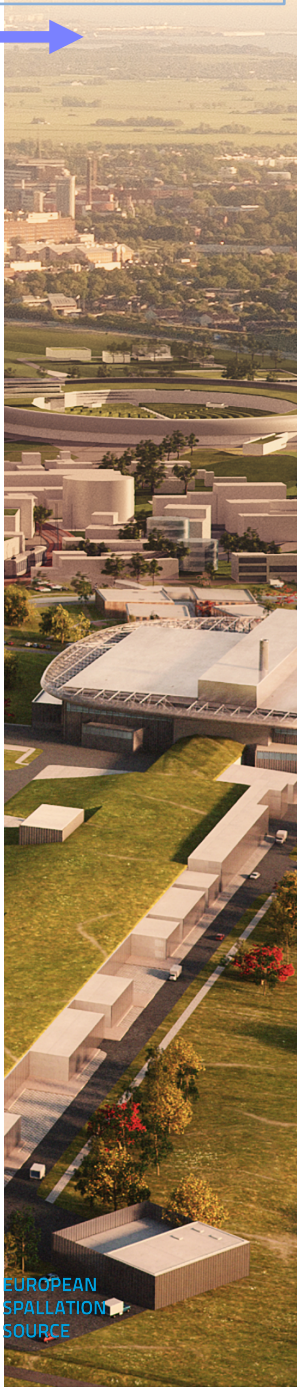
McStas - Mantid



ESS McStas Training 2016

May 30th - June 1st

EUROPEAN SPALLATION SOURCE

McStas

DTU PAUL SCHERRER INSTITUT PSI NEUTRONS FOR SCIENCE

EUROPEAN SPALLATION SOURCE

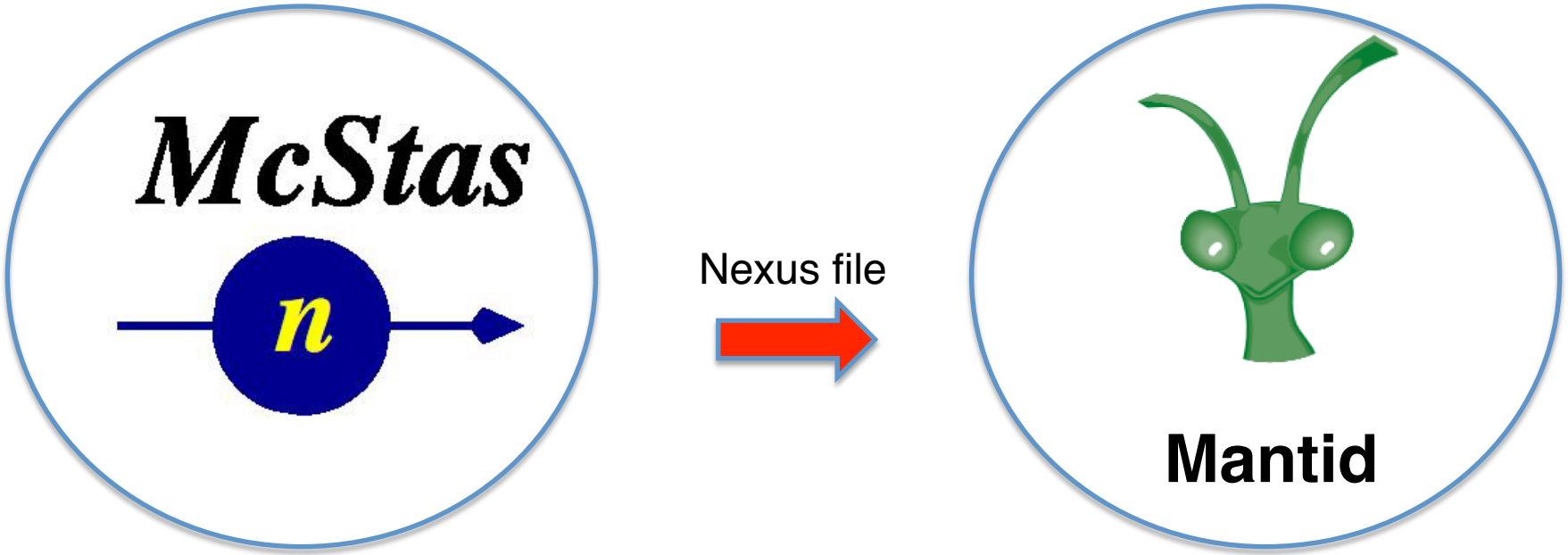
Exercise: McStas-Mantid

Purpose of the exercise is to be familiar with some McStas–Mantid key words

- Learn how to use McStas-Mantid interface
- Learn about the Nexus file format
- Learn about IDF (Mantid Instrument Definition file)
- Learn how-to use already developed (reduction) algorithms in Mantid
- Learn about Python scripting in Mantid

- McStas files:
  - templateSANS.instr
  - templatedSANS_Mantid.instr
  - templatedSasview_Mantid.instr

McStas-Mantid workflow



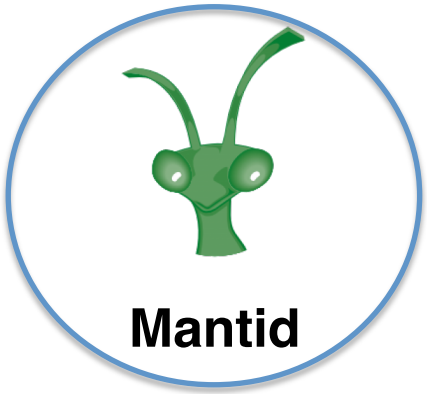
- The McStas Nexus file must contain:
- Event data, i.e each neutron has a pixel id and a time stamp
- An IDF
- McStas monitor_nD gives pixle id & time for each event
- mcdisplay can auto-generate an IDF

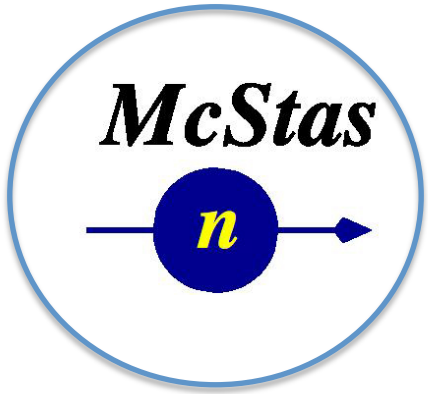
NeXus fileformat

- A number of large-scale neutron facilities use the NeXus data format for storing neutron data.
- NeXus is derived from the Hierarchical Data Format (HDF)
- Mantid uses the Nexus file format
- McStas can out put Nexus file format

Neutron information

Information only available on detector planes





# 2 paramtes	# 11 parameters
pixel id	
time	
	t: time
	r: coordinates x,y,z
	v: velocity vx,vy,vz
	s: spin sx, sy,sz
	p: neutron weight

Mantid: IDF & TOF

- 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.

McStas – Mantid: Rules I

How-to generate McStas event data for Mantid

Step 1. Compile McStas instrument code:

- mcstas templateSANS_Mantid.instr –trace

Step 2. Compile c code:

- gcc -o templateSANS_Mantid.out templateSANS_Mantid.c -lm -DUSE_NEXUS -lNeXus

Step 3. Generate IDF:

- mcdisplay templateSANS_Mantid.instr --format=Mantid -n0

Step 4. Run simulation:

- ./templateSANS_Mantid.out --format=Nexus

McStas – Mantid: Rules II

McStas event data conventions

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(….)"

Exercise I: McStas-Mantid

- Load templateSANS.instr
- Run simulation in mcgui (only ascii – no Nexus yet)
- Plot data

- Load templateSANS_Mantid.instr
- Run simulation in mcgui (only ascii – no Nexus yet)
- Plot data

- Compare results
- Whys does scattering pattern (and intensity) differ on the two versions?

Exercise II: McStas-Mantid

- Use templateSANS_Mantid.instr to make a Nexus file for Mantid
- Compile McStas code (See Rules I)
- Make IDF file
- Run simulation
- Start Mantid
- Load data into Mantid
- Play with Mantid interface

Exercise III: McStas-Mantid

- Use templateSANS_SasView.instr to make a nexus file for Mantid
- Compile McStas code (See Rules I)
- Make IDF file
- Run simulation
- Start Mantid
- Load data into Mantid
- Reduce event data in Mantid as described in the templateSANS_SasView.instr file

Exercise IV: McStas-Mantid

- Load ISIS_SANS2D.instr
- Edit *.instr file and make it ready for Mantid
- Use the Rules I & II
- Compile McStas code
- Make IDF file
- Run simulation
- Start Mantid
- Load data into Mantid
- Reduce data in Mantid
- Does data fit?

Exercise V: McStas-Mantid

- Write a python script in Mantid which will load and reduce the data
- Use data from templateSasView_Mantid.instr
- See link below about Mantid and Python
- TIP: one can save the “history” of used algorithms operations on an data set into a python file

Exercise VI: McStas-Mantid

- Write your own IDF file for templateSANS_Mantid.instr
- Look at the Mantid link on howto generate an IDF (See link below)
- Or search for IDF in Mantid search tool

Exercise VII: McStas-Mantid

- Download HDF view or nexpy (python package) to look inside a HDF file
- Open mccode.h5 from the templateSANS_Mantid.instr file and search for the IDF data
- Browse through the meta data in the file

Exercise VIII: McStas-Mantid

- Load templateSANS_Mantid.instr
- Make one simulation with Nexus output data for Mantid

- Remove the “Beam Stop” in the templateSANS_Mantid.instr file
- Make a second simulation with Nexus output data for Mantid

- Remove the “Sample” in the templateSANS_Mantid.instr file
- Make a thrid simulation with Nexus output data for Mantid

- Use the same “seed” for all simulations, eg. –seed=117
- Compare the three simulations in Mantid. When should they be equal?

Summary

- You should have learned how to use McStas and Mantid
- With a little training be convinced that many of Mantid algorithms can easily be used for virtual experiments (McStas simulations)

Links

McStas:
https://github.com/McStasMcXtrace/McCode/wiki/McStas-and-Mantid

IDF:
http://docs.mantidproject.org/nightly/concepts/InstrumentDefinitionFile.html

NeXus:
http://www.nexusformat.org

HDF view:
https://www.hdfgroup.org/HDF5/

Mantid and Python:
http://www.mantidproject.org/Python_In_Mantid