

Notions on McStas & Mantid

Kalliopi Kanaki
Jamboree Risø
September 5, 2016

Outline

- Brief introduction to McStas
- Interface with dgcode/Geant4

- Brief introduction to Mantid
- Interface with dgcode/Geant4

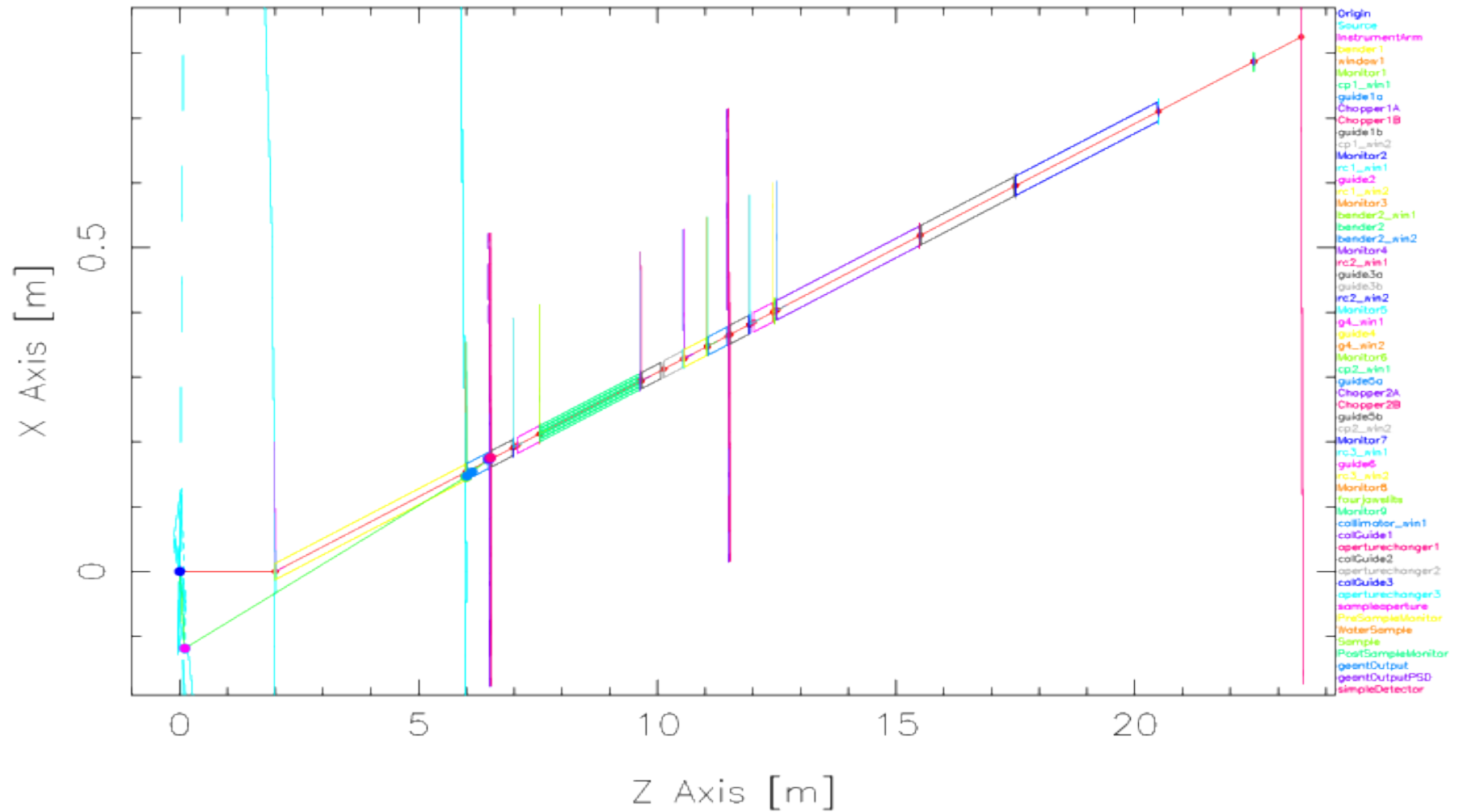
- McStas – Mantid interface without Geant4

McStas: A neutron ray-trace simulation package

- <http://mcstas.org/>, use latest version 2.3
- Used for instrument design and optimization
 - includes ESS source (pancake, butterfly moderators)
 - instrument components, e.g. benders, guides, choppers, collimators
 - sample models: either from McStas or extern sources, e.g. SasView for SANS
 - list of available samples: <https://ess-ics.atlassian.net/wiki/display/MCSTAS/McStas+pages>
- Well-documented how to install and run on multiple platforms (Linux, Mac)
- Plenty of advanced instrument files available from LoKI:
<https://bitbucket.org/essloki/loki-mcstas-master/src>
- Wiki documentation on how to run it on the DMSC cluster on several cores for high statistics production:
<https://ess-ics.atlassian.net/wiki/display/DG/How+to+work+at+the+DMSC#HowtoworkattheDMSC-McStasandMantid>
- Basic but non-interactive visualization tools available within McStas
- Analysis is preferable with monitor data dump from McStas + python/matlab/excel tools
 - python example analysis of L_monitor output:
dg_dgcode/packages/Projects/SansLoki/McStasLoki/scripts/overlayMonL

LoKI view in McStas

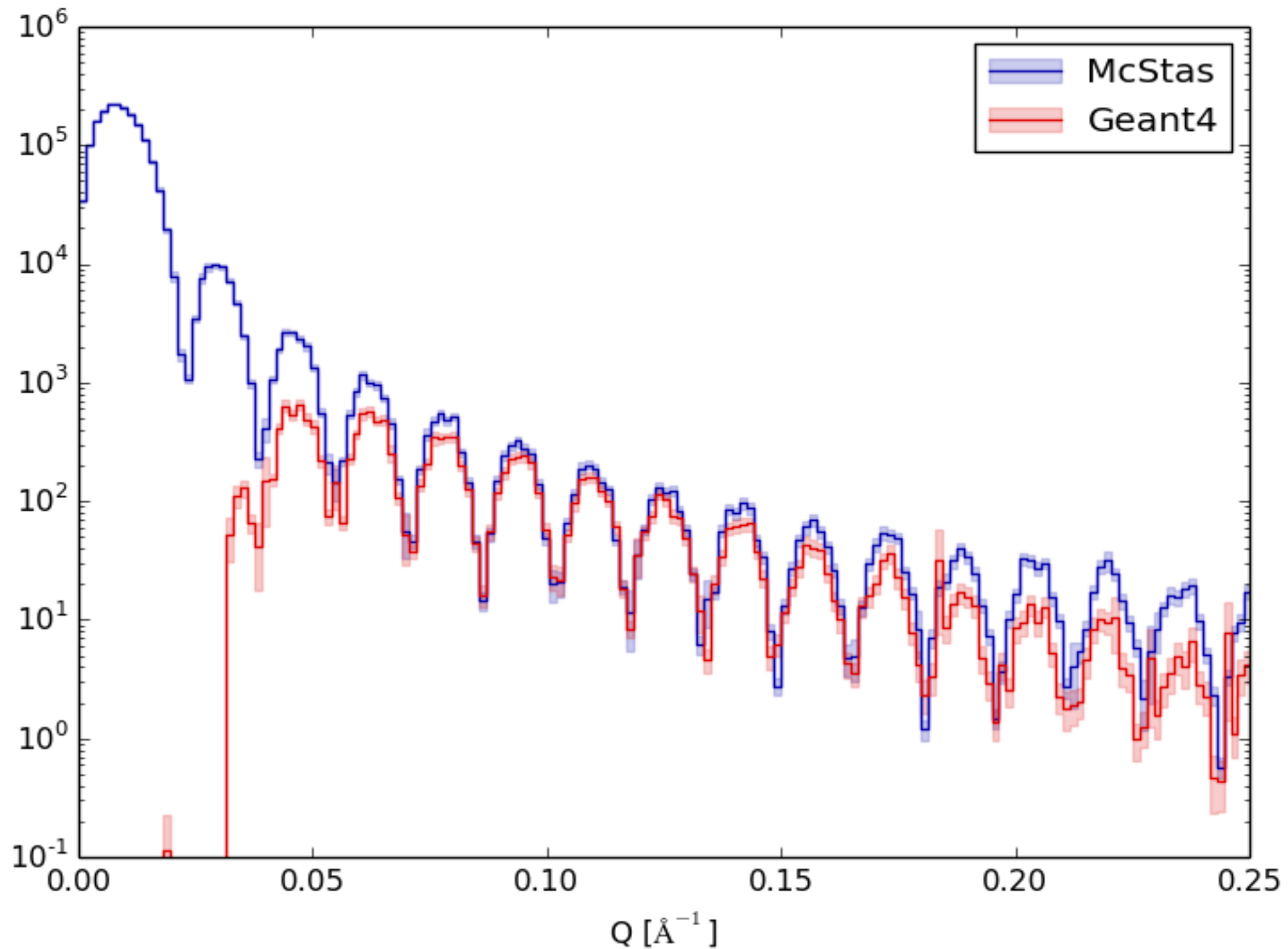
Z-X view: loki-master-model.out



McStas interface to Geant4

- Need for “realistic” Geant4 input with sample-related neutron properties for detector optimization → stop McStas simulation after scattering on sample and feed output to G4
- So far ASCII files from Monitor_nD componentn were used
 - too large and slower to read → abandoned
- Better solution available: MCPL format (Monte Carlo Particle List)
 - McStas components in place for use
 - Wiki documentation on how to read the mcpl files and run a G4 simulation with them
<https://ess-ics.atlassian.net/wiki/display/DG/McStas+to+Geant4+interface+via+the+MCPL+format>
 - use the cluster and python scripts to launch parallel processes (link and script to be added this week)

LoKI example: raw Q distribution at the sample and after detection



The Mantid Project

- <http://www.mantidproject.org/>
- Software package for visualization and data treatment of neutron instruments
- Runs on multiple platforms (Linux, Mac, Windows)
- GUI available for data handling for several default actions
- Python user interface for repetitive, elaborate, customized data analysis
- Recent trainings for ESS (McStas and Mantid):

<https://ess-ics.atlassian.net/wiki/display/DGPrivate/Seminars+and+Training+Material>

Mantid interface to Geant4

- Mantid needs 2 inputs to work with data (simulated or real):
 - an IDF (instrument definition file) containing a geometry description of the detector anode
 - a nexus file (hdf5) containing data and detector channel IDs
- Joined effort from DG and the Mantid team at ISIS to import the BandGEM detector geometry to Mantid, as the most complicated example available with new geometrical shapes, previously non-existent

<https://ess-ics.atlassian.net/wiki/pages/viewpage.action?pageId=12780504>

- New code features available in the master version

<http://download.mantidproject.org/> NOT in code release yet

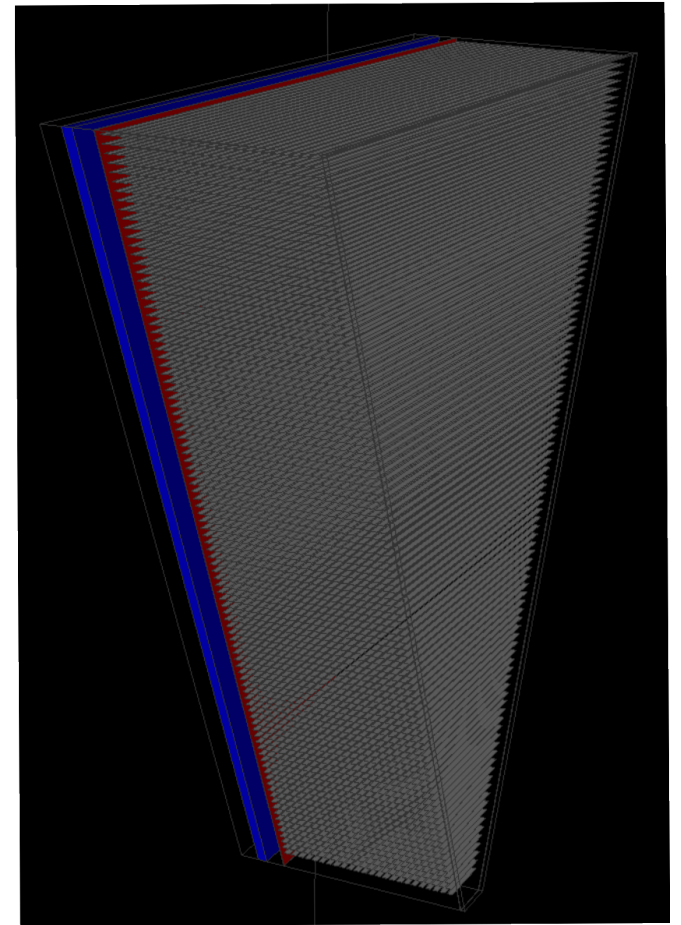
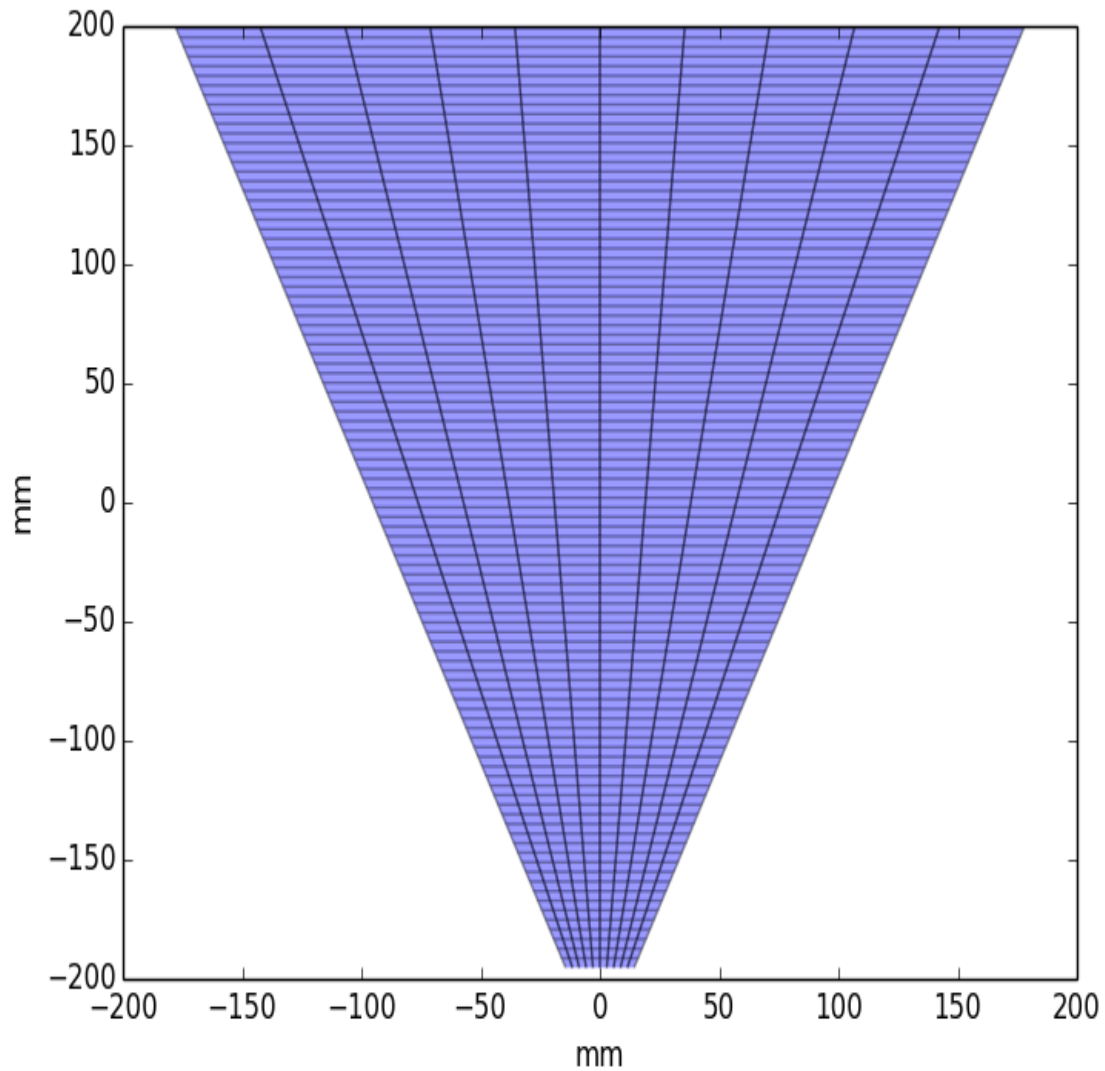
- Ultimate goals:
 - Visualization of detector geometry and sensitive area (event display)
 - Calibration and reduction routines for B10 detectors based on simulated data

The IDF: instrument definition file

- The IDF file is an XML document containing the geometry description of the detector (anode)
- Examples on how to build an IDF file from Geant4
 - He3: function writeMantidXML():
`dg_dgcode/packages/Projects/He3Tubes/G4GeoHe3Tubes/pycpp_GeoHe3Sans/geometry_module.cc`
(the XML geometry has to be practically redefined)
 - BandGEM: dump anode pad coordinates and let Mantid build the XML file externally → better way
`dg_dgcode/packages/Projects/BandGem/G4GeoBandGem/libsrc/BandGemFrame.cc`
- Instruction on building IDFs and validation tools

<http://docs.mantidproject.org/nightly/concepts/CreateanIDF.html#create-an-idf>

The BANDGEM anode



Mantid view of BandGEM/LoKI IDF

InstrumentWindow:ws

Render Pick Draw Inst

Full 3D

Axis View: Z-

Display Settings

Save image

1

Linear

1 n = 2

Autoscaling

0 0 Reset

Mouse Buttons: Left -- Rotation, Middle -- Zoom, Right -- Translate. Axes: X = Red; Y = Green; Z = Blue

?

McStas interface to Mantid

- Already available without the need for Geant4 in the middle (detector effects are omitted)
- Useful tool for instrument scientists to plan experiments but also for instrument design
- Requires the user to define the detector geometry in McStas for more complex cases, e.g. LoKI
- nexus files from McStas, prepared with an appropriate sample component, can be read and displayed in Mantid (paper submitted)

Mantid data view (QxQy) with BandGEM detector of an azimuthally asymmetric sample

The screenshot displays the MantidPlot software interface. At the top, the title bar reads "MantidPlot - untitled". Below it is a standard Ubuntu desktop environment with a terminal window showing the following output:

```
Results Log
Load successful, Duration 4.20 seconds
Load started
Load successful, Duration 45.31 seconds
```

The main window is titled "InstrumentWindow:EventData_mccode - Instrument". It features a central plot area showing a QxQy data view with a color scale ranging from 1e-09 to 0.01. The plot is divided into several sectors by black lines. To the left of the plot is a control panel with tabs for "Render", "Pick", "Draw", and "Instrument". The "Render" tab is active, showing options for "Full 3D", "Axis View: Z-", "Display Settings", and "Save image". A color scale legend is visible, with a value of 311e-09 at the bottom. Below the plot, there are fields for "Time-of-flight" (13882) and "14173.4", along with a "Reset" button. At the bottom of the window, a mouse button legend states: "Mouse Buttons: Left -- Rotation, Middle -- Zoom, Right -- Translate. Axes: X = Red; Y = Green; Z = Blue".

Overlaid on the right side of the main window is a "Take Screenshot" dialog box. It has a title bar with a close button and the text "Take Screenshot". The dialog contains the following options:

- Grab the whole screen
- Grab the current window
- Select area to grab

Below these options is a field for "Grab after a delay of 0 seconds". Under the "Effects" section, there are two checkboxes:

- Include pointer
- Include the window border

The "Apply effect:" dropdown is set to "None". A "Take Screenshot" button is located at the bottom right of the dialog.

On the far right of the interface, there are two panels. The top one is "Workspaces", which includes buttons for "Load", "Delete", "Group", "Sort", and "Save". Below it is a tree view showing a workspace named "mccode" containing several data files: "EventData_mccode", "EdetSample.dat_mccode", "Edet.dat_mccode", "PSD.dat_mccode", "psd2_av.dat_mccode", and "psd2.dat_mccode". The bottom panel is "Algorithms", which has an "Execute" button and a list of algorithm categories: "Arithmetic", "CorrectionFunctions", "Crystal", "DataHandling", "Diagnostics", "Diffraction", "Events", "Examples", "Inelastic", "MDAlgorithms", "Muon", "Optimization", and "PythonAlgorithms".

At the bottom of the interface is a "Script Interpreter" window with the following text:

```
object? -> Details about 'object', use 'object??' for extra details.
%guiobj -> A brief reference about the graphical user interface.

In [1]:
```

Summary

- McStas-Geant4-Mantid interfaces are under development to match the needs of B10 detectors
- McStas input to Geant4 is an excellent tool for large detector optimization → read documentation and come to the experts for support
- Opportunity and necessity to help the Mantid people write the data reduction routines for B10 detectors
 - the geometry input has made great progress
 - data + channel ID input from Geant4 to follow by the end of the year
- In my view this is a concrete and sound methodology for taking the new technologies to the top of readiness scale → DG/LoKI has paved the way
- A workshop on detectors/Mantid may be organized this fall