

# McStas - Mantid

Torben Nielsen

Anders Markvardsen

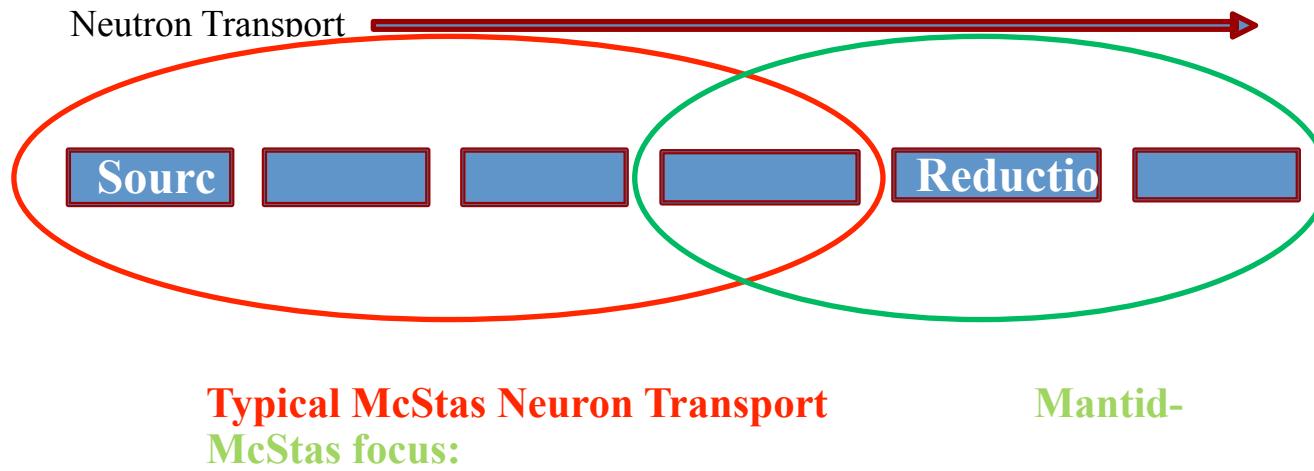
Peter Willendrup

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# Comparison

*Classic McStas*

Post processing:



mcstas - plot



mcstas - transport

*Mantid-McStas*

Post processing:



mantidplot



mcstas - transport

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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

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# Illustration: simplified SANS

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

McStas tutorial: sim... x +

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

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McStasMcXtrace / McCode

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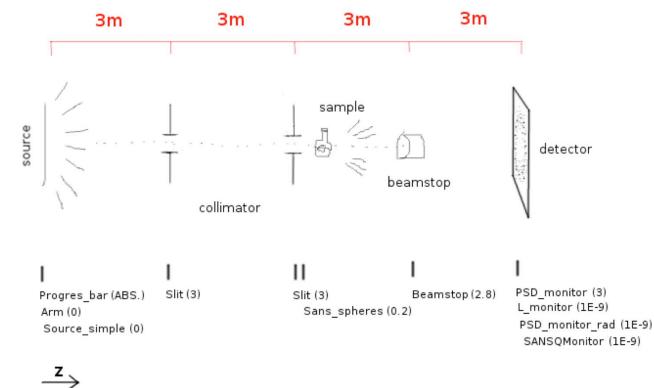
Code Issues 69 Pull requests 0 Projects 0 Wiki Pulse Graphs

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.



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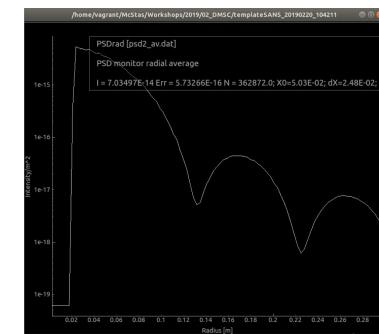
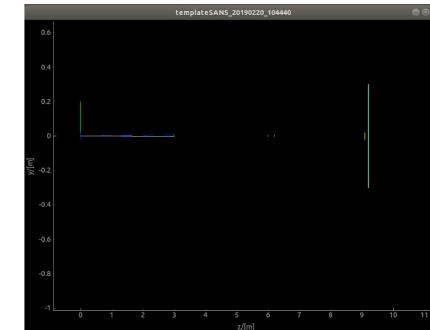
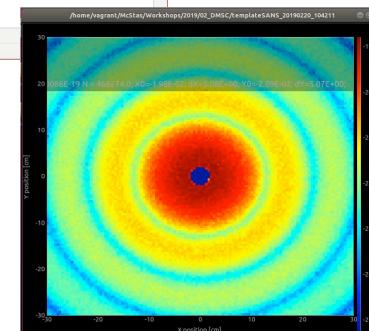
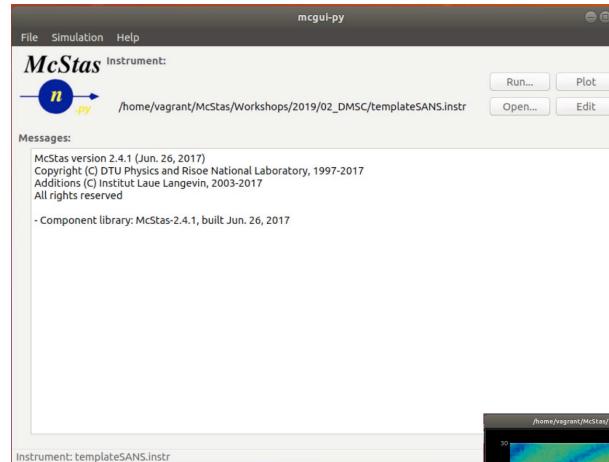
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**McStas**



R=150, phi=0.1,

## McStas GUI:



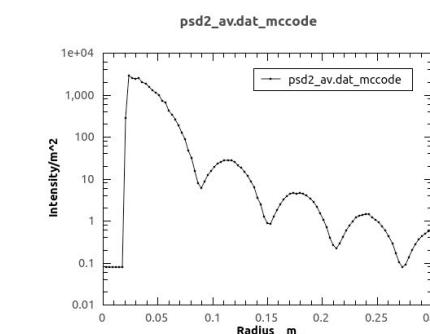
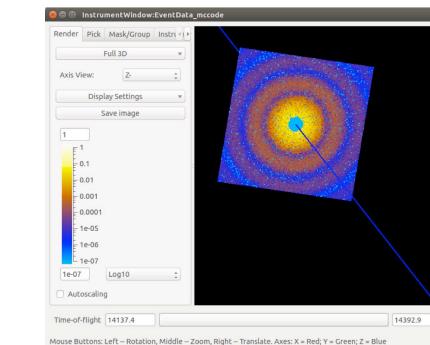
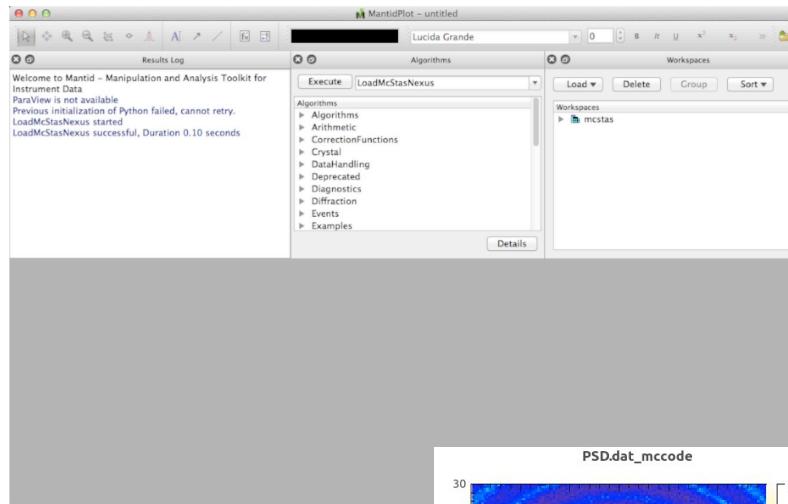
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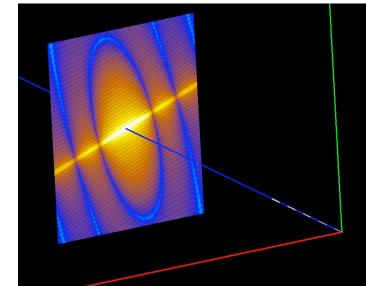
*McStas*



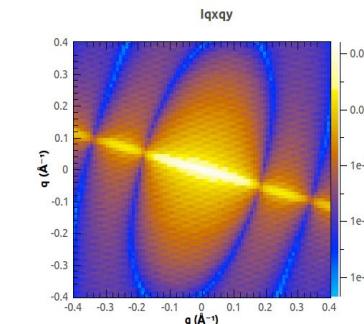
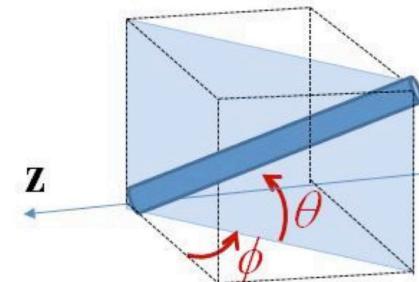
# Mantid GUI:



## Example: Usage of Mantid

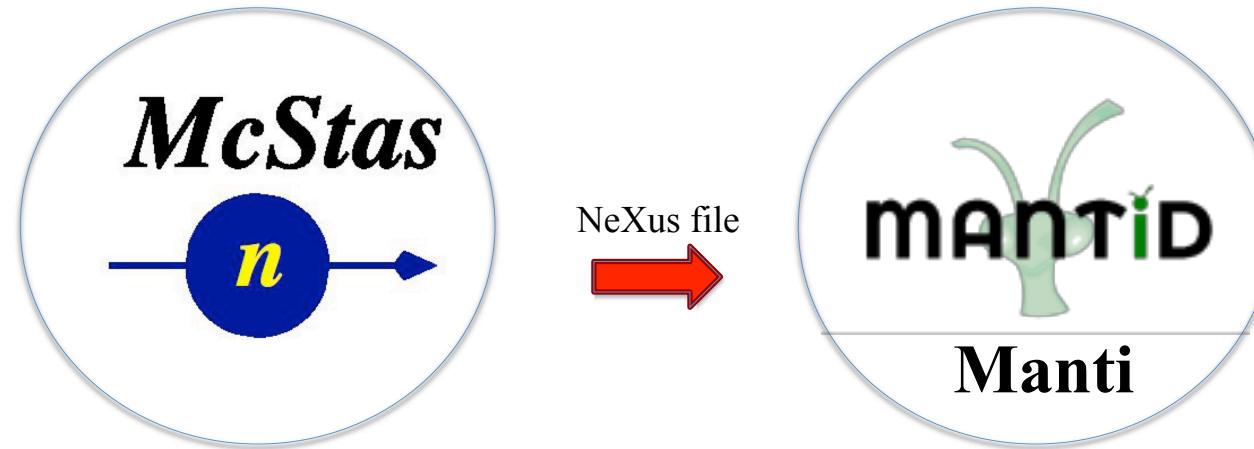


- McStas –Mantid
- 2D scattering kernel from SasView



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## The NeXus



- The McStas Nexus file must contain:
- Event data, i.e. each neutron has a pixel id and a time stamp

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**McStas**



# McStas NeXus

HDFView 2.9

Recent Files /home/ub/tmp/McStas\_Event/McStas/Exp\_Data/mccode.h5

Table View - 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

|    | 0           | 1            | 2            | 3    | 4       | 5   |
|----|-------------|--------------|--------------|------|---------|---|
| 0  | 3.185987... | -0.01450...  | 0.007932...  | 0.0  | 18717.0 | 0.025524...   |
| 1  | 3.192848... | 0.141796...  | 0.347311...  | 1.0  | 31227.0 | 0.046068...   |
| 2  | 2.989055... | -0.01409...  | -5.33756...  | 2.0  | 18333.0 | 0.025703...   |
| 3  | 3.001396... | -0.00520...  | -0.01711...  | 3.0  | 17759.0 | 0.025671...   |
| 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 | 0.041376...   |
| 7  | 0.022012... | 0.058801...  | -0.08114...  | 7.0  | 15195.0 | 0.088100...   |
| 8  | 6.984646... | 0.012643...  | -0.03070...  | 8.0  | 17      | Text View - data - /entry1/instrument/instrument_xml/ - mccode.h5                   |
| 9  | 8.530934... | -0.00867...  | 0.012712...  | 9.0  | 18      | Text  |
| 10 | 0.009140... | -0.07853...  | -0.07291...  | 10.0 | 19      | Data selection: [0] ~ [0]   |
| 11 | 7.150334... | -0.01082...  | 0.005151...  | 11.0 | 18      | <?xml version="1.0" encoding="UTF-8"?>  |
| 12 | 0.001010... | 0.457856...  | 0.087702...  | 12.0 | 21      | <!-- IDF generated using McStas McDisplay and the Mantid backend -->                |
| 13 | 0.004965... | 0.003146...  | -0.04262...  | 13.0 | 16      | <!-- For help on the notation used to specify an Instrument Definition File see     |
| 14 | 8.629457... | -0.03193...  | -0.02392...  | 14.0 | 17      | <a href="http://www.mantidproject.org/IDF">http://www.mantidproject.org/IDF</a> --> |
| 15 | 7.072494... | 0.015294...  | -0.01158...  | 15.0 | 17      | <instrument name="ISIS_SANS2d_Mantid.out" valid-from="1900-01-31 23:59:59"          |
| 16 | 3.898581... | -2.38144...  | 0.011657...  | 16.0 | 18      | valid-to="2100-01-31 23:59:59" last-modified="Tue Apr 4 14:17:50 2017">             |
| 17 | 3.479036... | -0.02370...  | -0.00281...  | 17.0 | 18      | </defaults>   |
| 18 | 5.870513... | 0.0066430... | 0.006773...  | 18.0 | 18      | <length unit="meter"/>  |
| 19 | 0.010325... | -0.07164...  | -0.01926...  | 19.0 | 17      | <angle unit="degree"/>  |
| 20 | 3.191063... | -0.00829...  | -0.00252...  | 20.0 | 18      | <reference-frame>   |
| 21 | 3.746034... | -0.00570...  | 0.011052...  | 21.0 | 18      | <!-- The z-axis is set parallel to and in the direction of the beam. The            |
| 22 | 0.003724... | 0.036904...  | 0.029156...  | 22.0 | 19      | y-axis points up and the coordinate system is right handed. -->                     |
| 23 | 3.316878... | -0.00442...  | 1.6097504... | 23.0 | 18      | <along-beam axis="z"/>  |
| 24 | 0.023456... | -0.03083...  | 0.084904...  | 24.0 | 21      | <pointing-up axis="y"/>   |
| 25 | 0.001505... | 0.031248...  | -0.02562...  | 25.0 | 17      | <handedness val="right"/>   |

IDF xml

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## IDF xml data, TOF and



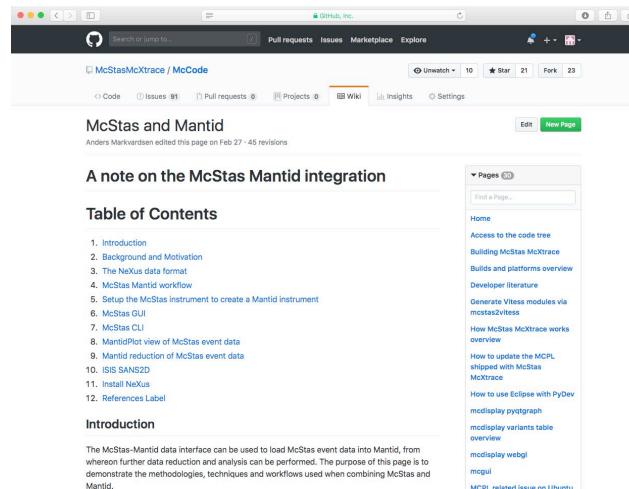
- Mantid's IDF store geometry information used in TOF analysis
- This implies parsing information about:
  - where the neutron source is located,

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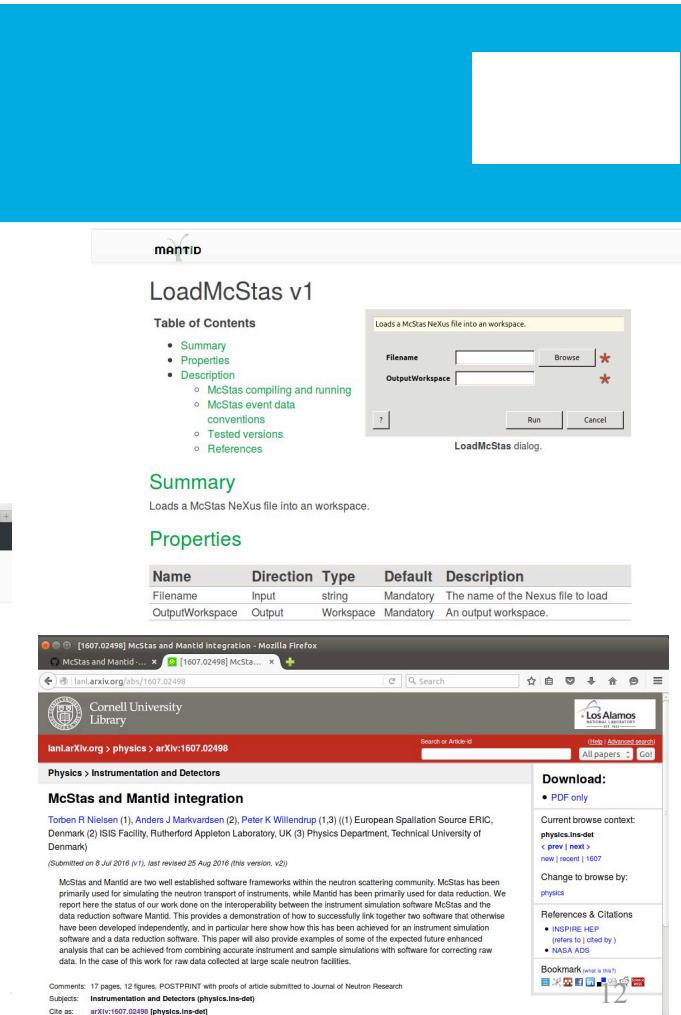


# How to use: Online

- GithubMcStas wiki pages
- Archive - lanl.arXiv.org



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



The top part of the image shows the 'LoadMcStas v1' dialog box, which allows users to load a McStas Nexus file into a workspace. It has fields for 'Filename' and 'OutputWorkspace' with a 'Browse' button, and buttons for 'Run', 'Cancel', and a help icon. Below this is a 'Summary' section describing the dialog's function. The bottom part shows a screenshot of an arXiv.org article page titled 'McStas and Mantid integration' by Torben R Nielsen et al. The page includes details about the software integration, download options (PDF only), and citation information.

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## McStas event



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(.... )**”

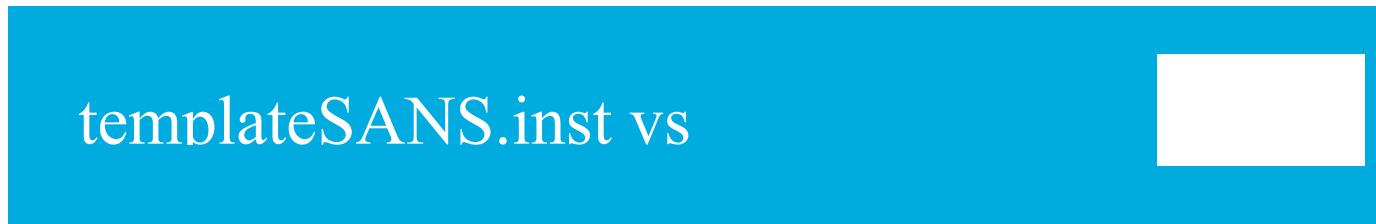
In the McStas instrument file the source must be named  
**“sourceMantid”**

- E.g. “**COMPONENT sourceMantid= Source\_simple(.... )**”

In the McStas instrument file the sample must be named  
**“sampleMantid”**

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*McStas*



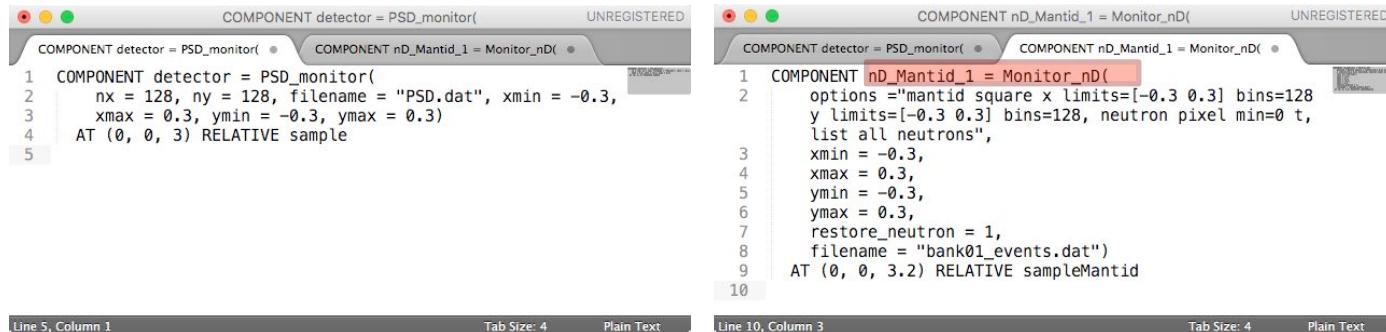
```
templateSANS.instr x templateSANS_Mantid.instr x UNREGISTERED
1 DEFINE INSTRUMENT templateSANS(lambda=6, dlambd=0.05, r=100, PHI=1e-3, Delta_Rho=0.6, sigma_abs=0.5)
2
3 TRACE
4
5 COMPONENT a1 = Progress_bar()
6 AT (0,0,0) ABSOLUTE
7
8 COMPONENT arm = Arm()
9 AT (0, 0, 0) ABSOLUTE
10
11 COMPONENT 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



```

COMPONENT detector = PSD_monitor( UNREGISTERED
COMPONENT nD_Mantid_1 = Monitor_nD( UNREGISTERED
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 detector = PSD_monitor( UNREGISTERED
COMPONENT nD_Mantid_1 = Monitor_nD( UNREGISTERED
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

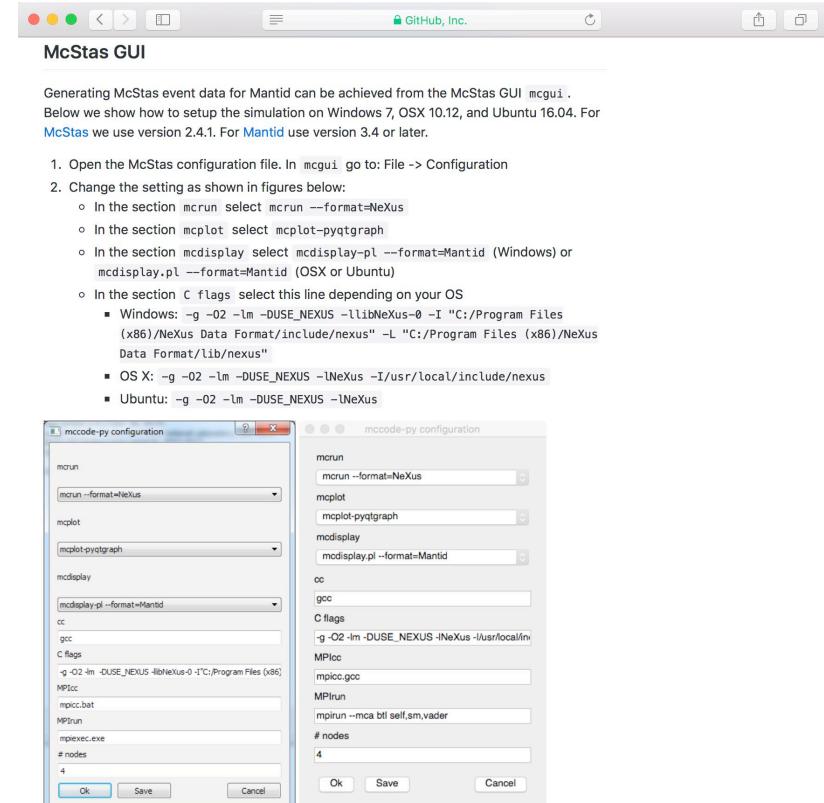
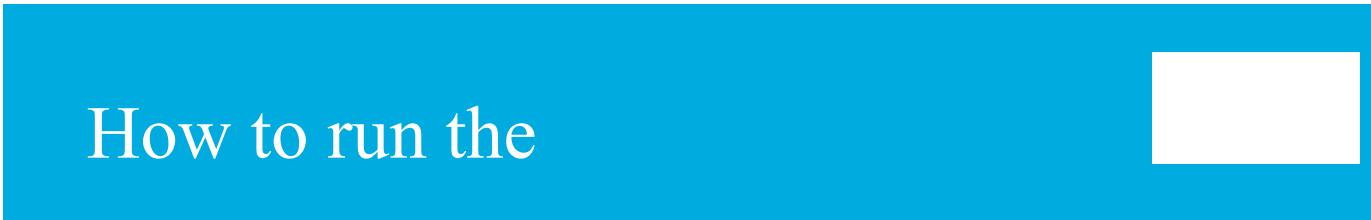
```

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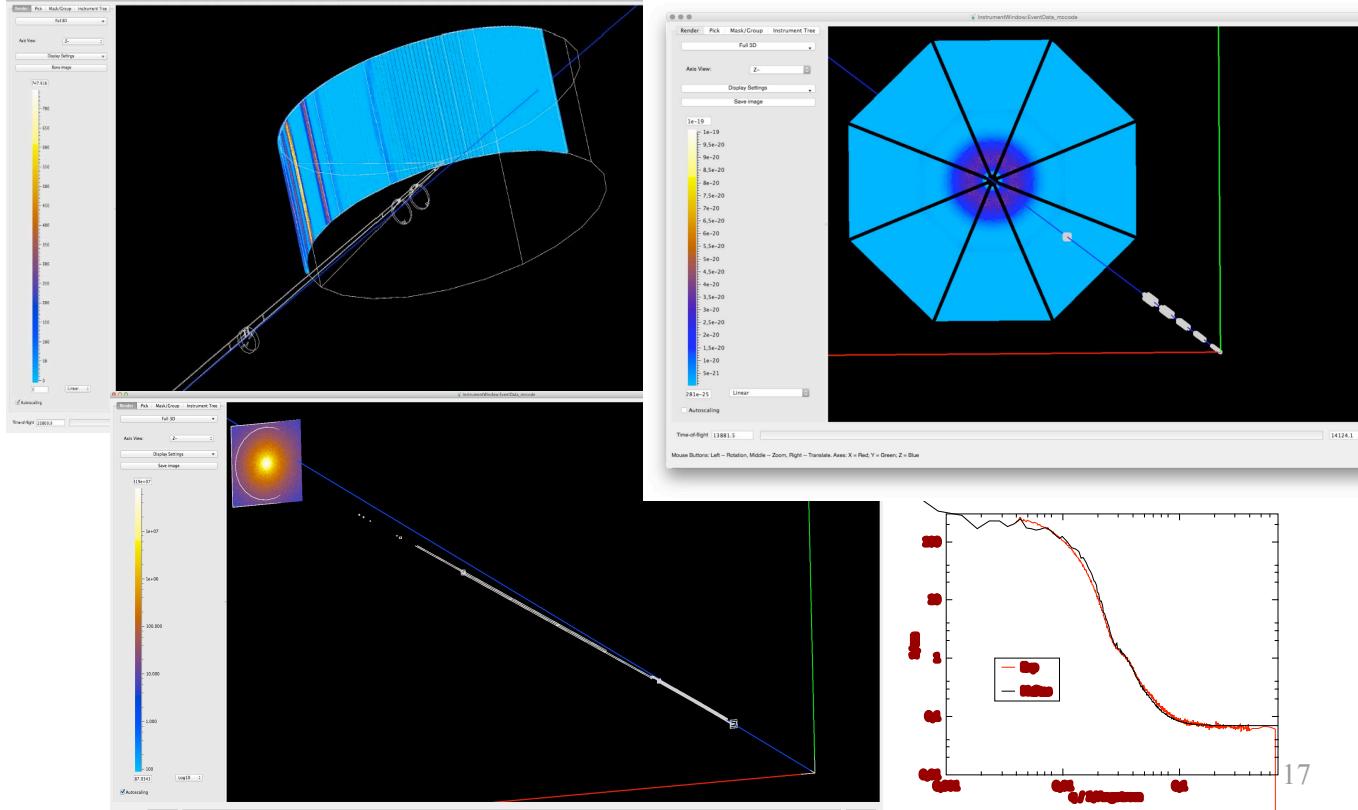


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Wikipage on GitHub

# Examples of detectors: IN5

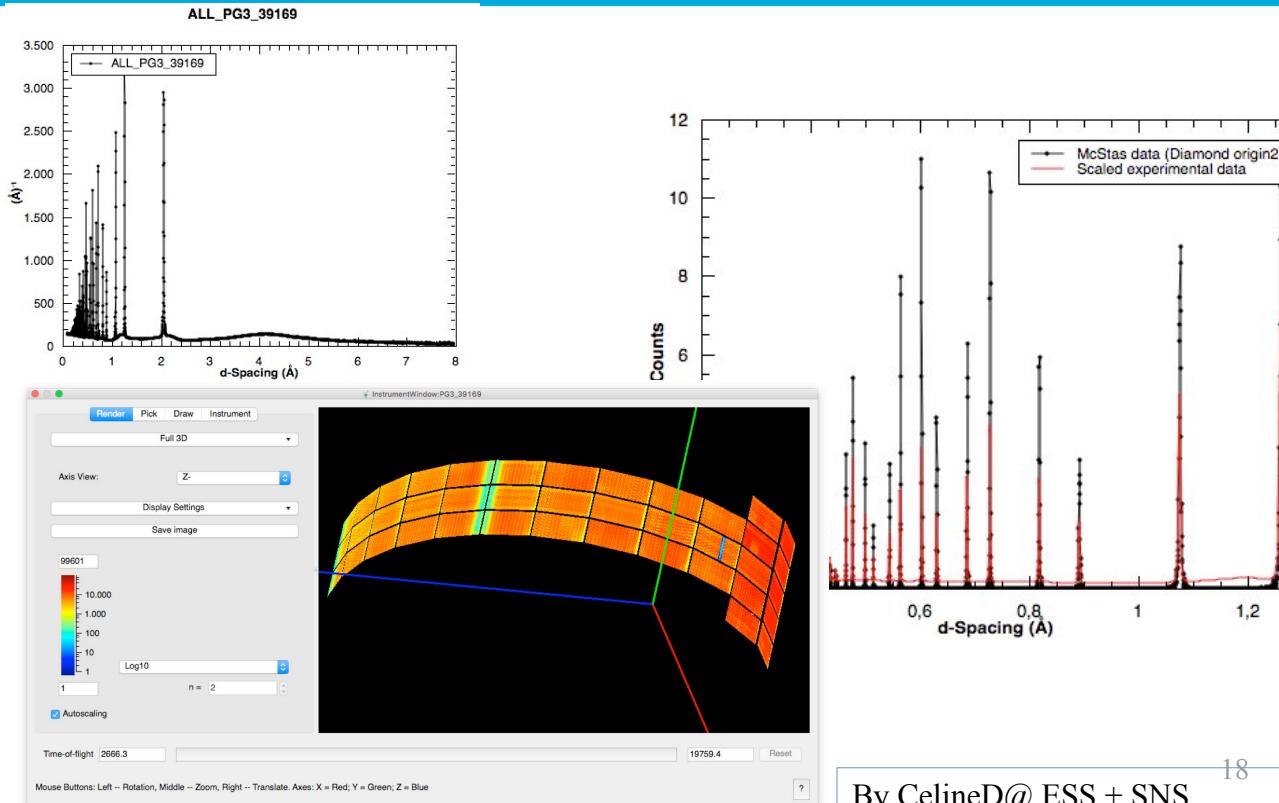


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**McStas**



## McStas and experimental data:

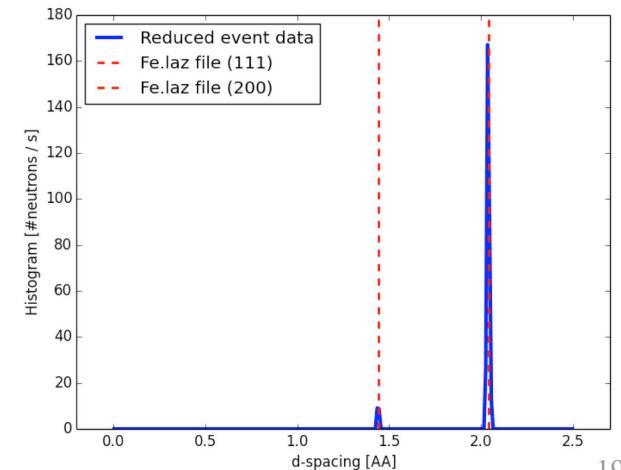
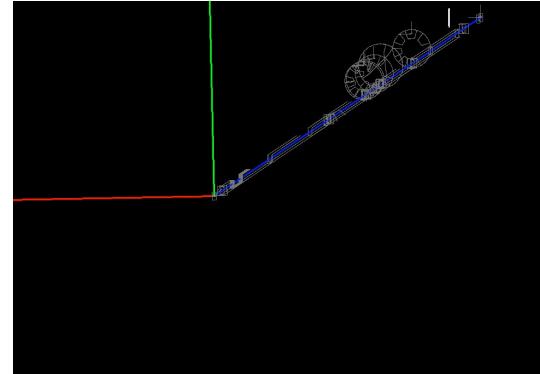


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By CelineD@ ESS + SNS



## Example –V20 –Powder



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## Summar



1. Easier to post-process (event) data than making a completely new McStas simulation / component
  - E.g.:
  - Rebinas needed
  - Sum selective over detectors
  - Use already developed methods in Mantid

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