCode Watch 6 Star 11 Fork 16

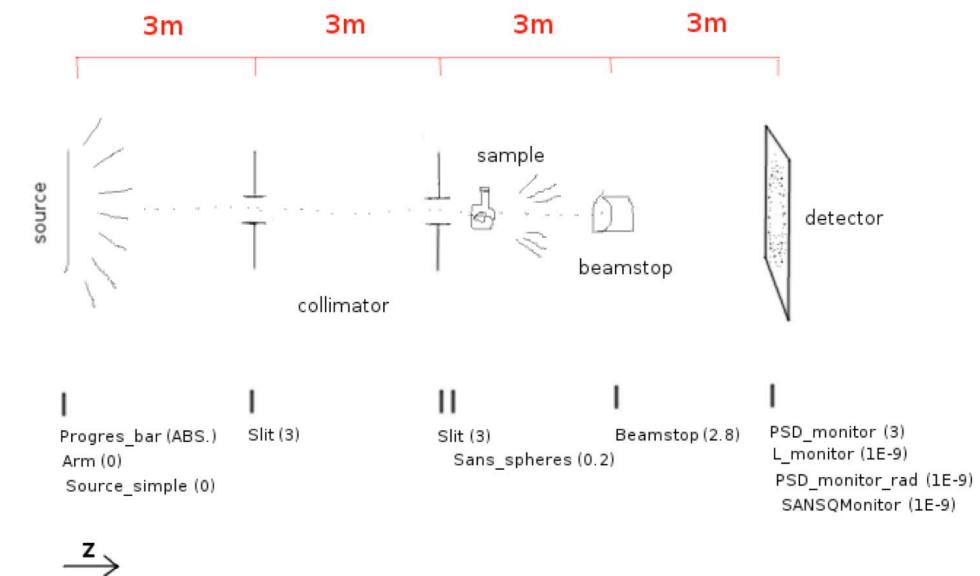
Code Issues 69 Pull requests 0 Projects 0 Wiki Pulse Graphs

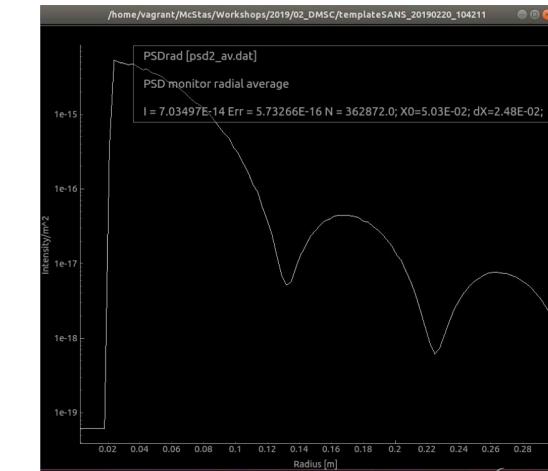
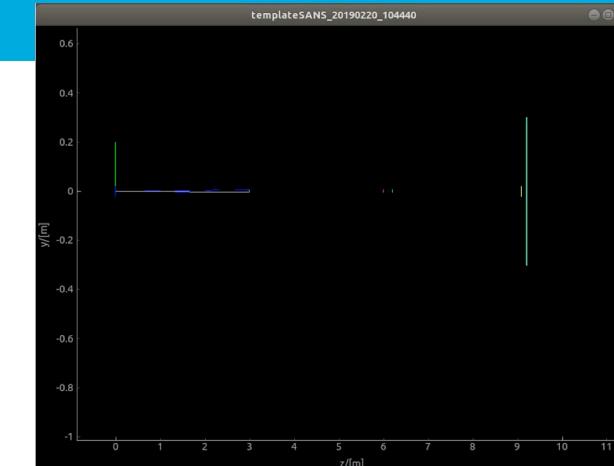
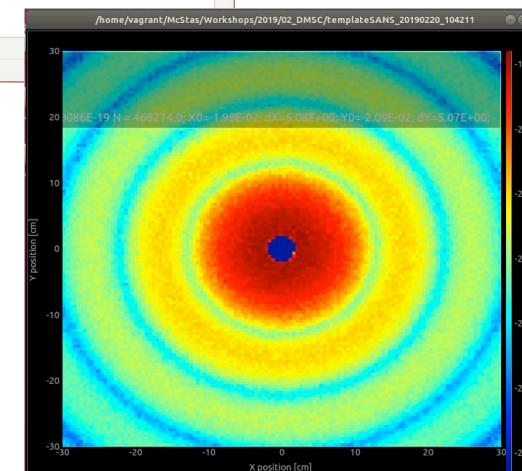
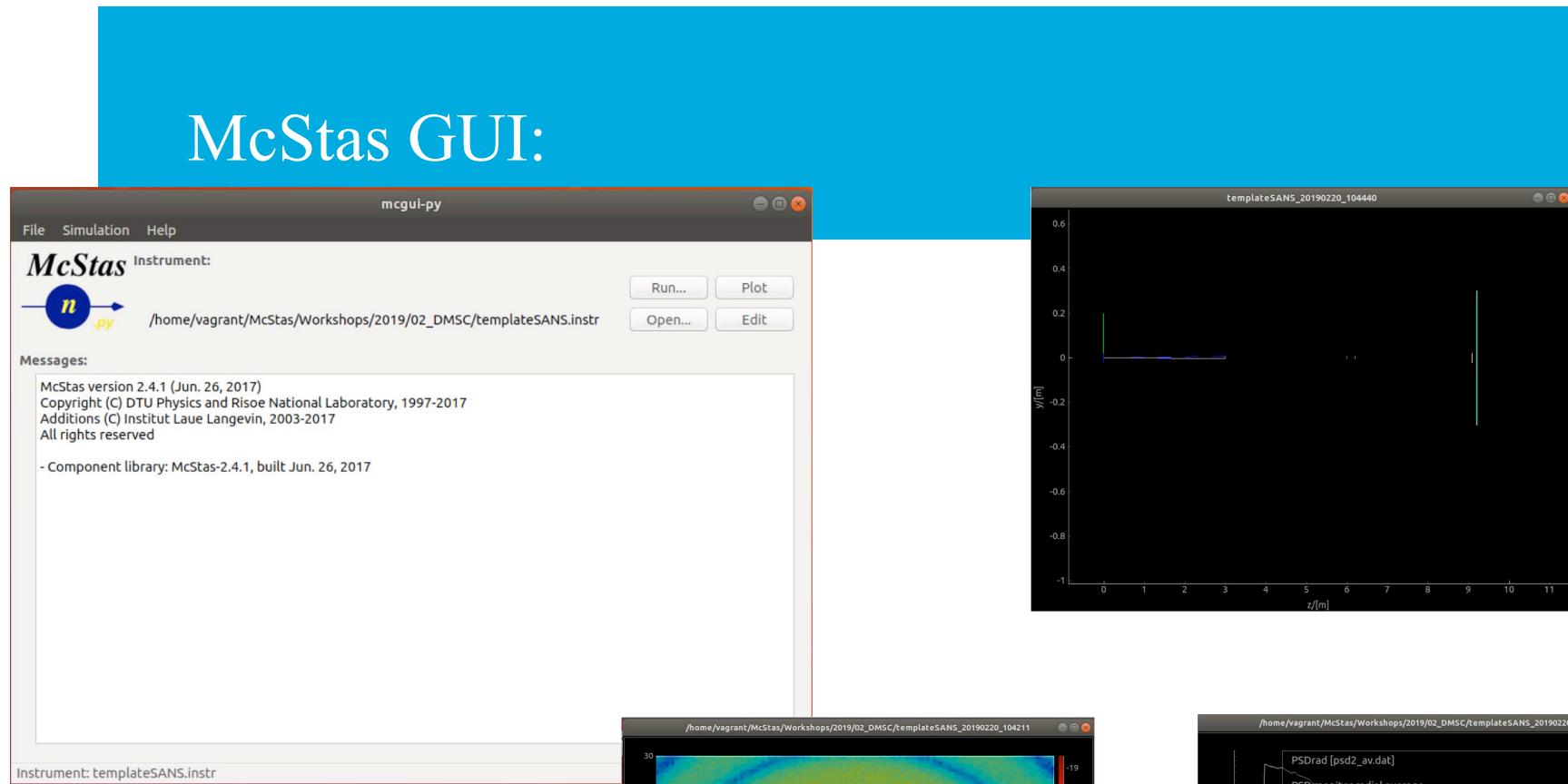
## McStas tutorial: simplified SANS instrument

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

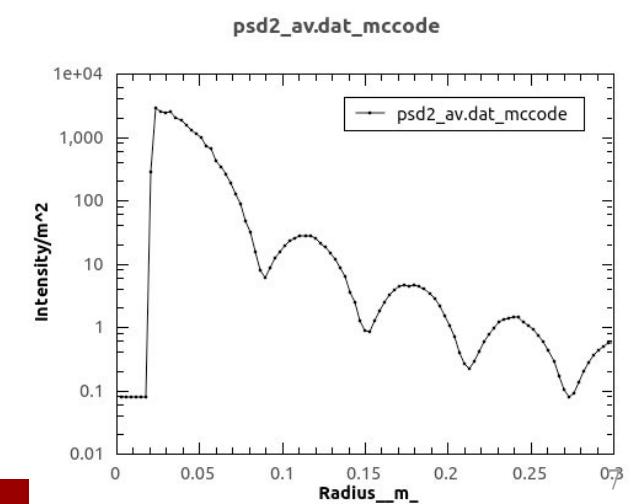
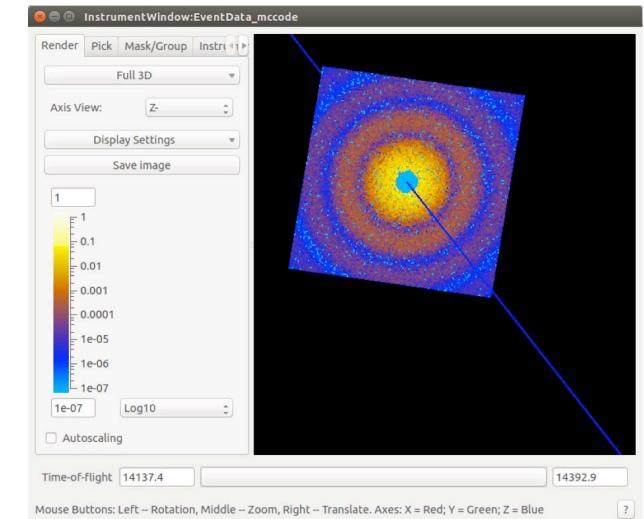
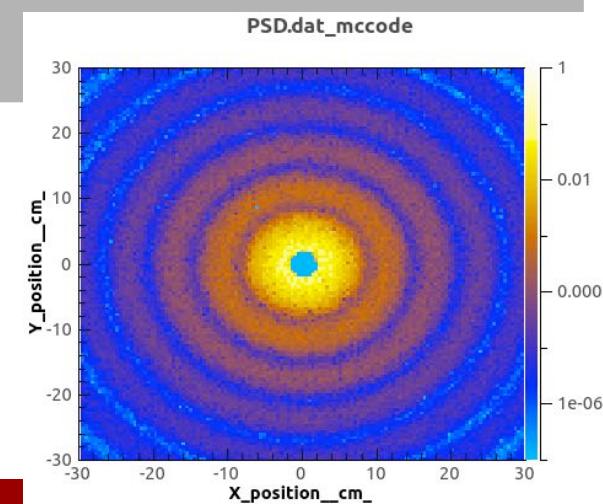
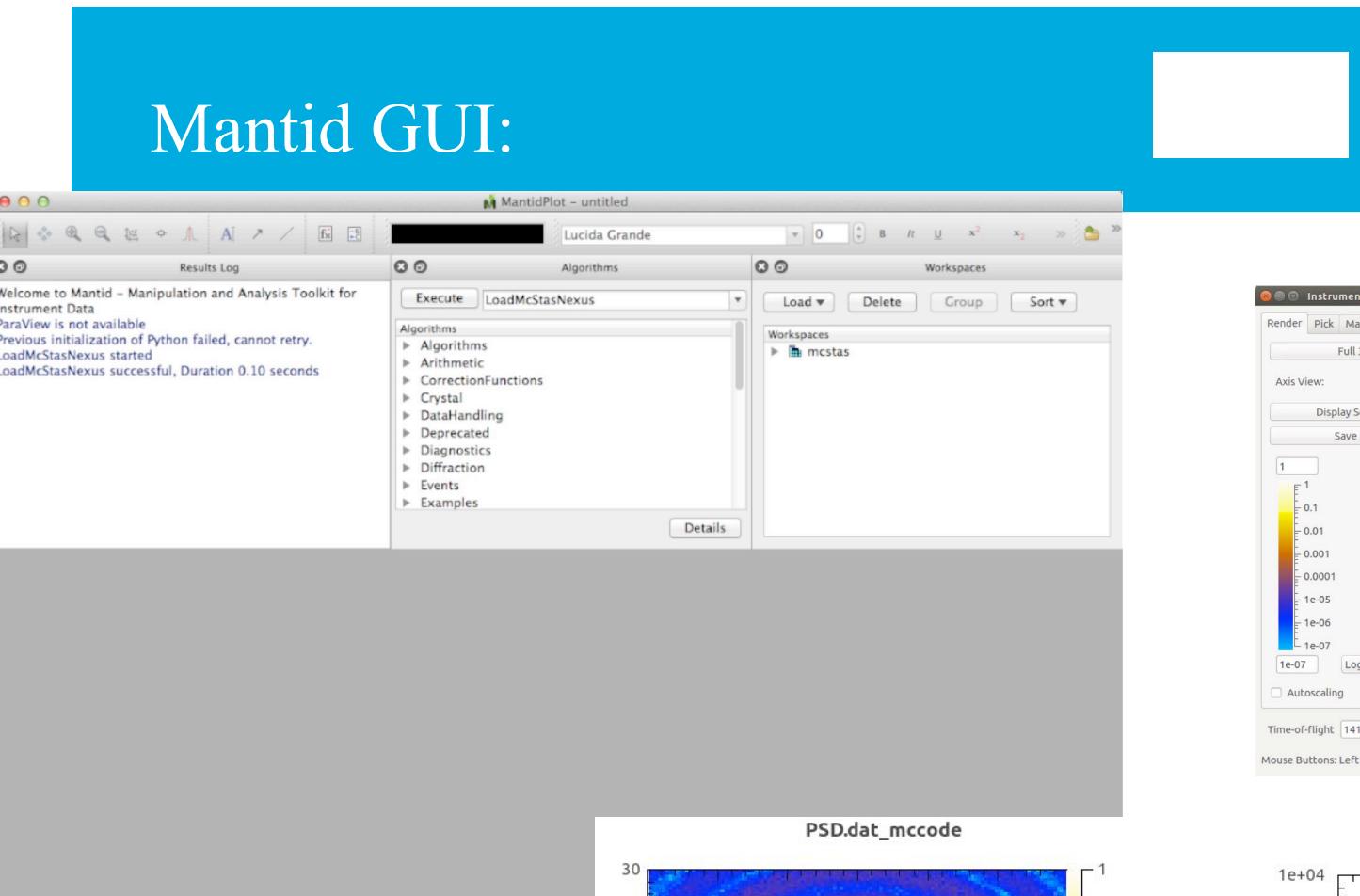
In this tutorial, you will write a simplified SANS instrument. When you have completed this tutorial, you will have learned the basics of mcstas.

- Requirements: mcstas 2.2a.



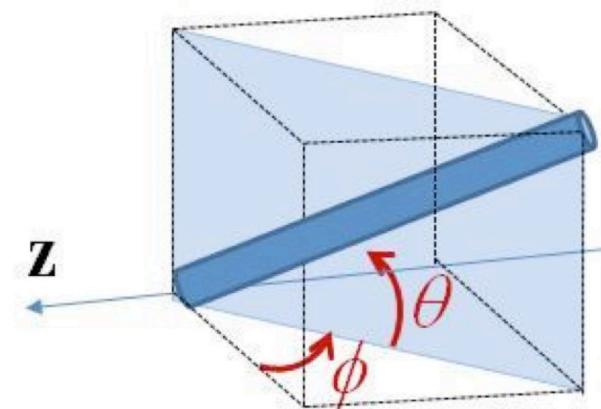


R=150,phi=0.1, d=1,a=0

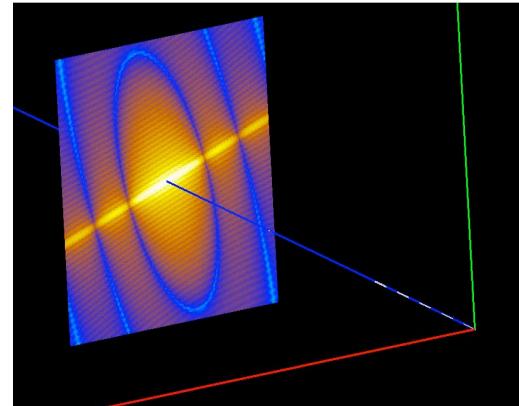
**McStas**



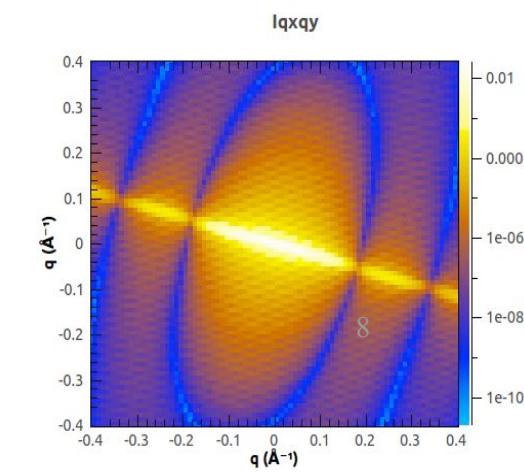
2021 Virtual  
ISIS  
McStas  
School



## Example: Usage of Mantid

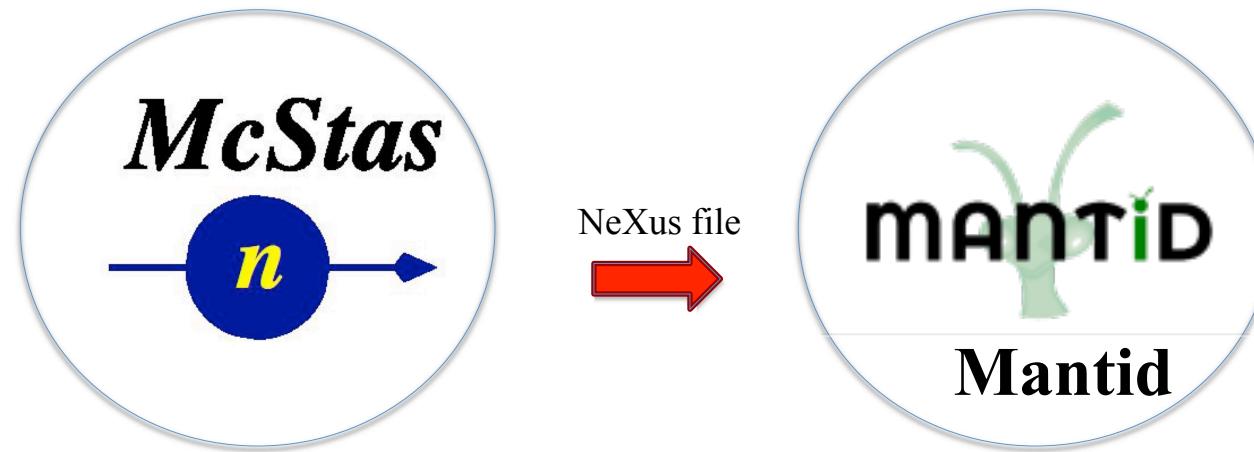


- McStas –Mantid
- 2D scattering kernel from SasView
- 2D reduction in Mantid: Qxy
- Can be send back to SasViewfitting





## 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

Instrument XML Data

TextView - data - /entry1/instrument/instrument\_xml/ - mccode.h5

Data selection: [0] ~ [0]

```
<?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>
```

Log Info Metadata

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

10



## 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  $k_f$



## 2021 Virtual ISIS McStas School

# 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](https://lanl.arxiv.org/abs/1607.02498)
- Built-into Mantid

**McStas and Mantid**  
Anders Markvardsen edited this page on Feb 27 · 45 revisions

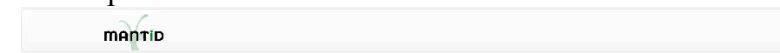
**A note on the McStas Mantid integration**

**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 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

Loads a McStas Nexus file into an workspace.

Filename	<input type="text"/>	Browse	*
OutputWorkspace	<input type="text"/>	*	
<input type="button" value="?"/>		<input type="button" value="Run"/>	<input type="button" value="Cancel"/>

LoadMcStas dialog.

### Summary

Loods 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.

**[1607.02498] McStas and Mantid integration - Mozilla Firefox**

lanl.arxiv.org/abs/1607.02498

Cornell University Library

Search or Article-id

Download:

- PDF only

Current browse context: physics.ins-det

< prev | next >  
new | recent | 1607

Change to browse by: physics

References & Citations

- INSPIRE HEP (refers to | cited by)
- NASA ADS

Bookmark (what is this?)

Comments: 17 pages, 12 figures, POSTPRINT with proofs of article submitted to Journal of Neutron Research

Subjects: Instrumentation and Detectors (physics.ins-det)



# 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(.... )**”

13



# templateSANS.instr vs templateSANS\_Mantid.instr

templateSANS.instr x templateSANS\_Mantid.instr x UNREGISTERED

```

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.instr x templateSANS\_Mantid.instr x UNREGISTERED

```

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 cql12
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
12

```

Line 10, Column 3 Tab Size: 4 Plain Text



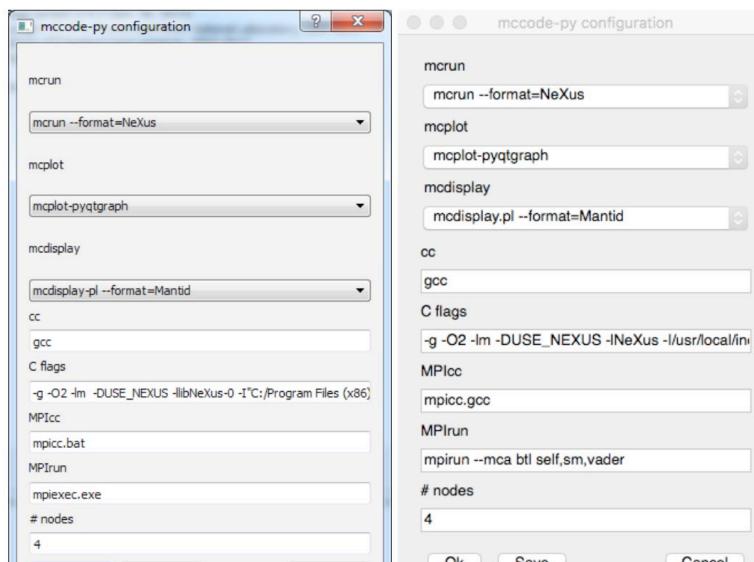
# How to run the simulation



## 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`

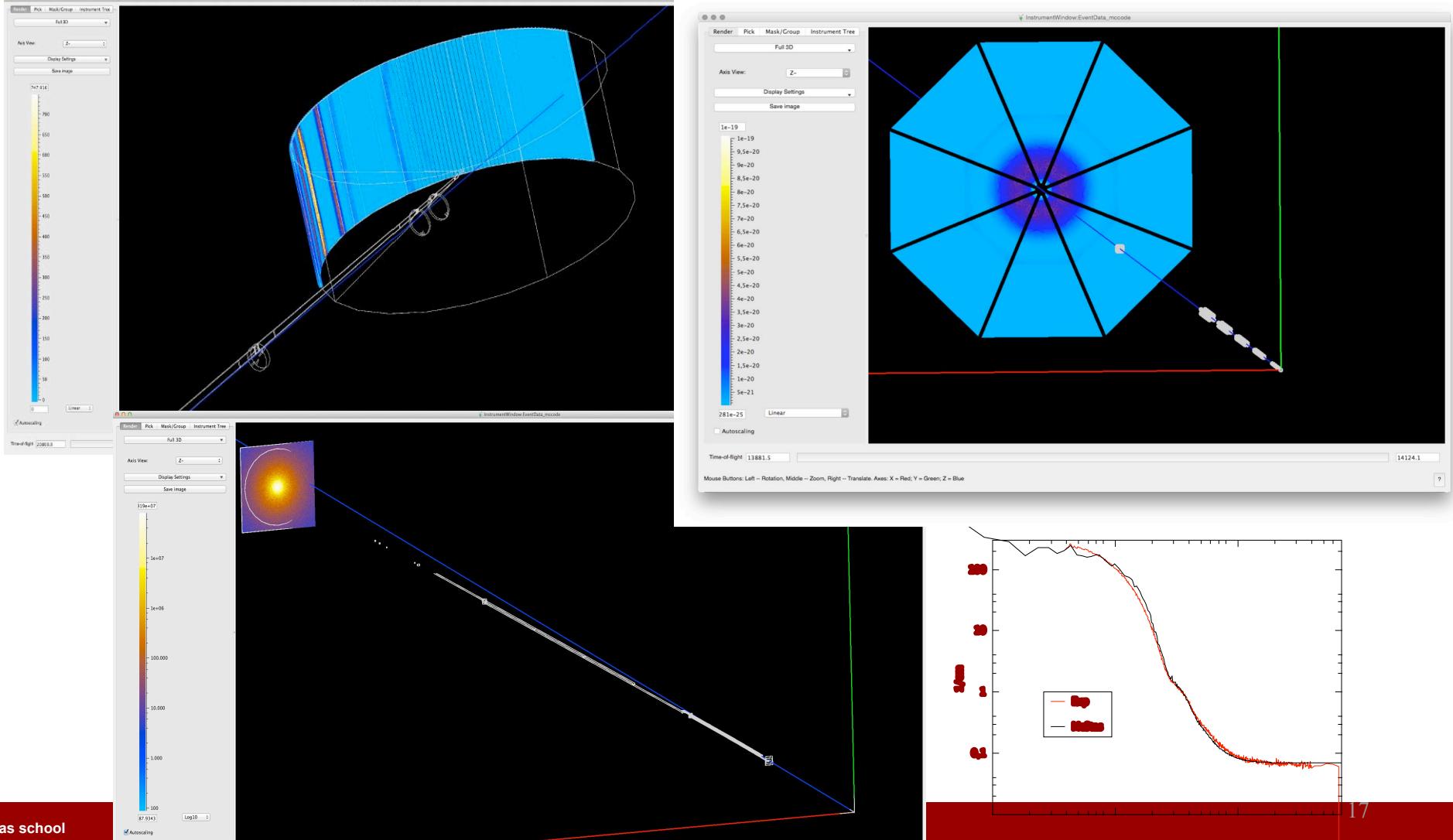


Wikipedia on GitHub



2021 Virtual  
ISIS  
McStas  
School

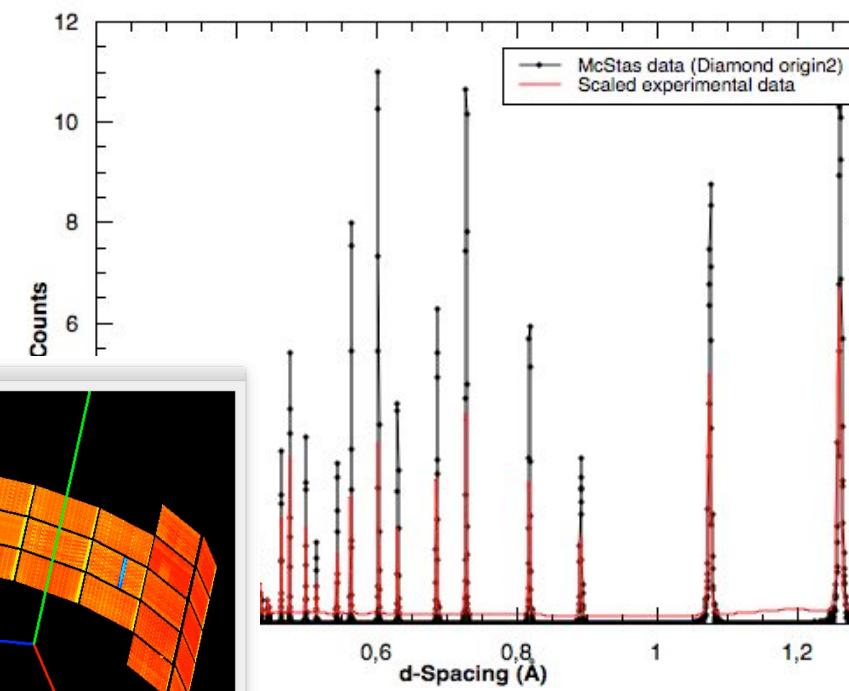
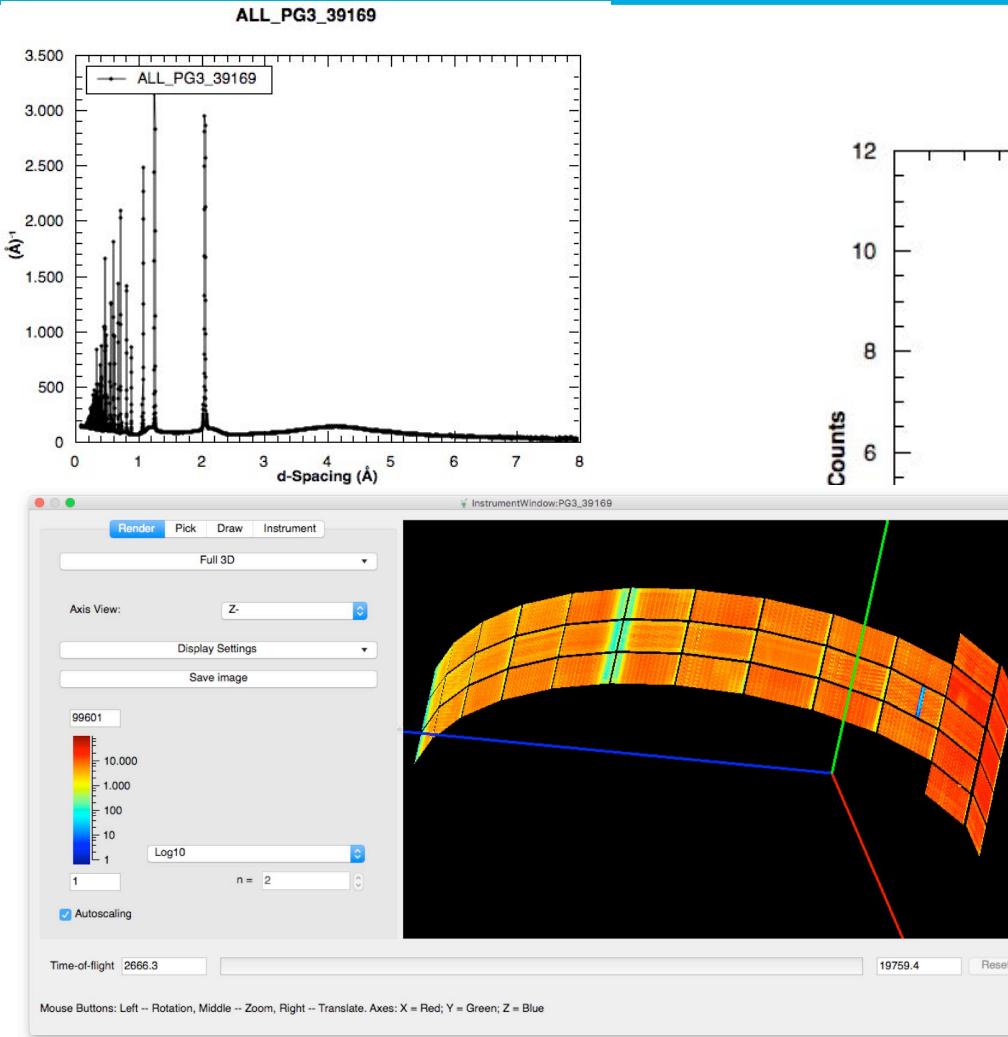
# Examples of detectors: IN5 (ILL), LoKI (ESS), SANS2D (ISIS)





2021 Virtual  
ISIS  
McStas  
School

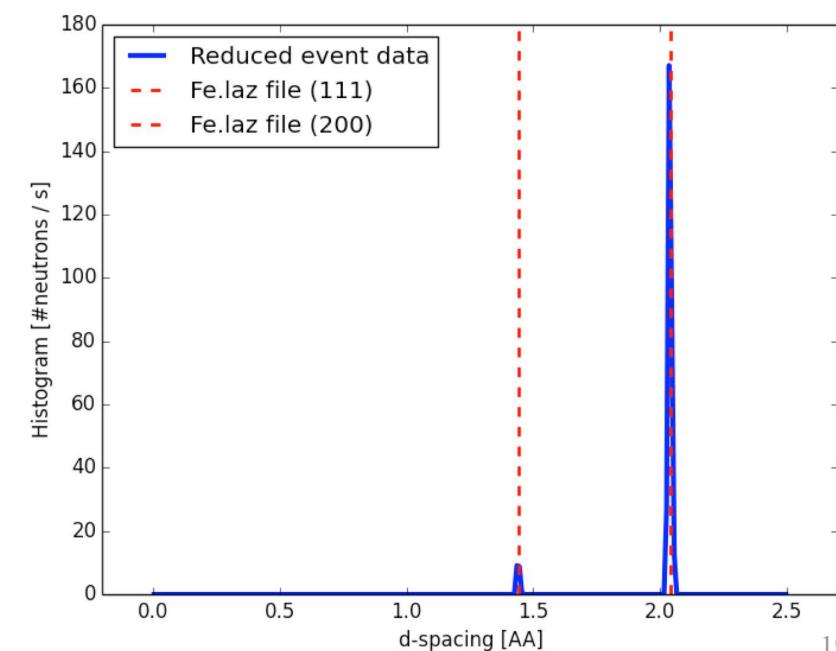
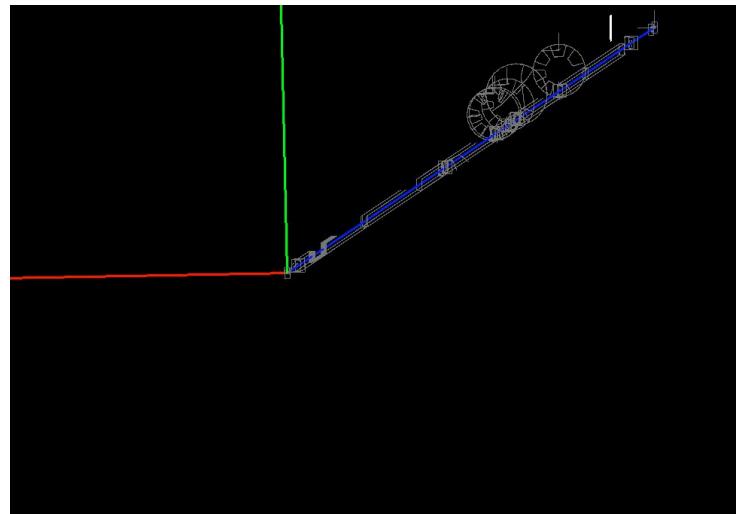
# McStas and experimental data: POWGEN



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

20