# Notions on McStas & Mantid

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# Outline

- Brief introduction to McStas
- Interface with dgcode/Geant4

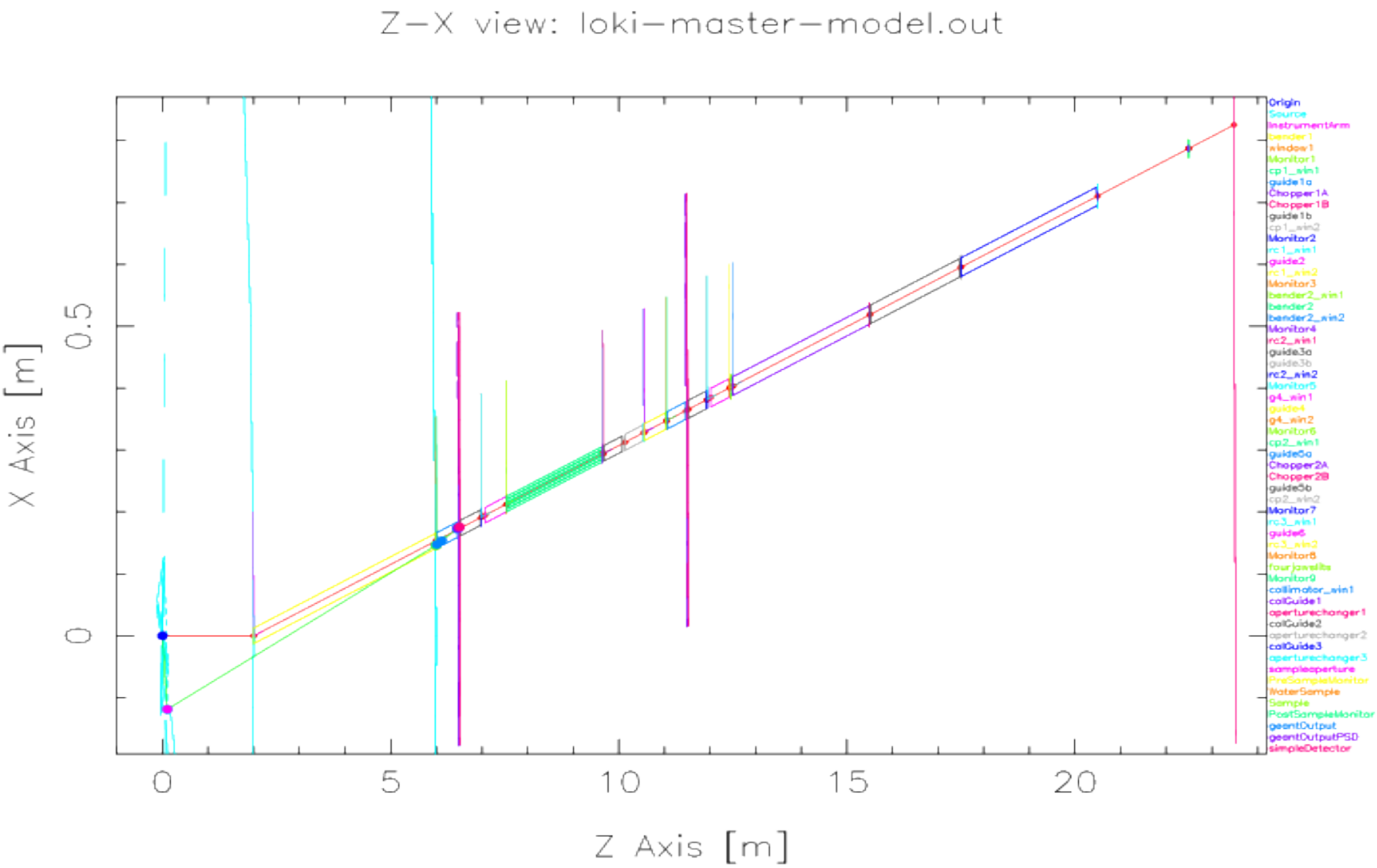
- Brief introduction to Mantid
- Interface with dgcode/Geant4

- 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

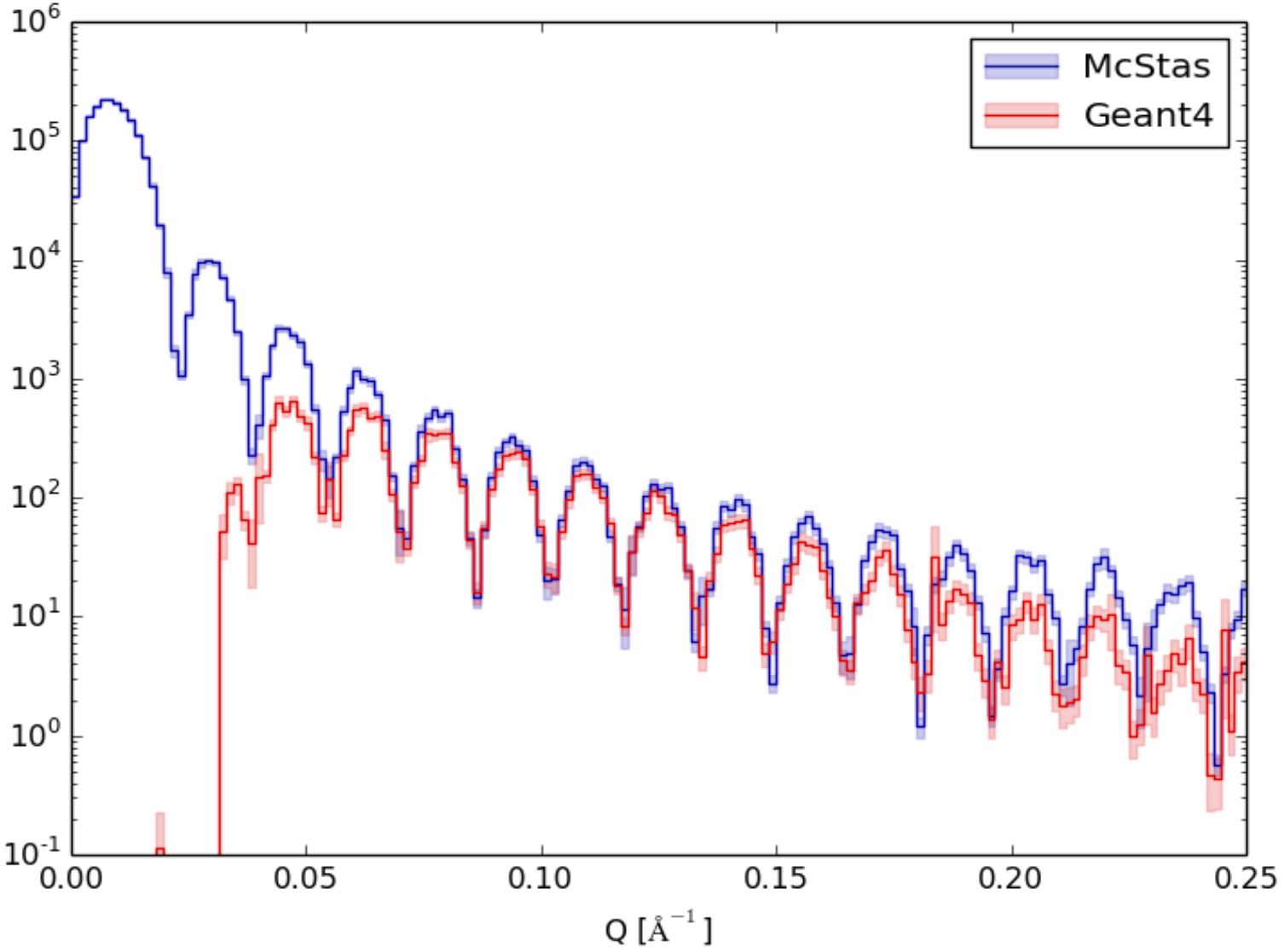


# McStas interface to Geant4

- 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():

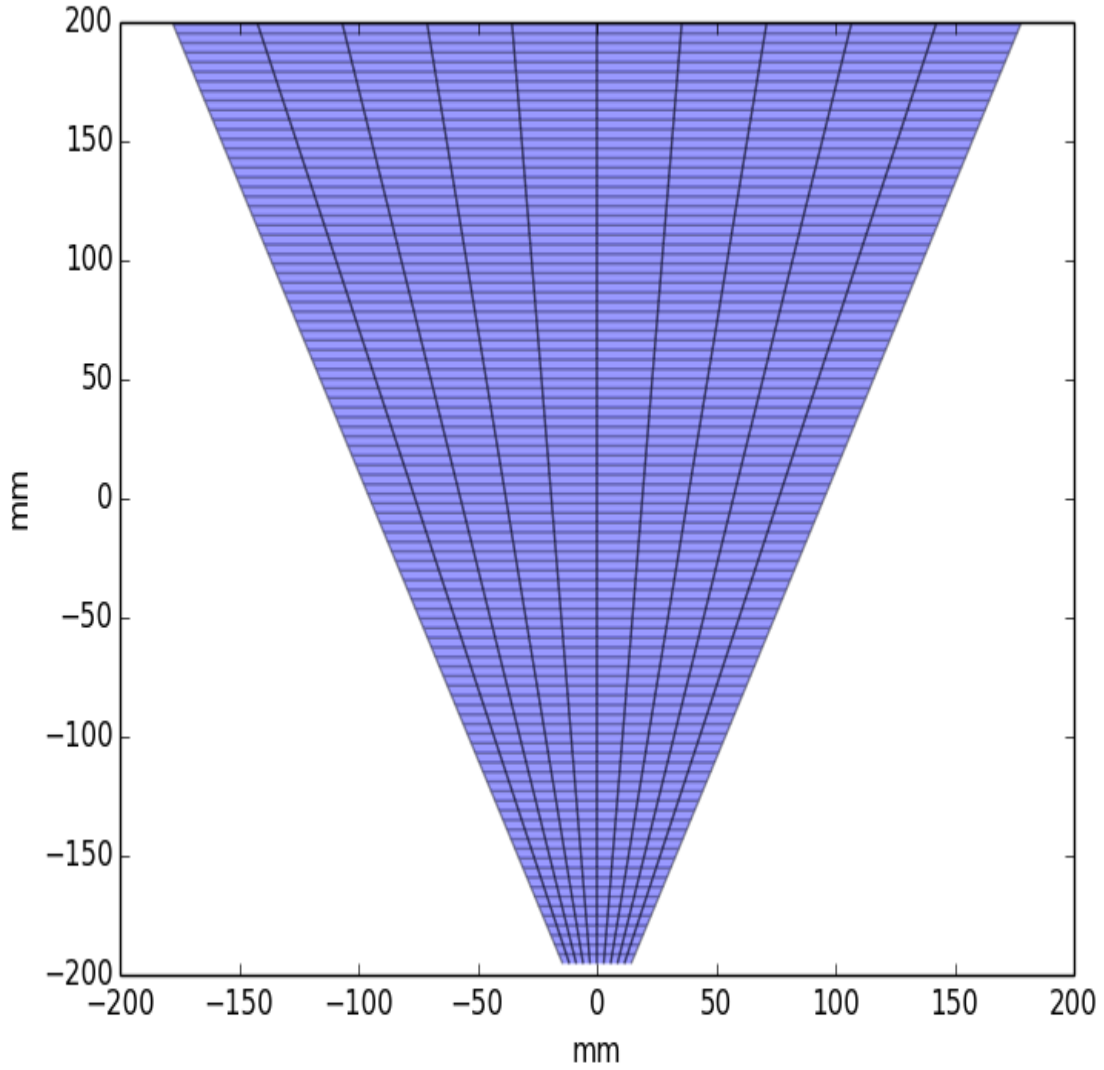
    dg_dgcode/packages/Projects/He3Tubes/G4GeoHe3Tubes/pycpp_GeoHe3Sans/geometry_module.cc

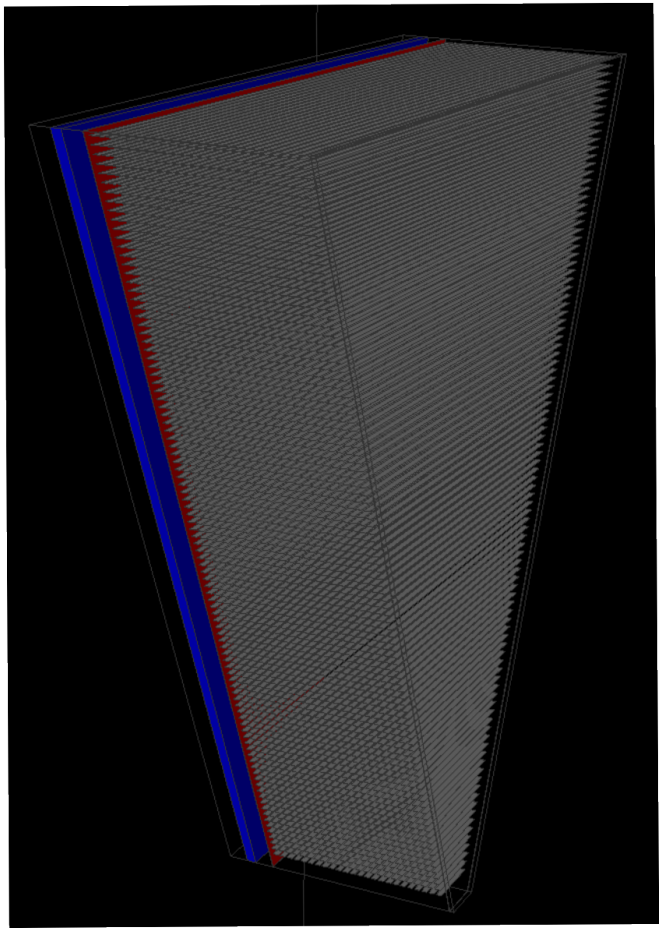
    (the XML geometry has to be practically redefined)
  - BandGEM: dump anode pad coordinates and let Mantid build the XML file externally → better way

    dg_dgcode/packages/Projects/BandGem/G4GeoBandGem/libsrc/BandGemFrame.cc
- Instruction on building IDFs and validation tools

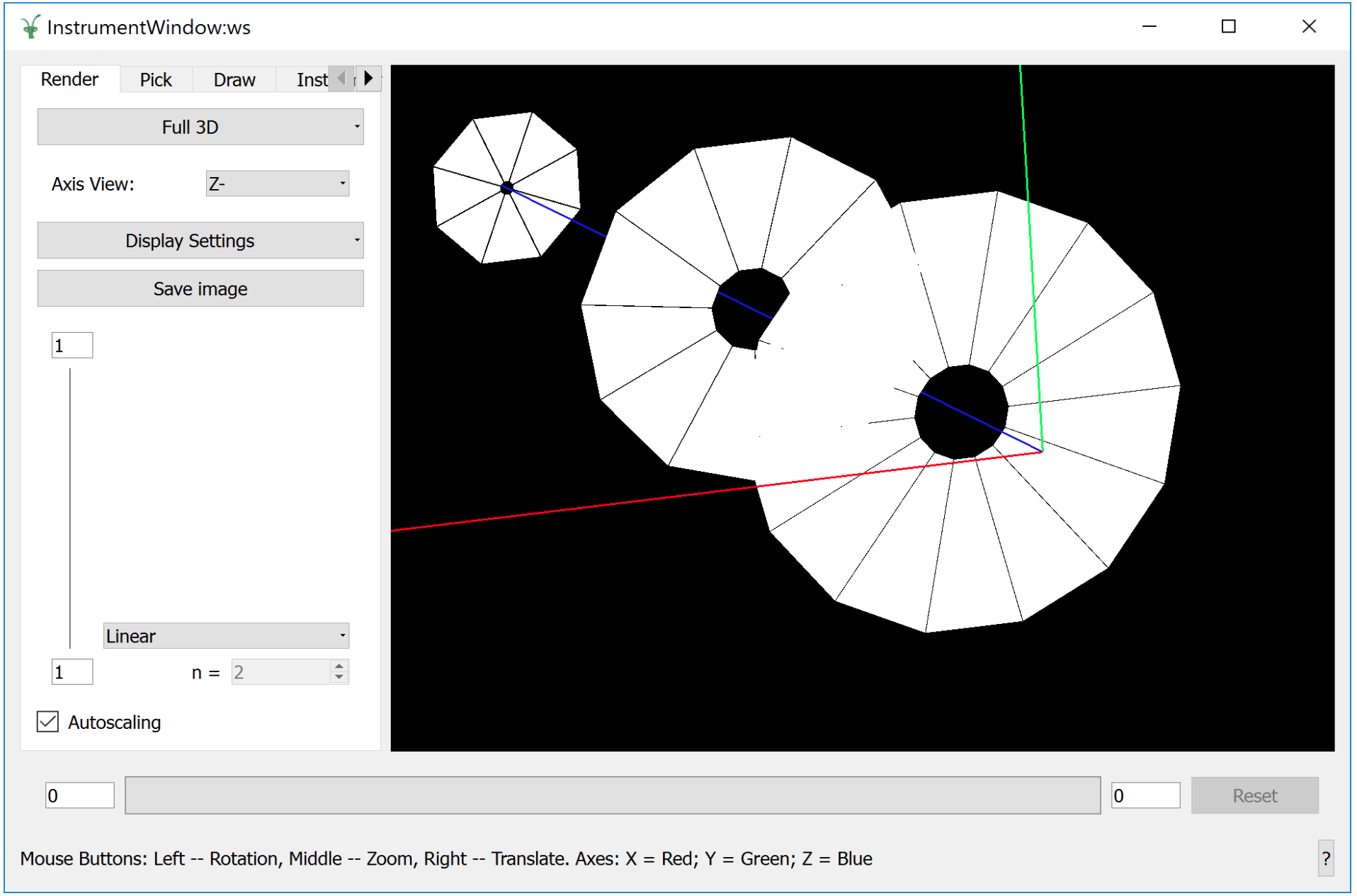
  http://docs.mantidproject.org/nightly/concepts/CreateanIDF.html#create-an-idf

# The BANDGEM anode



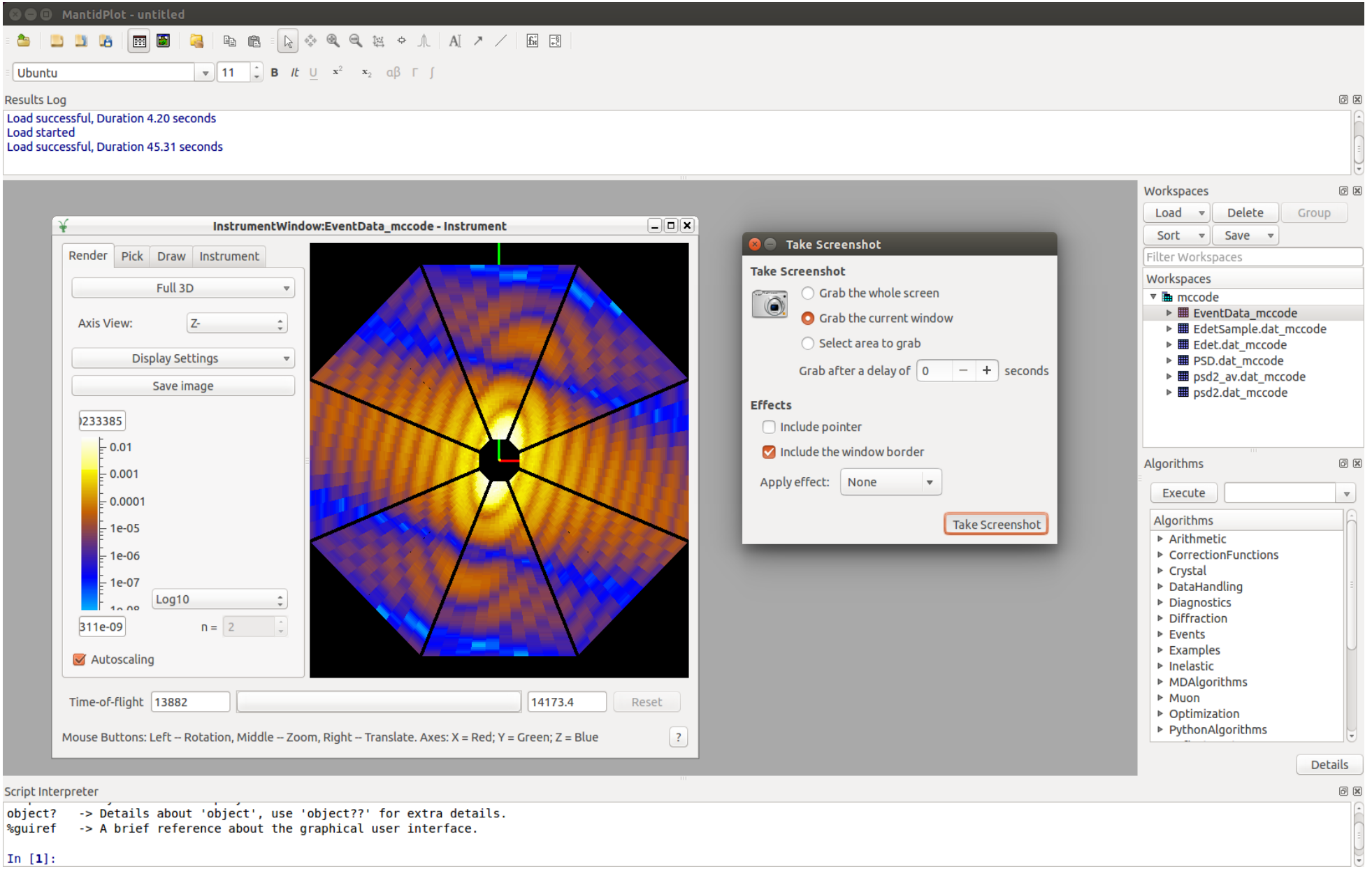
# Mantid view of BandGEM/LoKI IDF



# 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



# Summary

- McStas-Geant4-Mantid intefaces 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