Downloaded from orbit.dtu.dk on: Apr 20, 2024

DTU Library

New developments in the McStas neutron instrument simulation package

Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Klinkby, Esben Bryndt; R. Nielsen, Torben; Farhi, E.; Filges, U.; Lefmann, K.

Publication date:
2014

Link back to DTU Orbit

Citation (APA):
Willendrup, P. K. (Author), Bergbäck Knudsen, E. (Author), Klinkby, E. B. (Author), R. Nielsen, T. (Author), Farhi, E. (Author), Filges, U. (Author), & Lefmann, K. (Author). (2014). New developments in the McStas neutron instrument simulation package. Sound/Visual production (digital)

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

New developments in the McStas neutron instrument simulation package

Peter Willendrup[1,2], Erik Knudsen[1], Esben Klinkby[3,4], Torben R Nielsen[2], E Farhi[5], U Filges[6], K Lefmann[7]

[1]NEXMAP, Physics Department, Technical University of Denmark, Denmark

[2]ESS Data Management & Sofware Center, Denmark

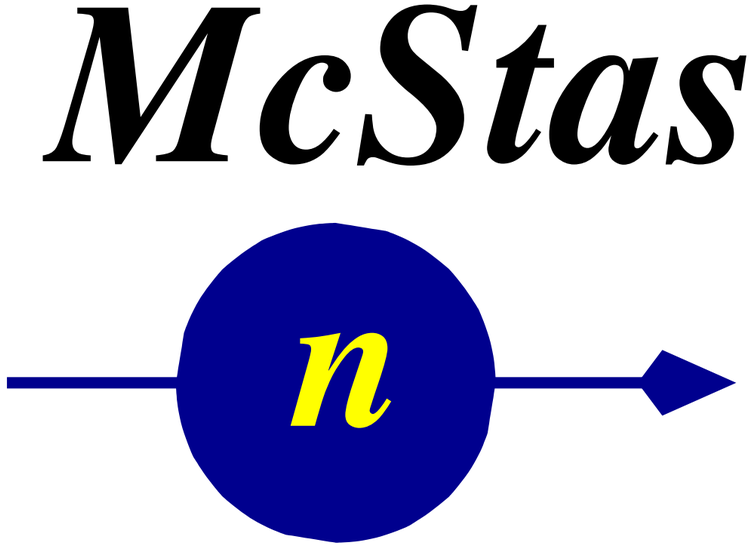
[3]Center for Nuclear Technologies, Technical University of Denmark, Denmark

[4]ESS Neutronics Group, Sweden

[5]CS-group, Institut Laue-Langevin (ILL), France

[6]LDM, Paul Scherrer Institute (PSI), Switzerland

[7]eScience and Nano-Science centers, Niels Bohr Institute (NBI), Denmark



Agenda

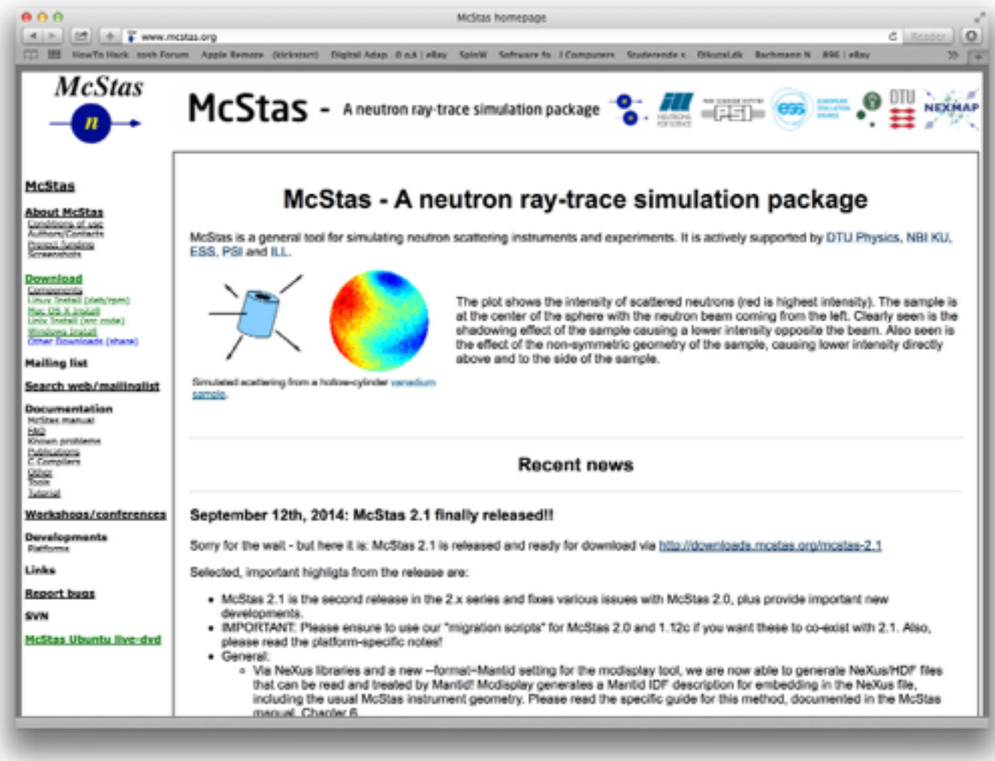
- A brief introduction to McStas, Monte Carlo & raytracing

- Highlighted new features in McStas 2.1
  - McStas-MCNP for background estimates
  - McStas-Mantid event processing
  - Speedup in Single_crystal.comp

McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH, **ESS**
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students

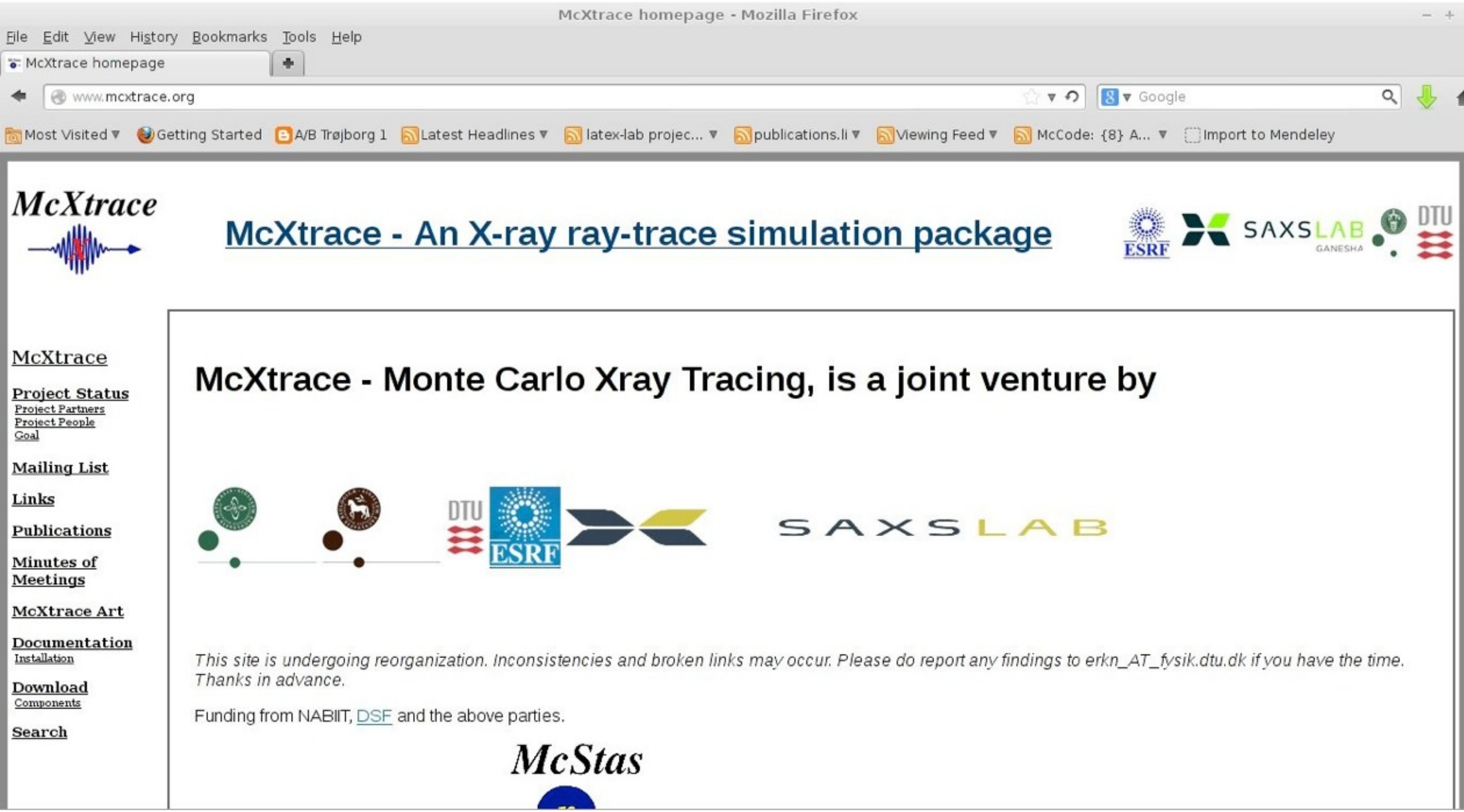
GNU GPL license
Open Source



Project website at
http://www.mcstas.org

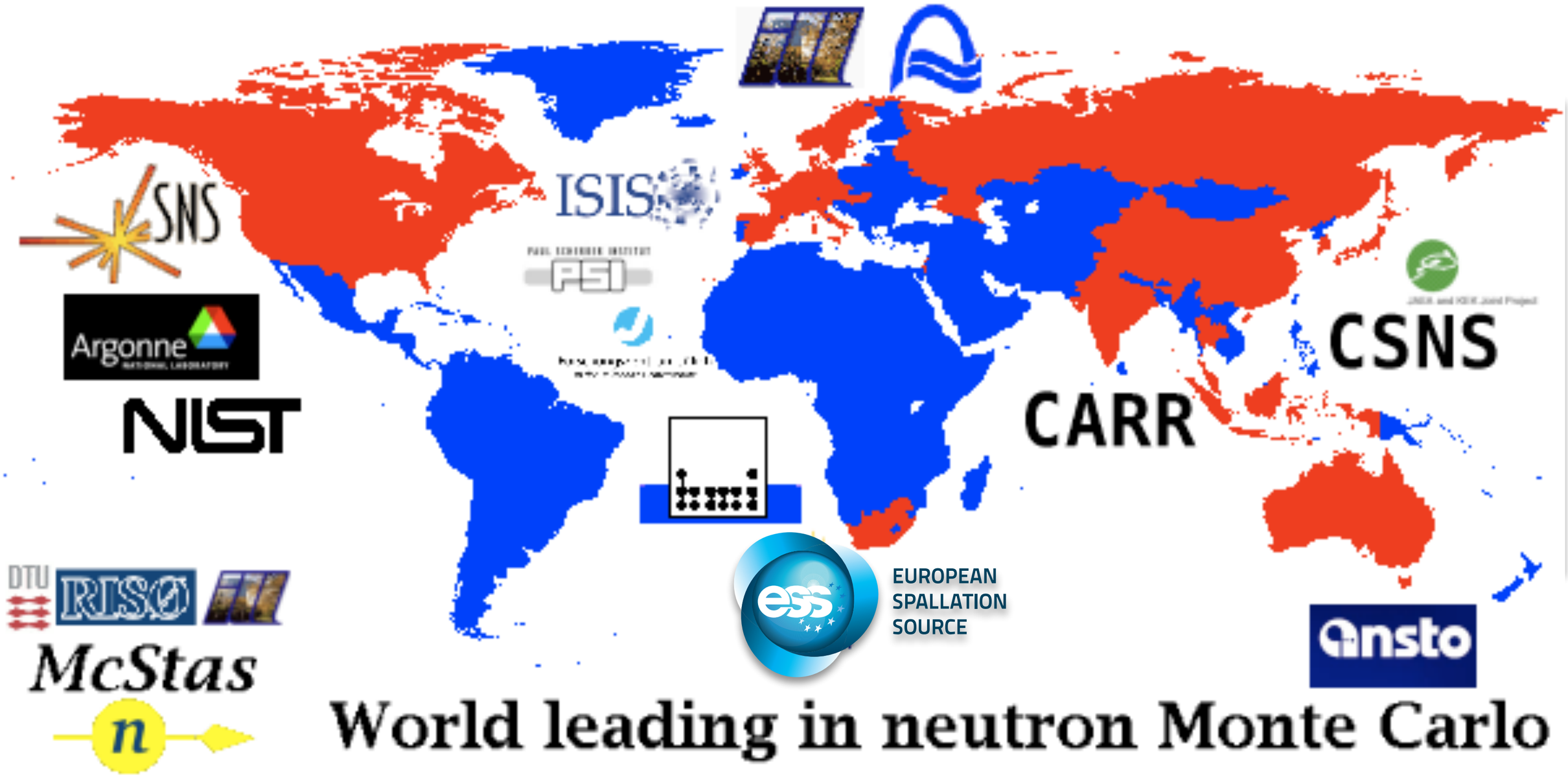
mcstas-users@mcstas.org mailinglist

New developments in McStas



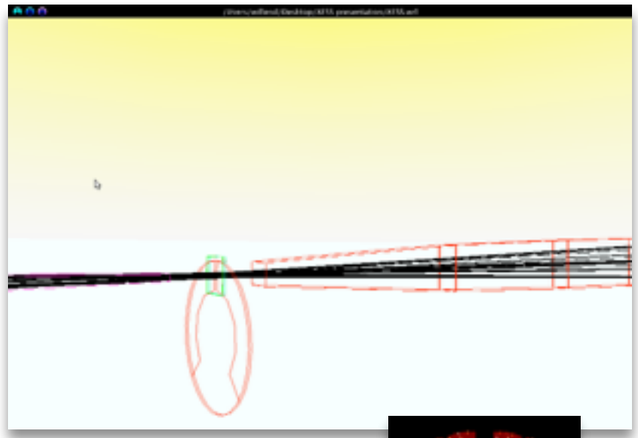
New developments in McStas

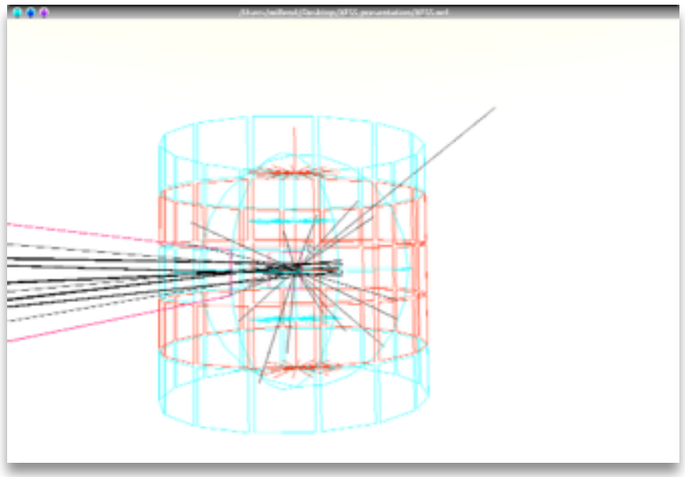
McStas Introduction

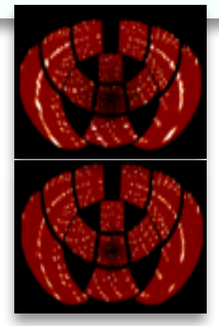


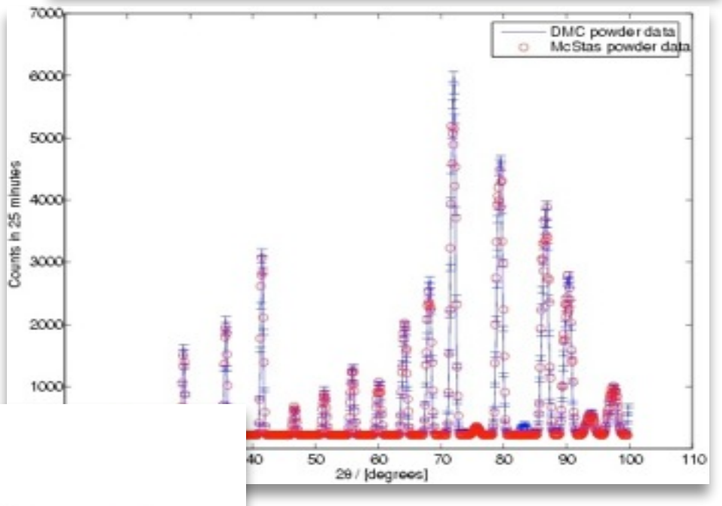
New developments in McStas

What is McStas used for?



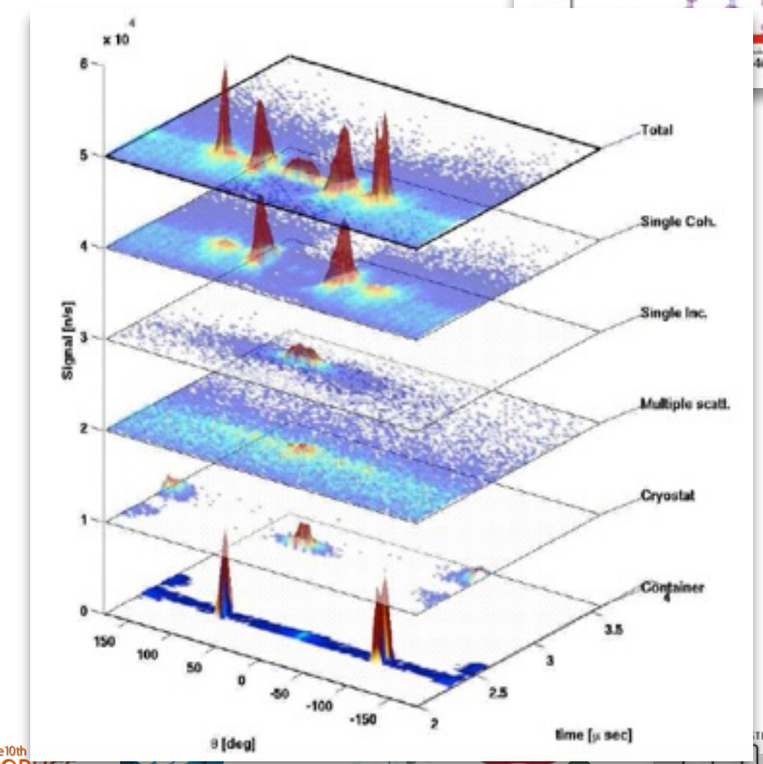


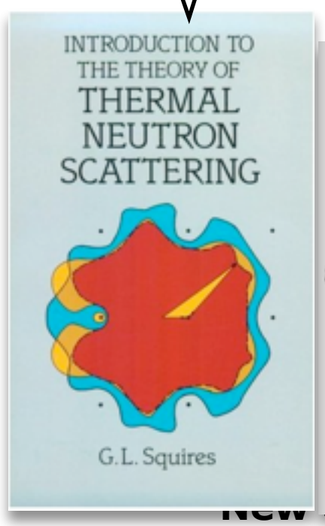


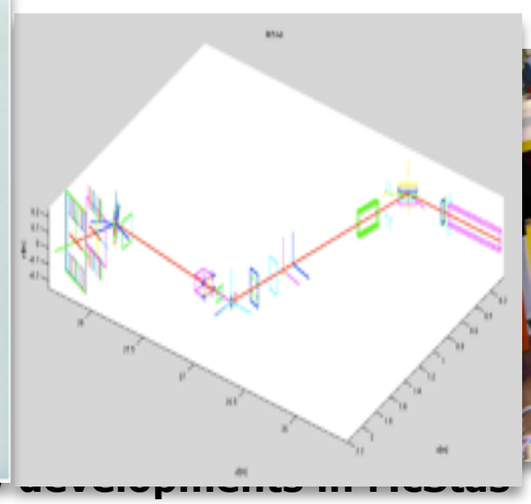


- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)

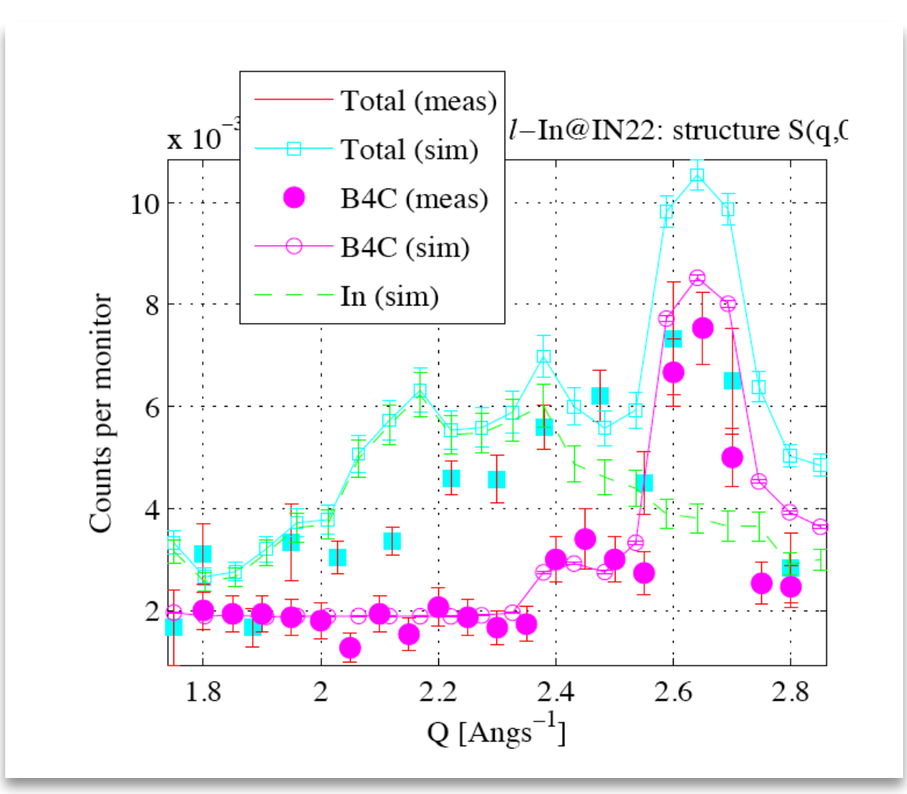




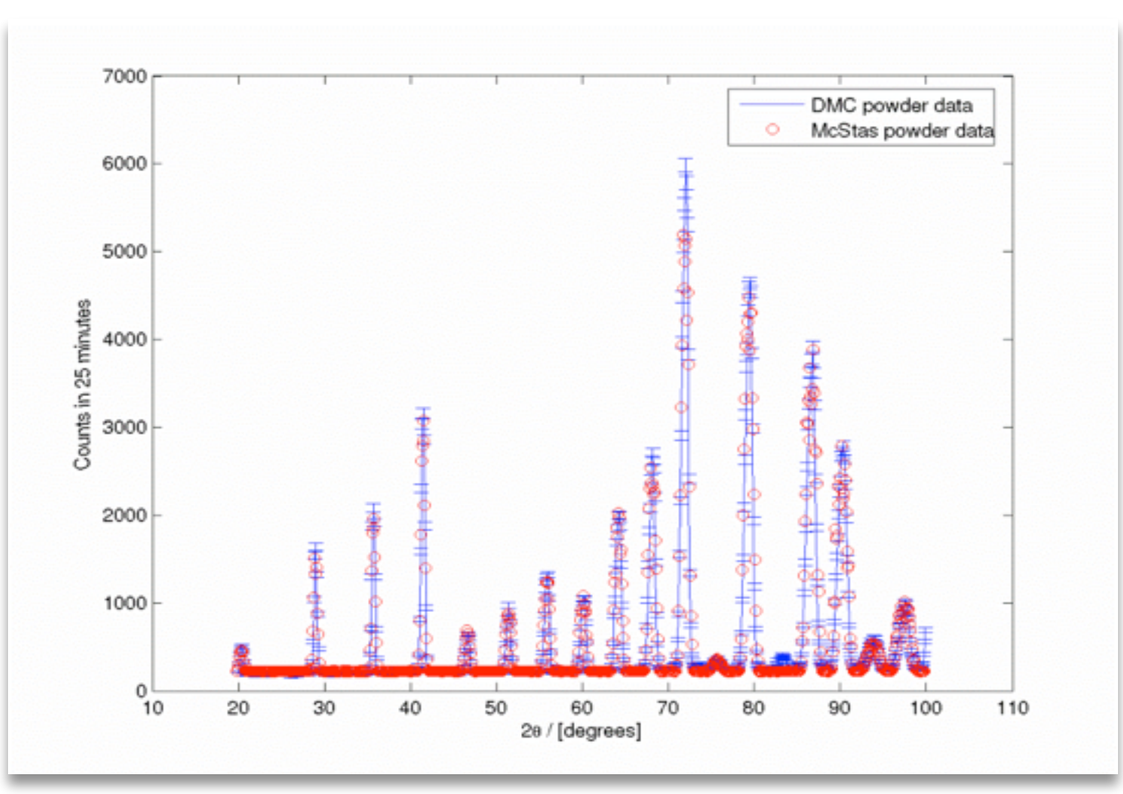


Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agrees very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable



E. Farhi, P. Willendrup et al., in preparation



P. Willendrup et al., Physica B, 386, (2006), 1032.

New developments in McStas

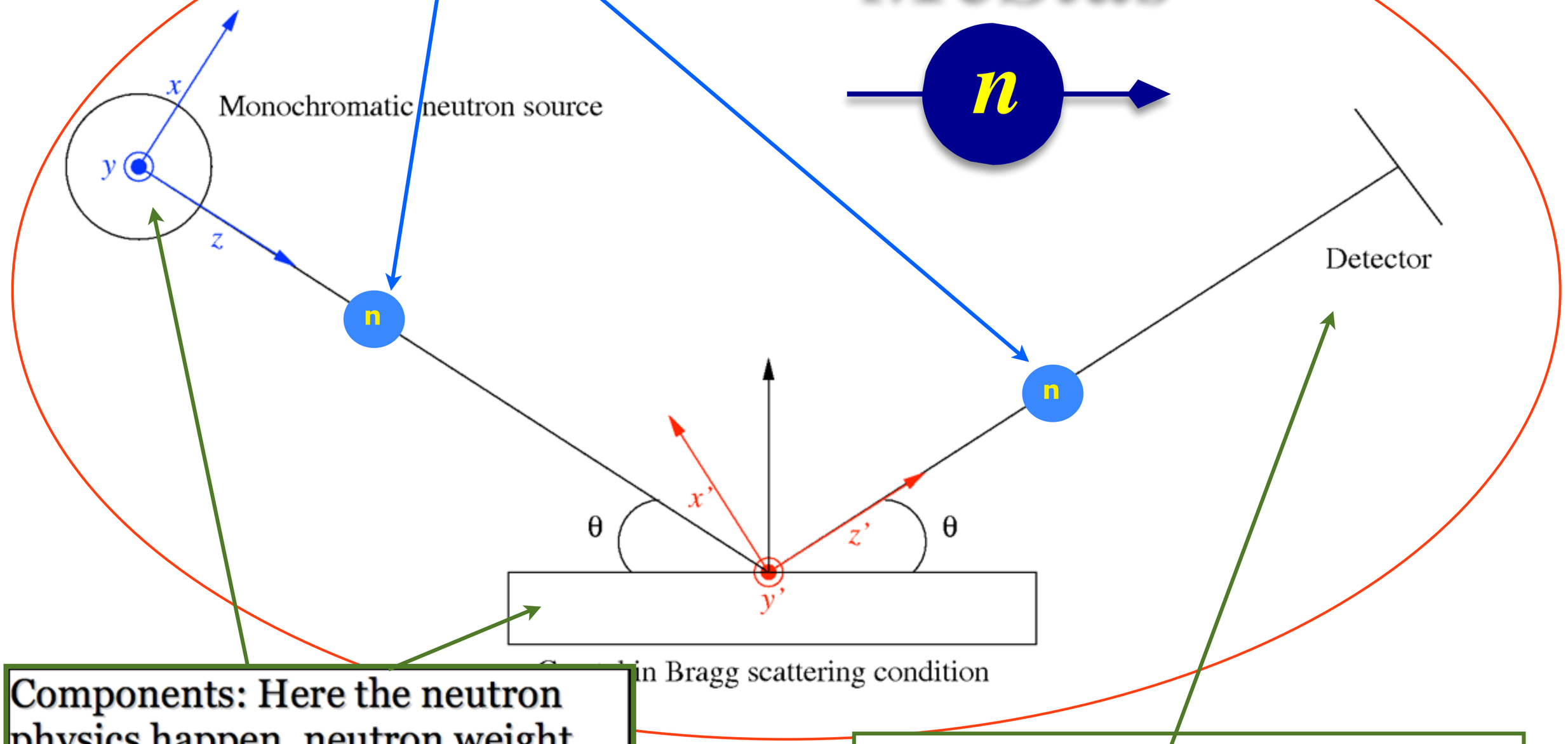
Neutron ray/package:

Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity (v_x,v_y,v_z)
Spin (s_x,s_y,s_z)

Time (t)

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.

McStas

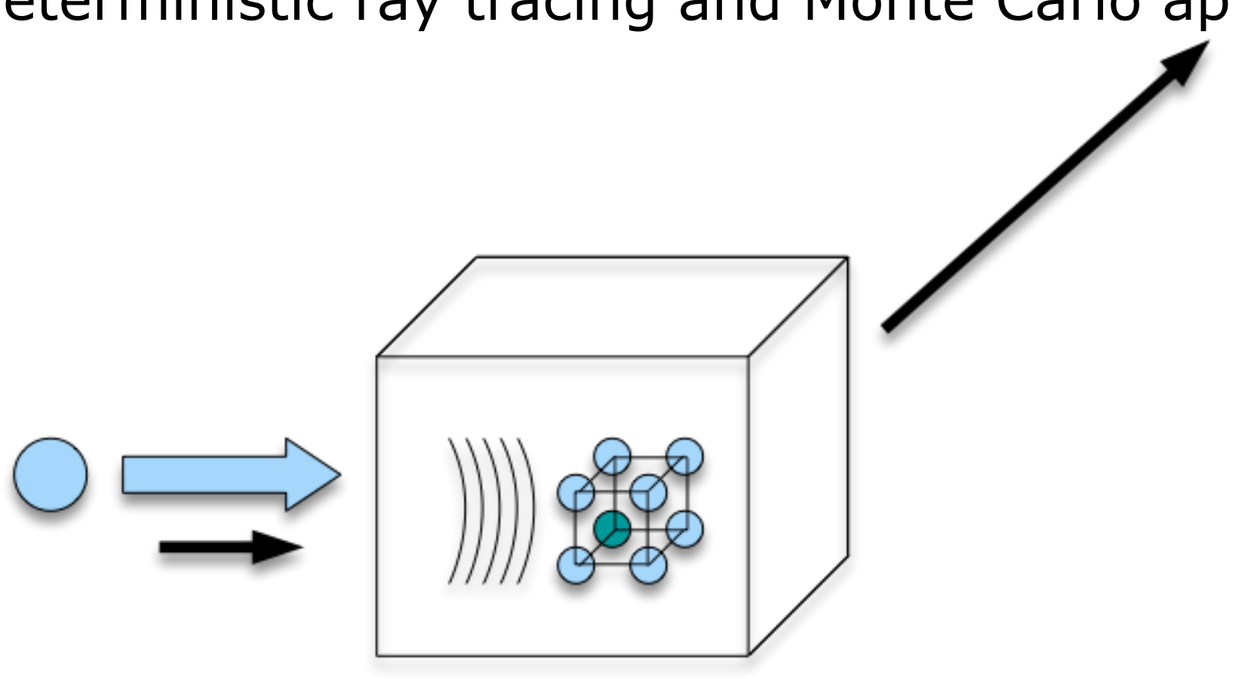


Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.

Local, internal coordinate system!

Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of "complicated" distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



- Result: A realistic and efficient transport of neutrons in the thermal and cold range

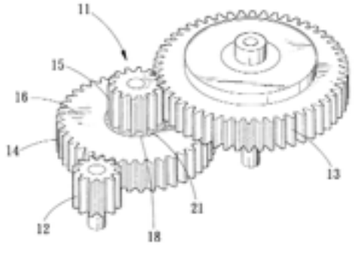
McStas overview

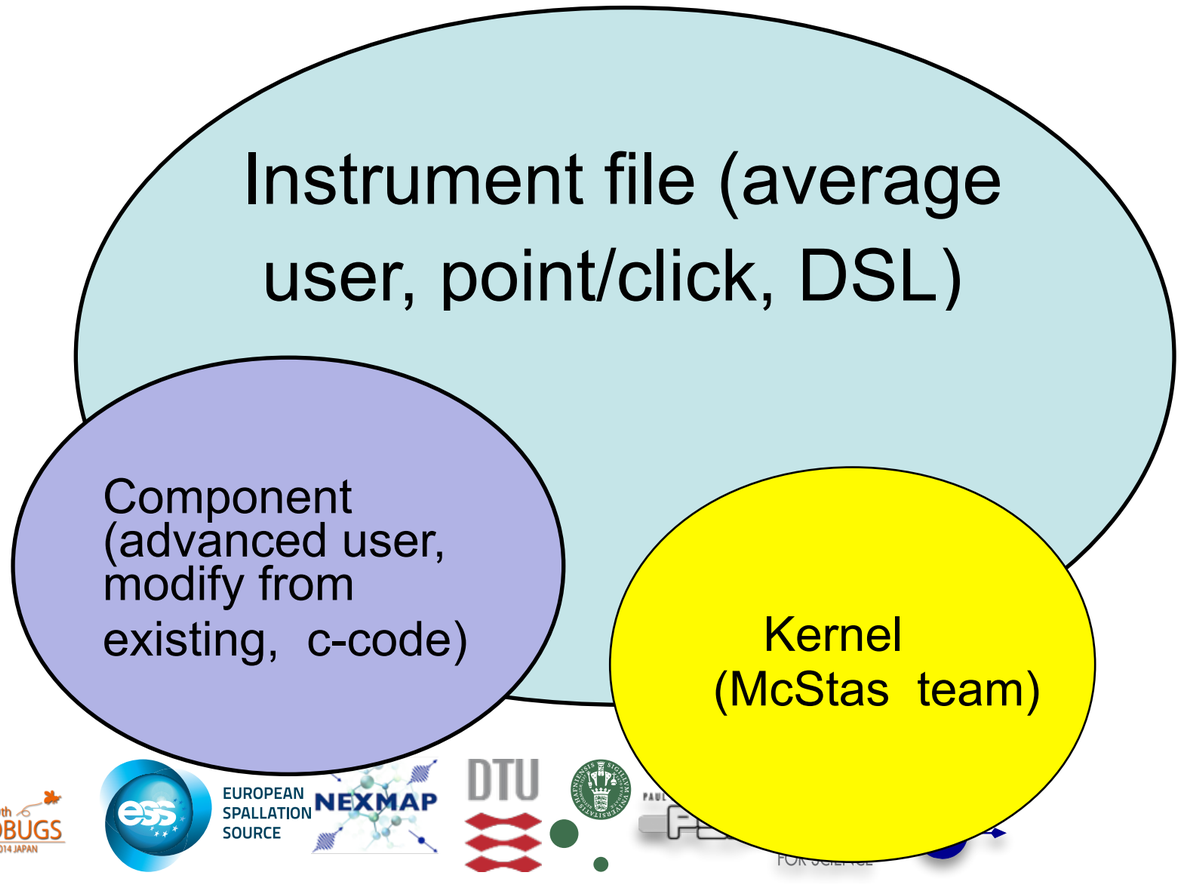
- Portable code (Unix/Linux/Mac/Windoze)

- Ran on everything from iPhone to 1000+ node cluster!

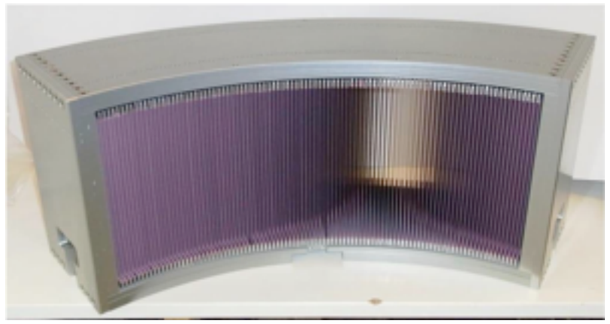
- 'Component' files (~150) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps

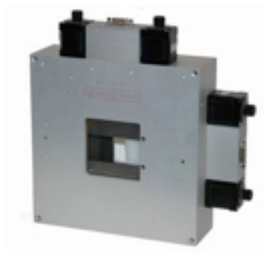
- DSL + ISO-C code gen.

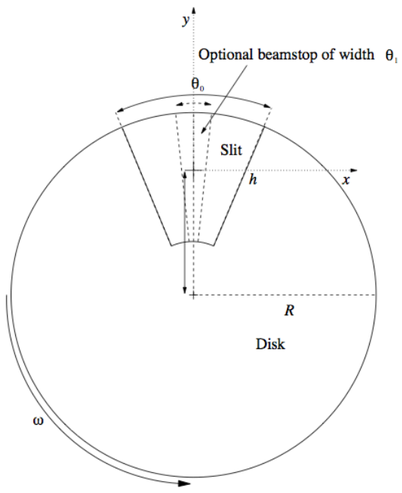


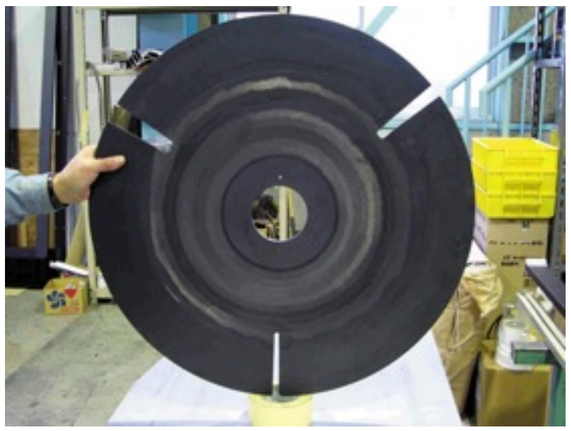


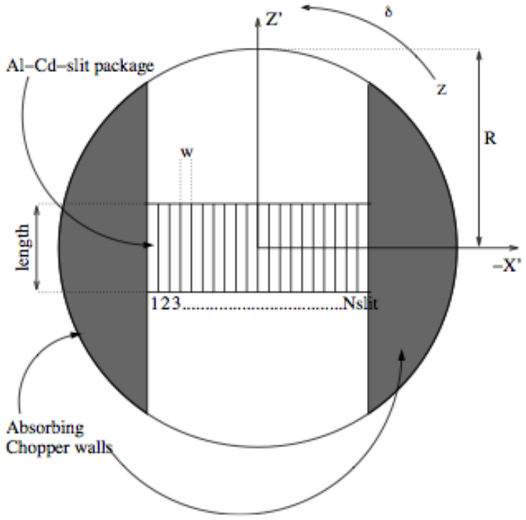
Neutron optics and other instrument components

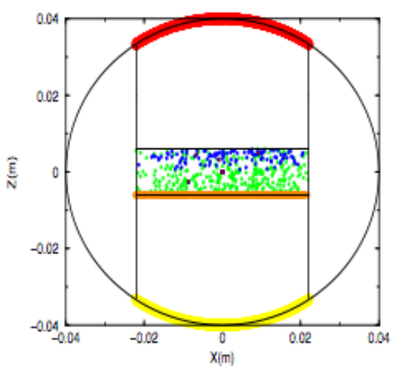


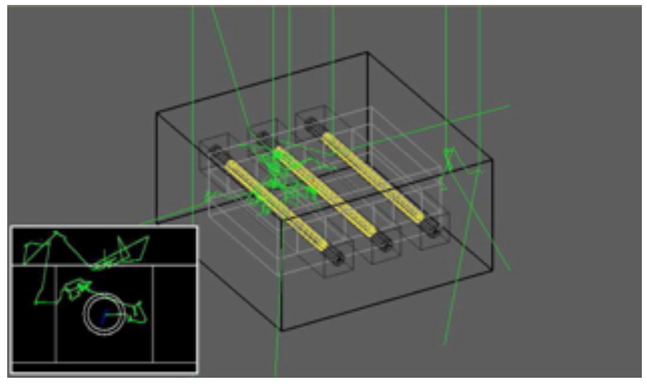










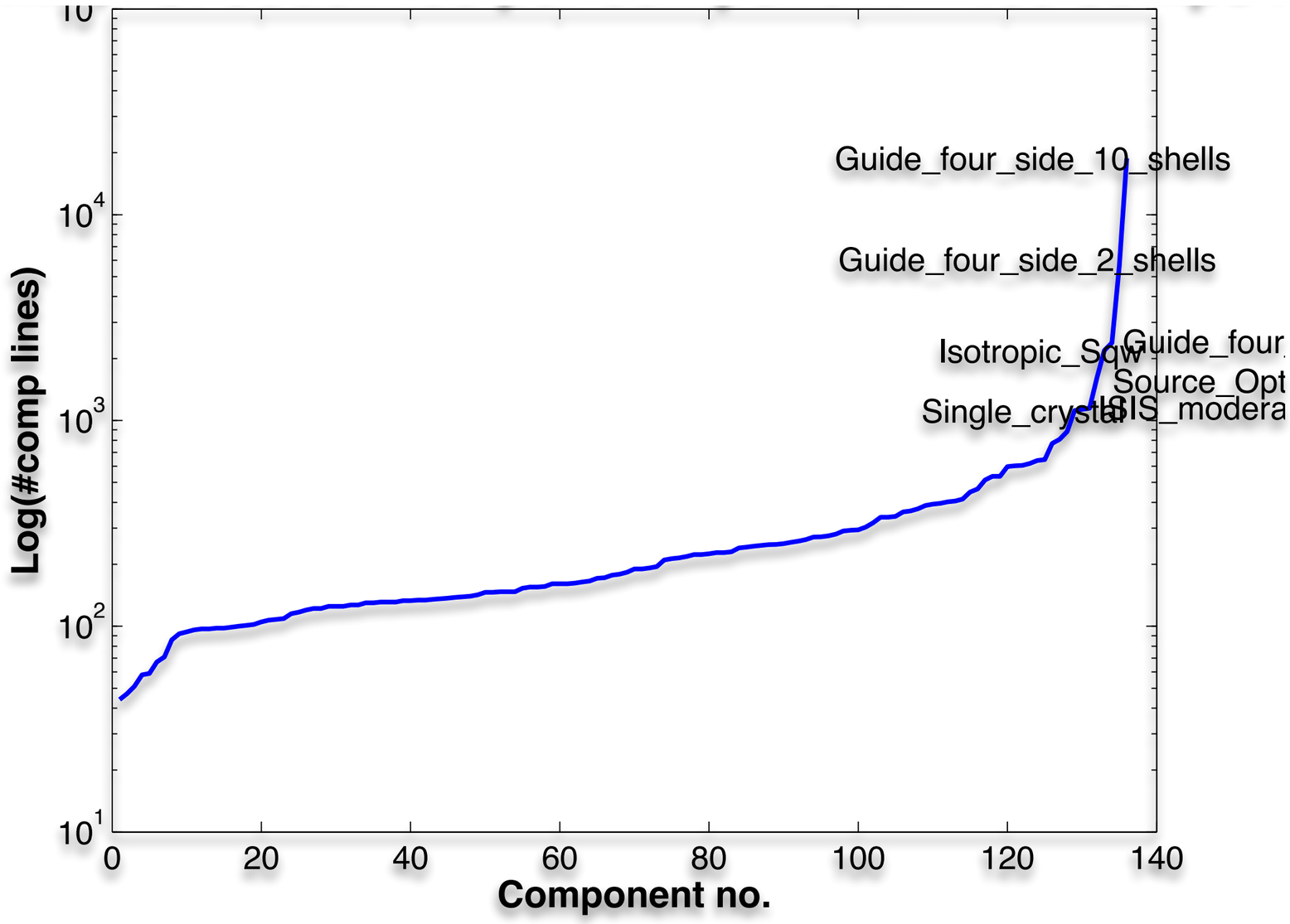


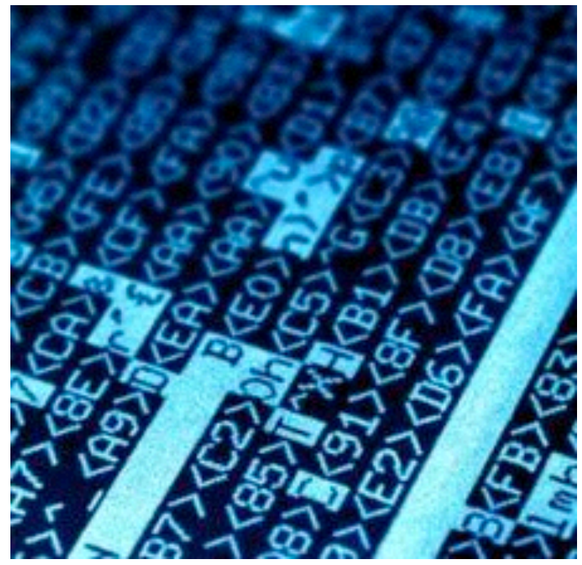
New developments in McStas

Writing new comps or understanding existing is not that complex...

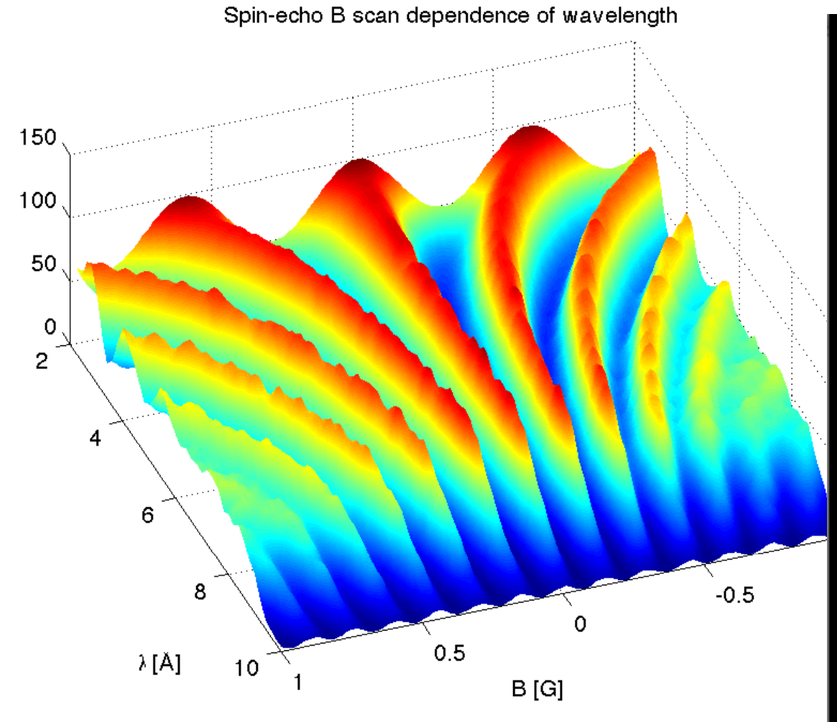
- Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

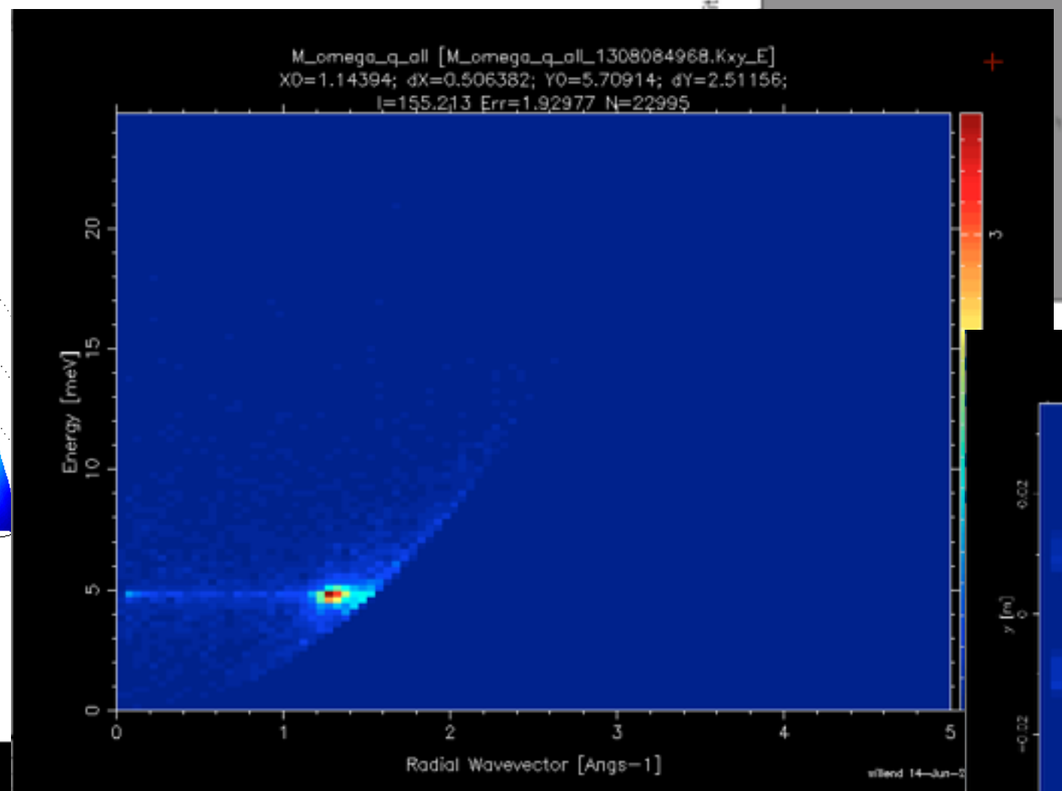
Number of lines of code per component - 165 comps in total

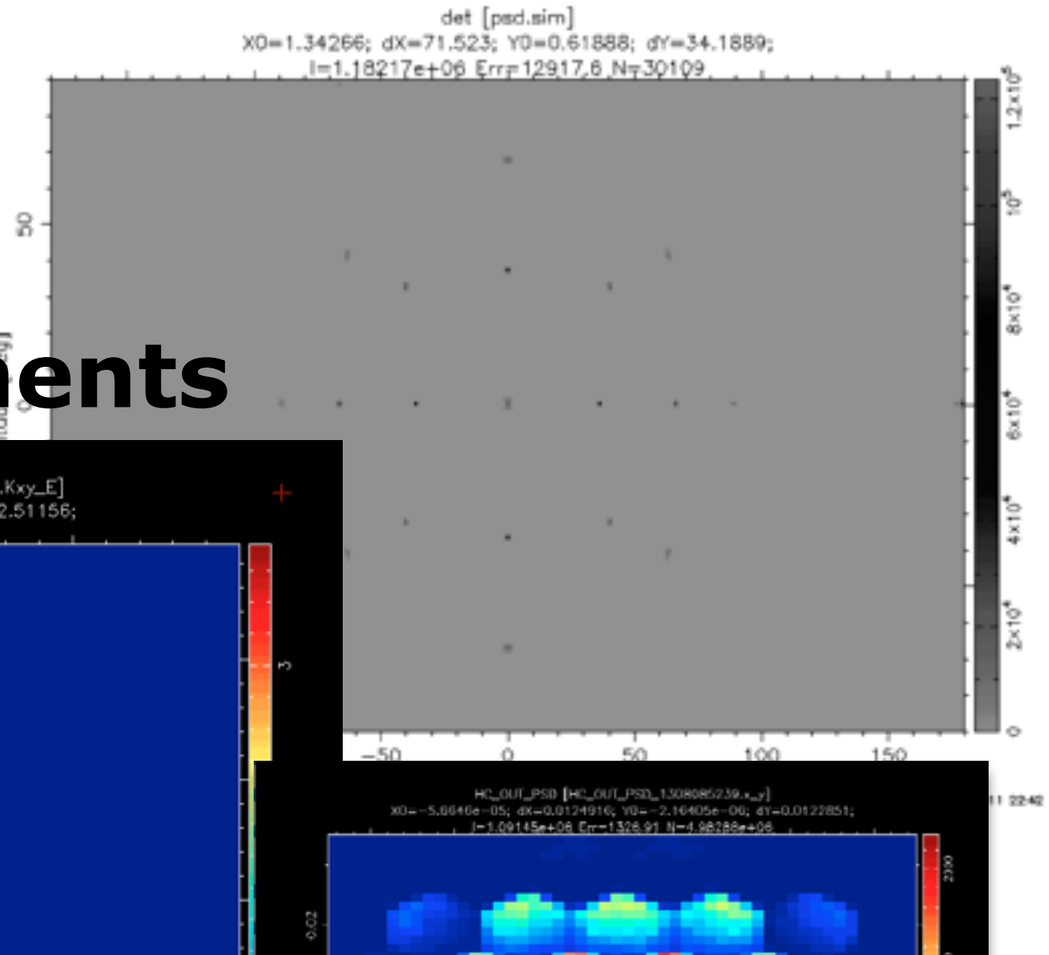


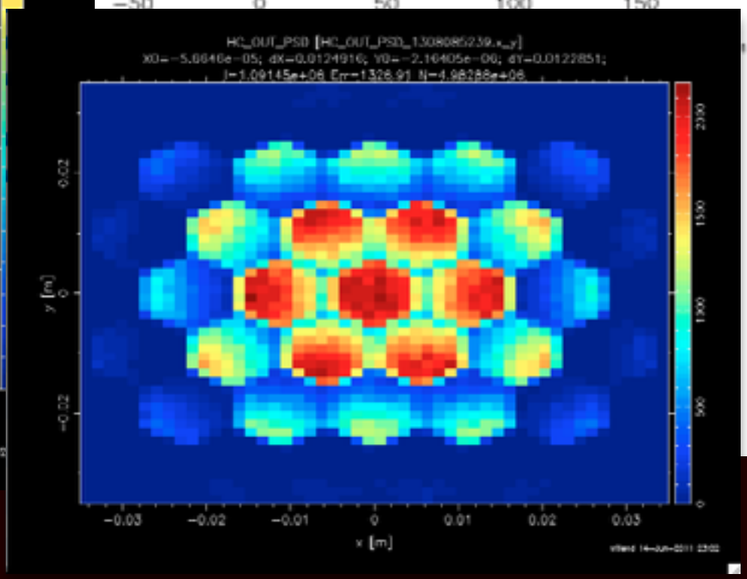


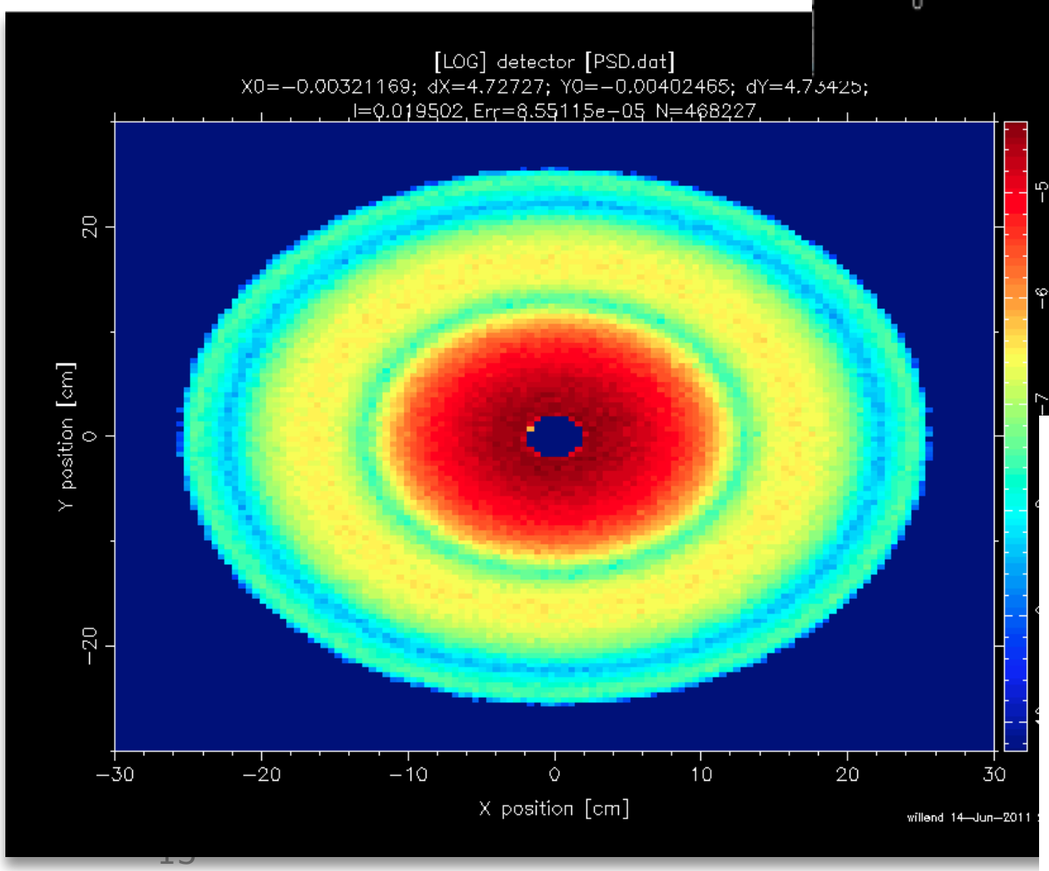
Example suite: 123 instruments

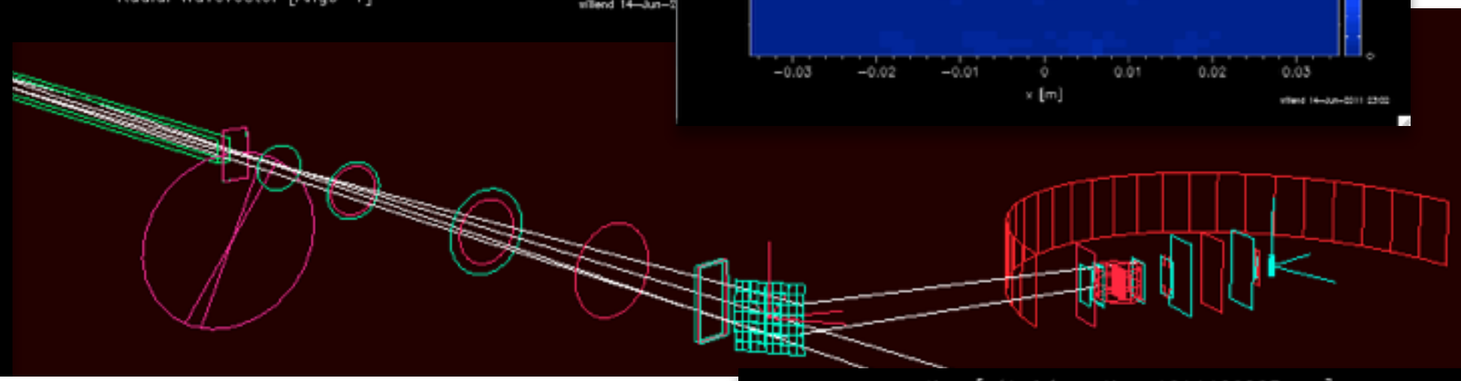


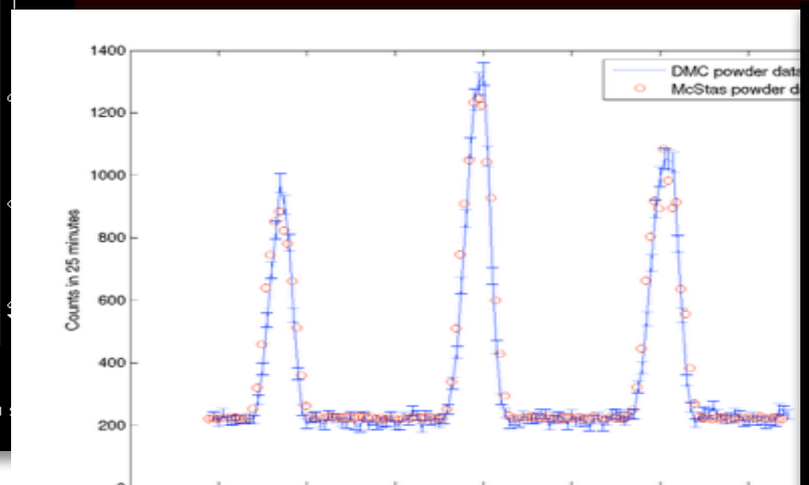


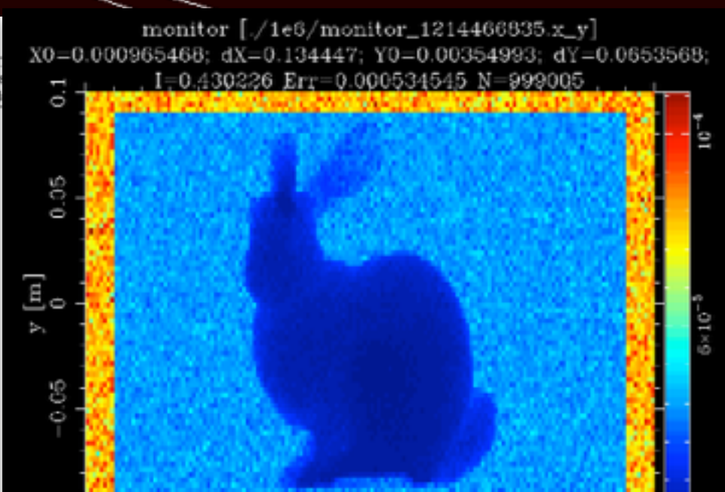




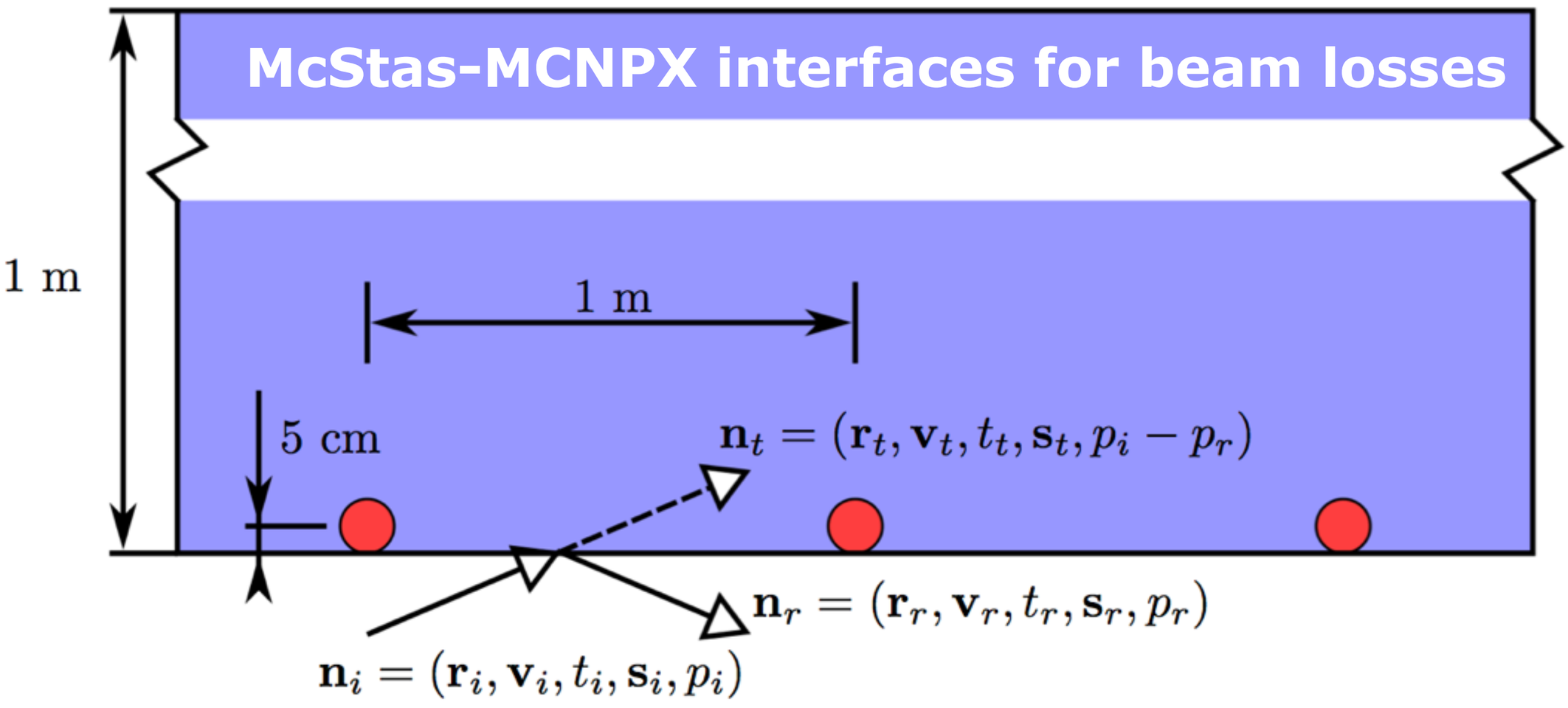








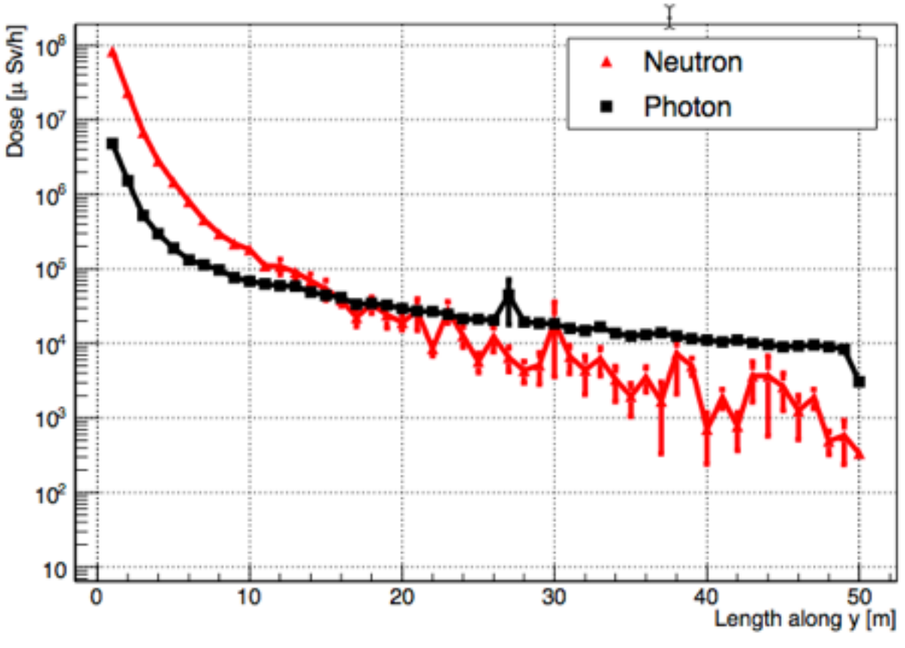
McStas-MCNPX interfaces for beam losses

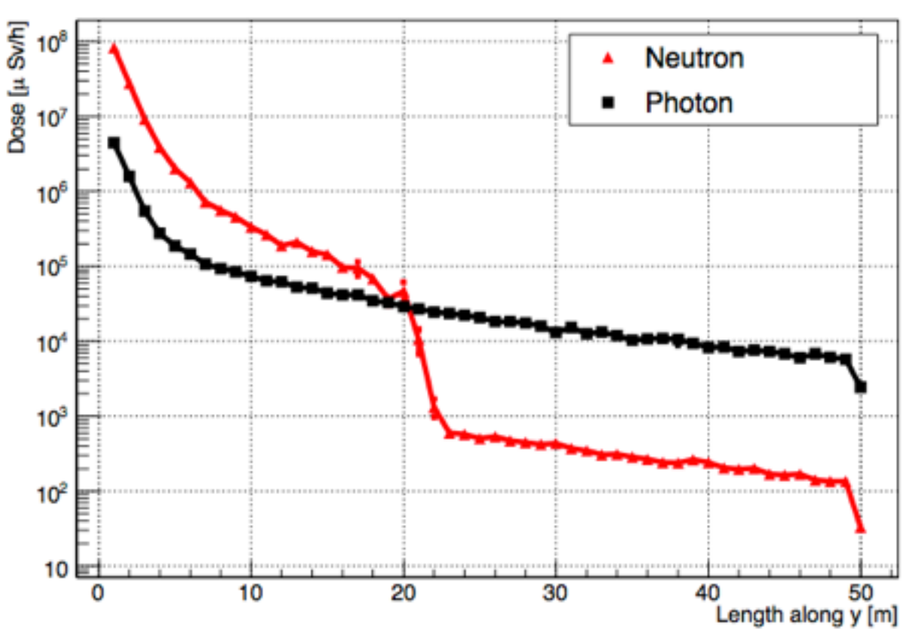


MCNPX

SSR SSW

McStas

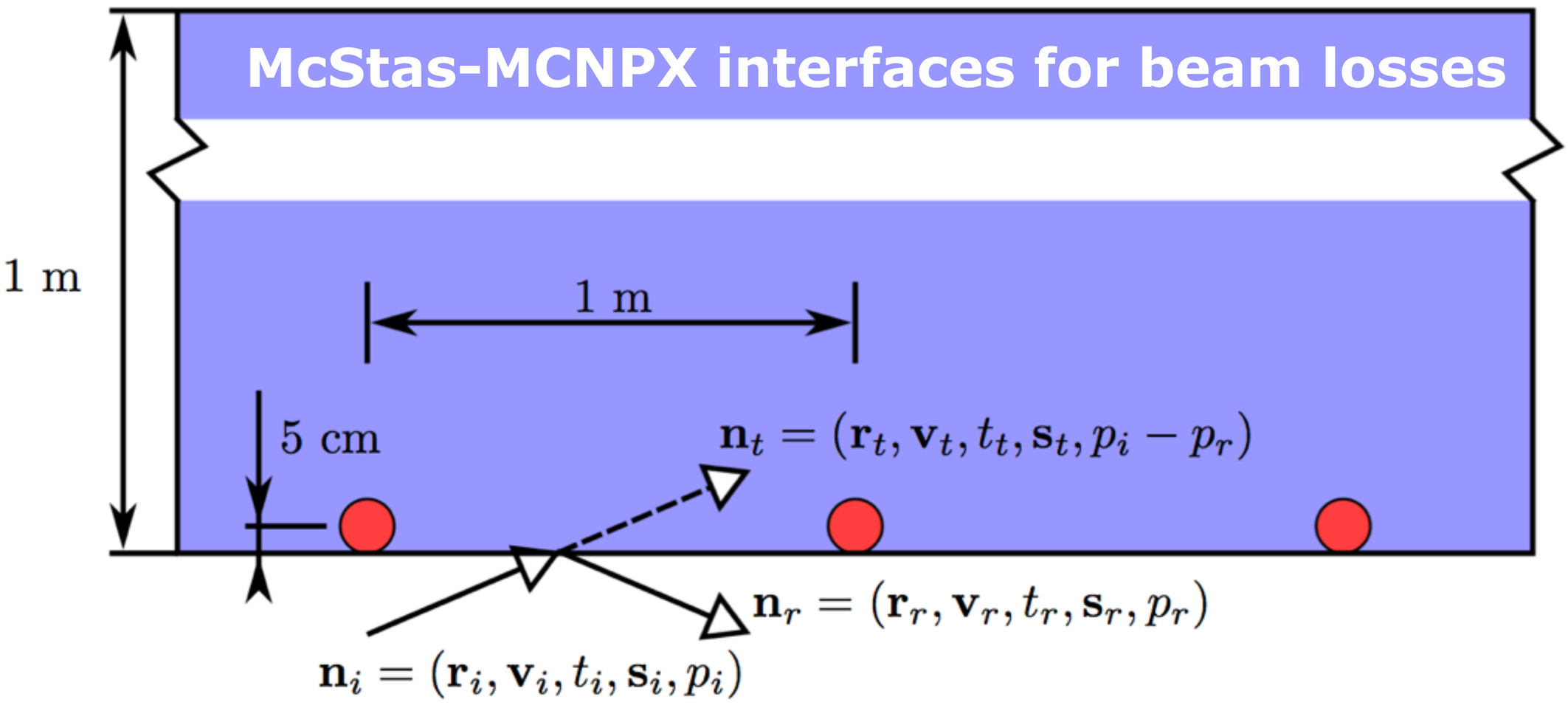




Collaboration
DTU Nutech
DTU Fysik
ESS

PSI NEUTRONS FOR SCIENCE McStas

McStas-MCNPX interfaces for beam losses

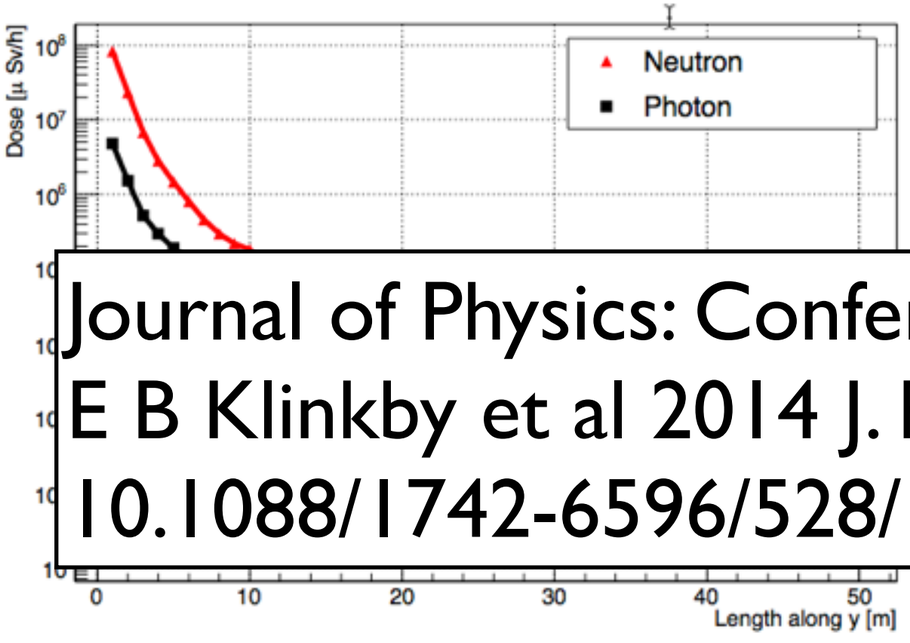


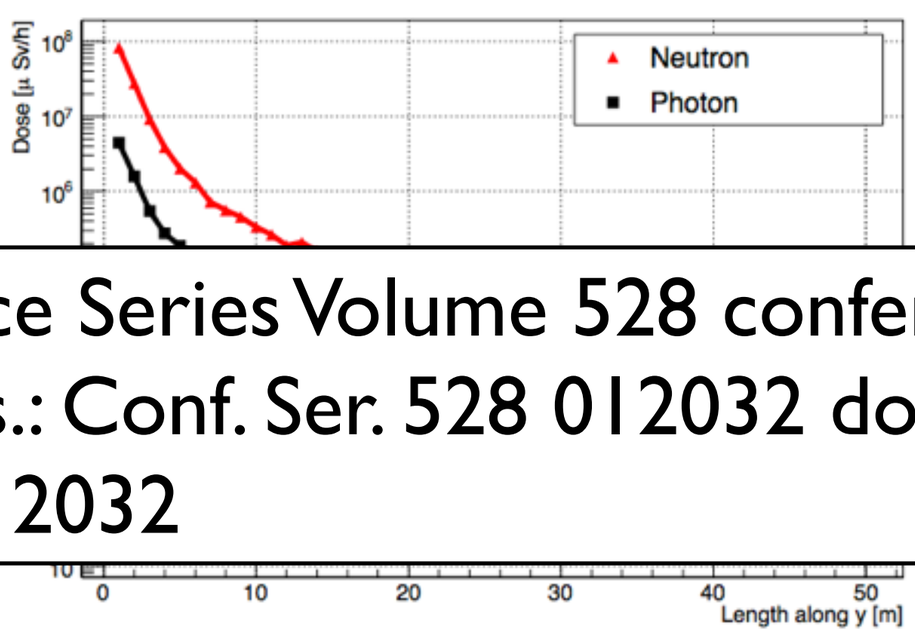
MCNPX

SSR SSW

McStas

Use: Check the Scatter_logger.comp in the McStas distribution





Journal of Physics: Conference Series Volume 528 conference 1
E B Klinkby et al 2014 J. Phys.: Conf. Ser. 528 012032 doi: 10.1088/1742-6596/528/1/012032

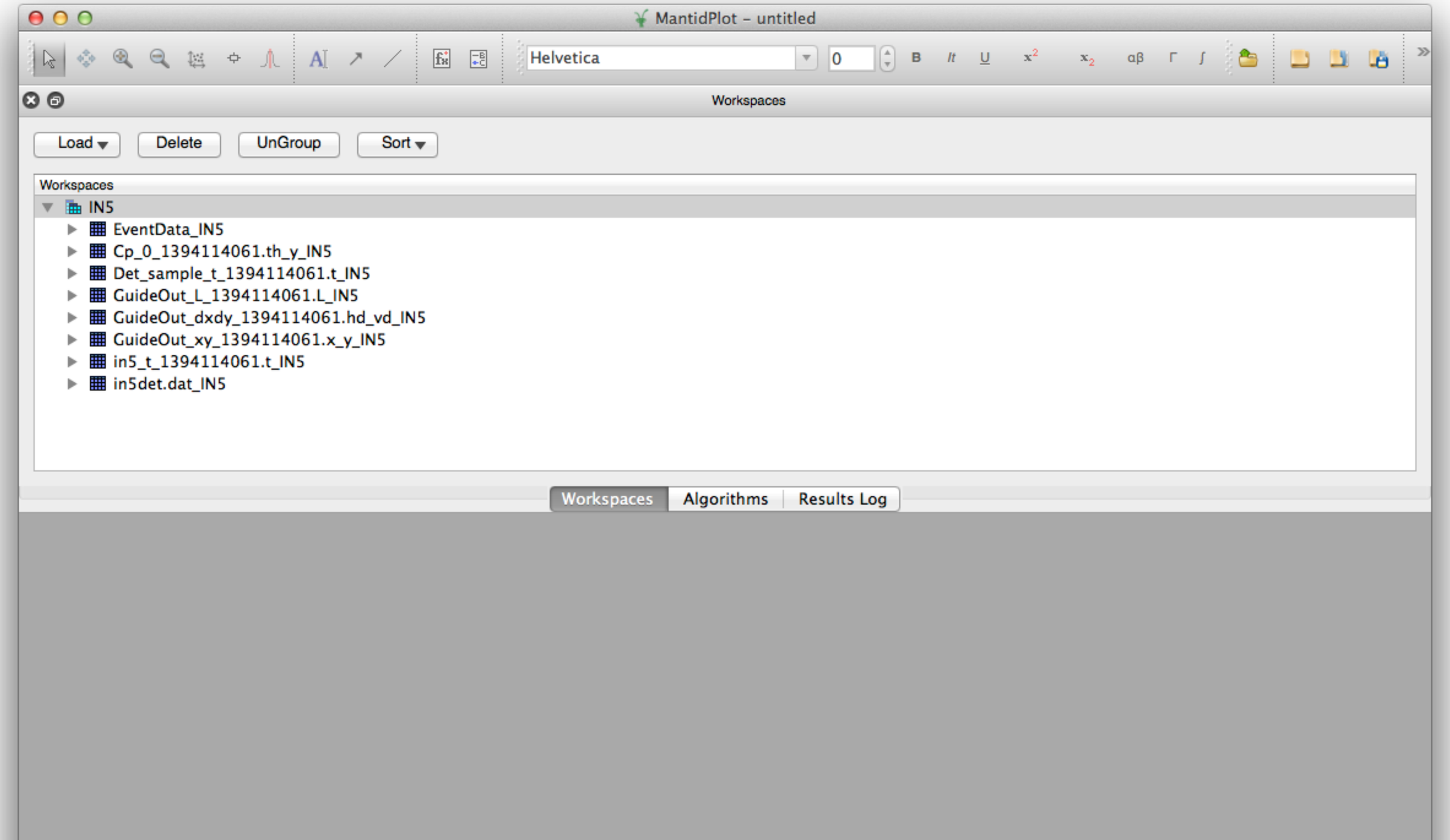
Future: Geant4, PHITS?

Collaboration
Nutech
Fysik

PSI NEUTRONS FOR SCIENCE McStas

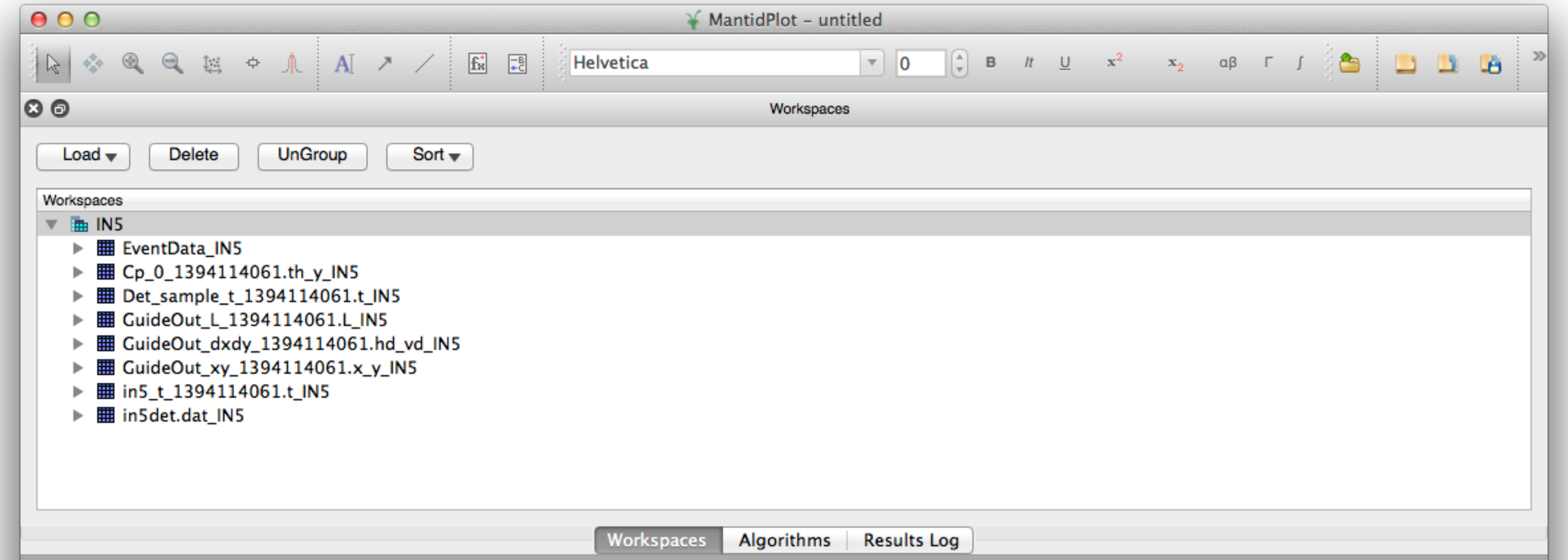
McStas-Mantid event processing facilitated by:

Special labels in component list
Special Monitor_nD paramers
IDF autogenerated by “mcdisplay” run
NeXus output and LoadMcStas Mantid algorithm



McStas-Mantid event processing facilitated by:

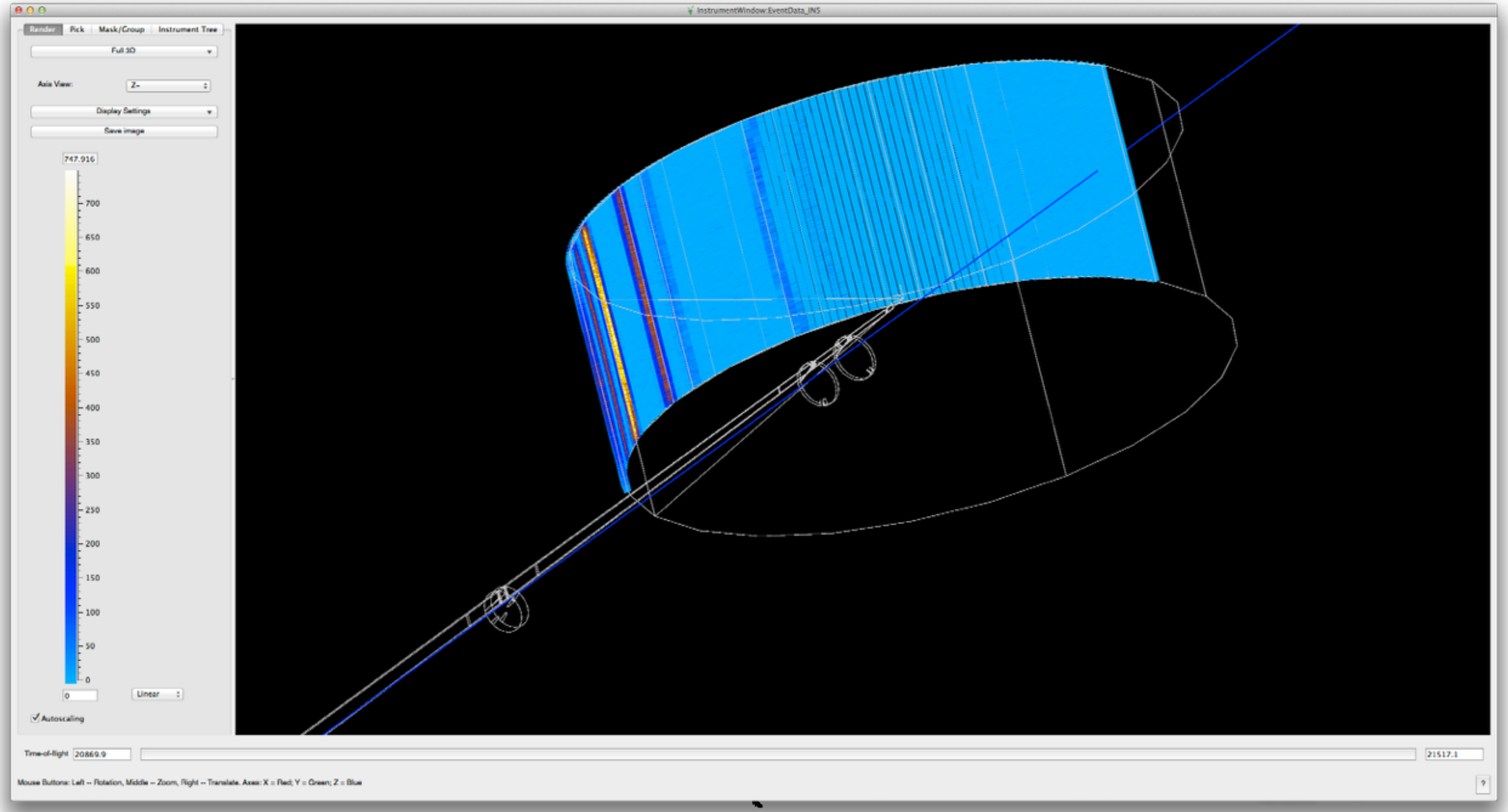
Special labels in component list
Special Monitor_nD paramers
IDF autogenerated by “mcdisplay” run
NeXus output and LoadMcStas Mantid algorithm



Use: Check out templateSANS_Mantid from the McStas distribution - fully functional reduction

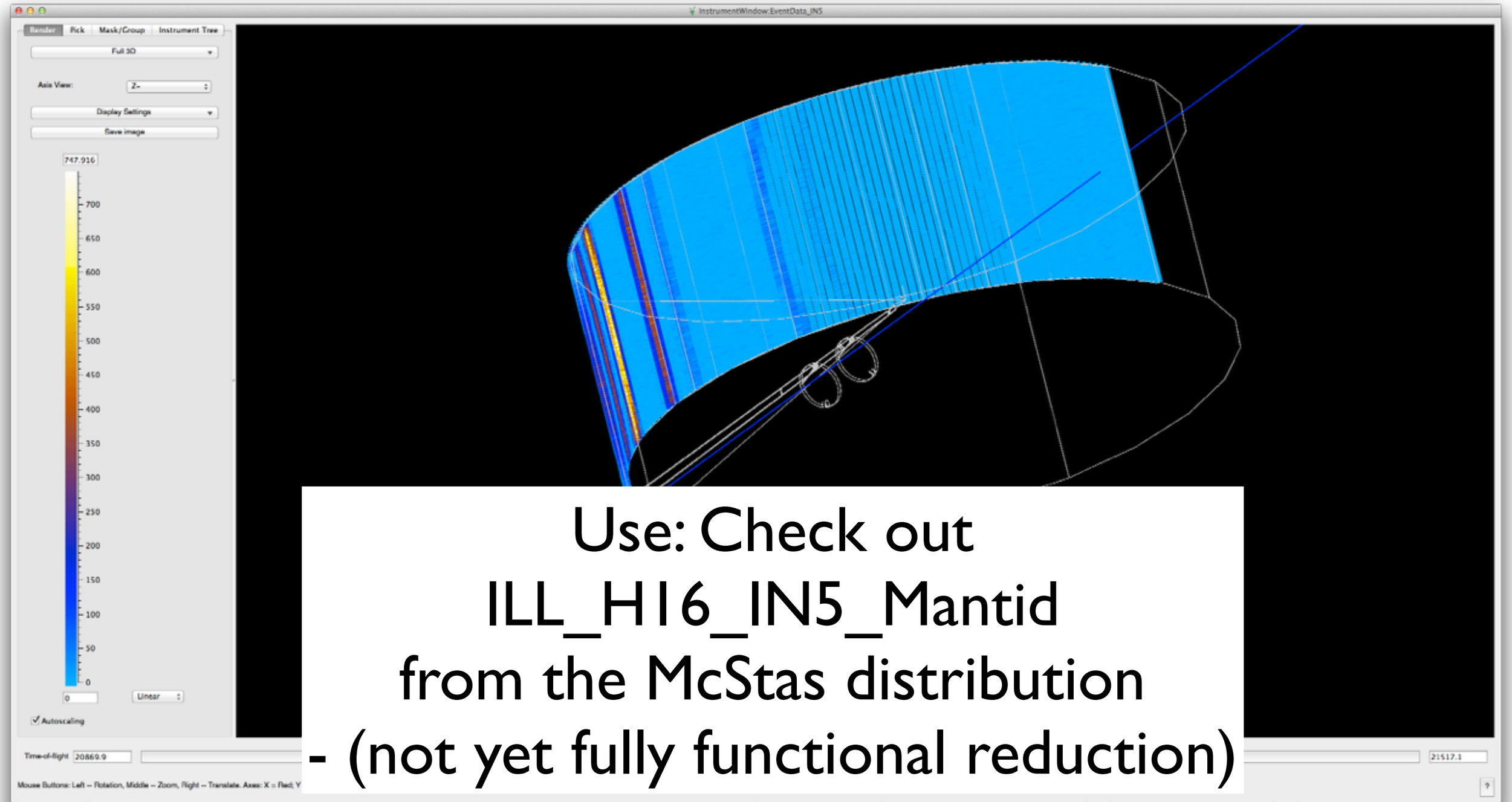
Events shown on the full instrument

- The event data from McStas should look something like this in “full 3D” - you may have to move/zoom a bit about



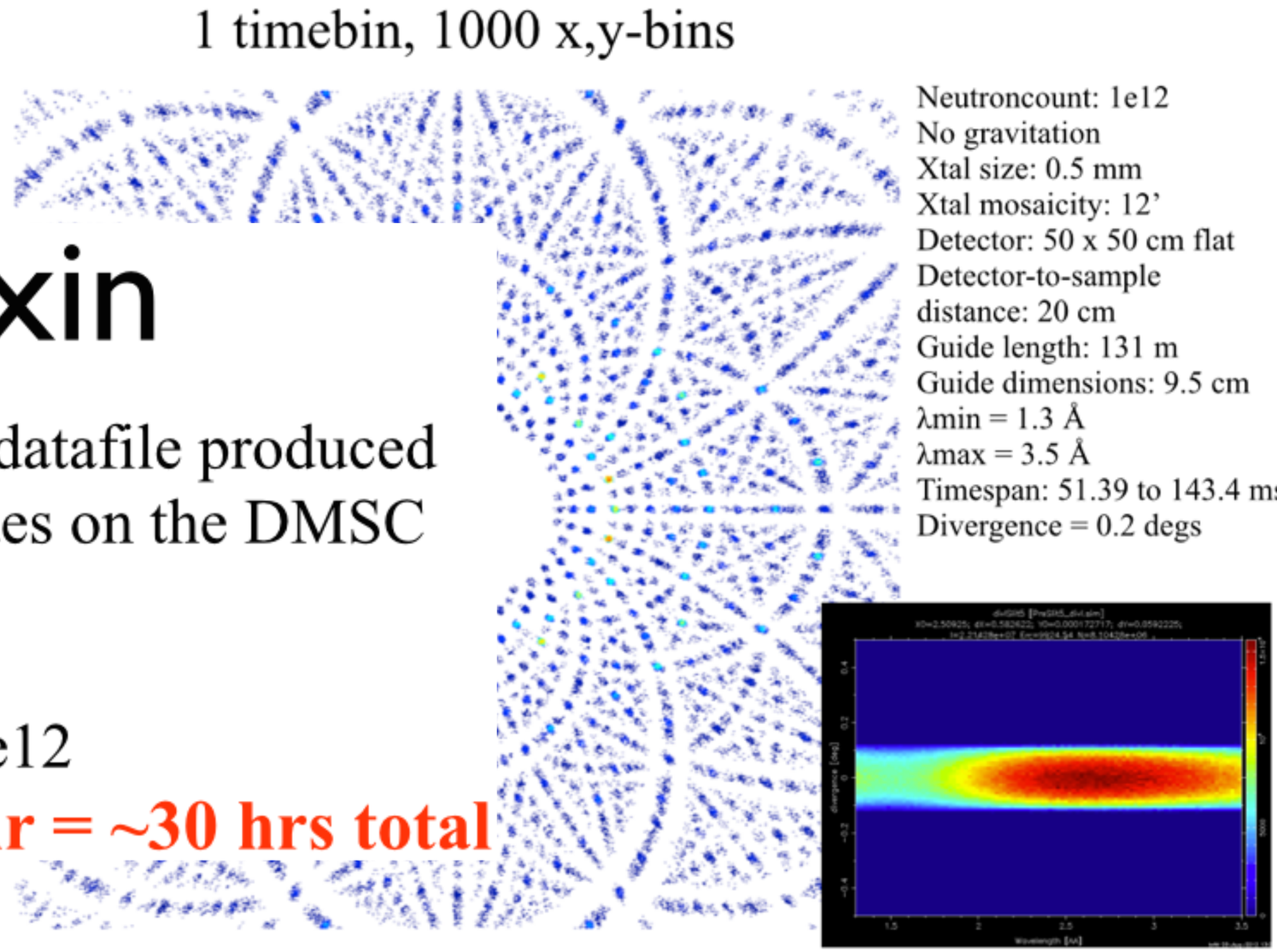
Events shown on the full instrument

- The event data from McStas should look something like this in “full 3D” - you may have to move/zoom a bit about



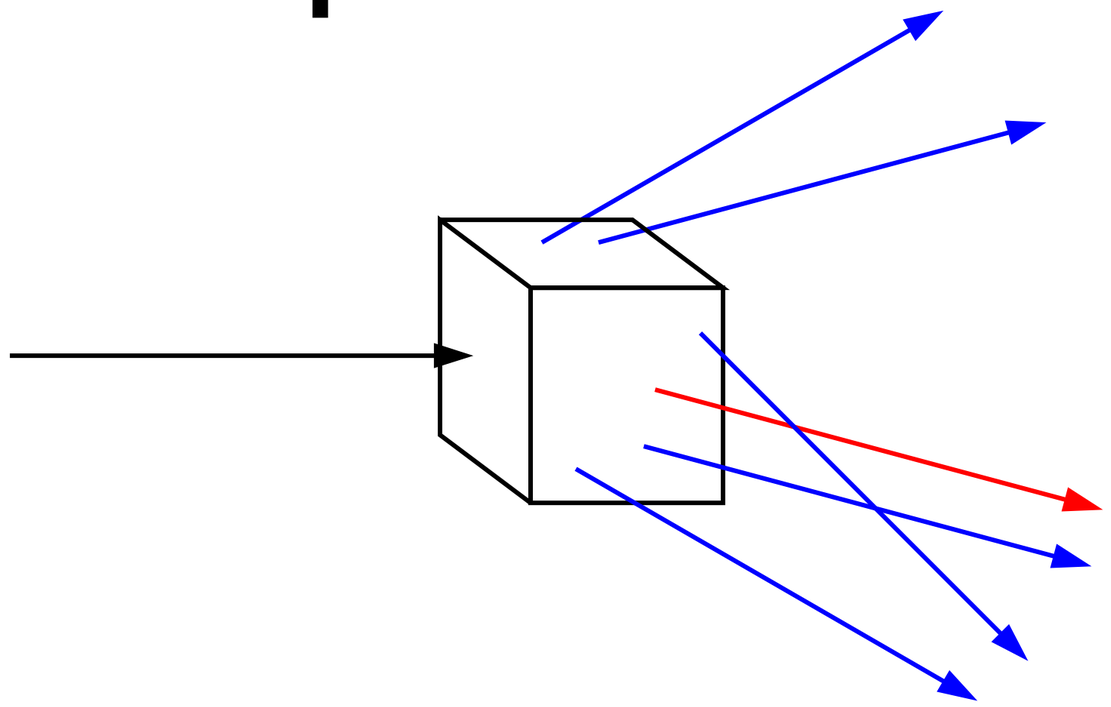
Problem: McStas Single_crystal.comp "slow" for large unit cell diffraction studies

- Example: Rubredoxin



- Reflection list ~ 124 K reflections (still "small" in the PX world!!)

Algorithm improvement: **Use incoming neutrons more efficiently - scatter each one on all possible reflections**



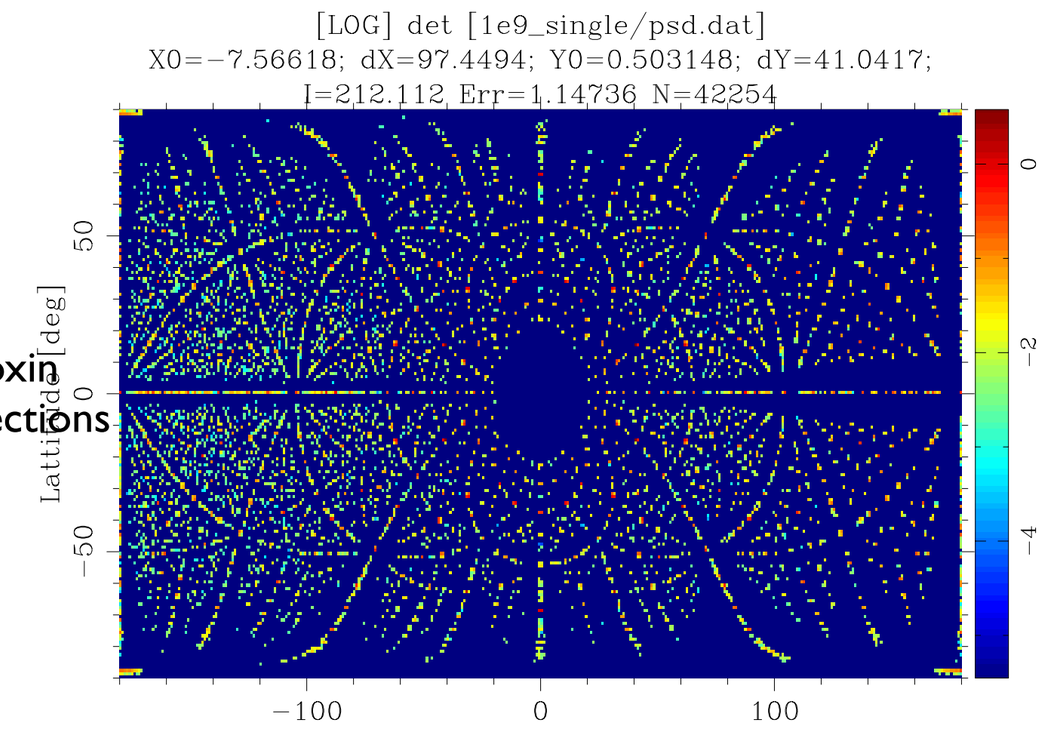
- **Red**: Original algorithm, one incoming neutron used only once
- **Blue**: Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of "active"** diffraction **spots** - in the case Rubredoxin this is around **50**!

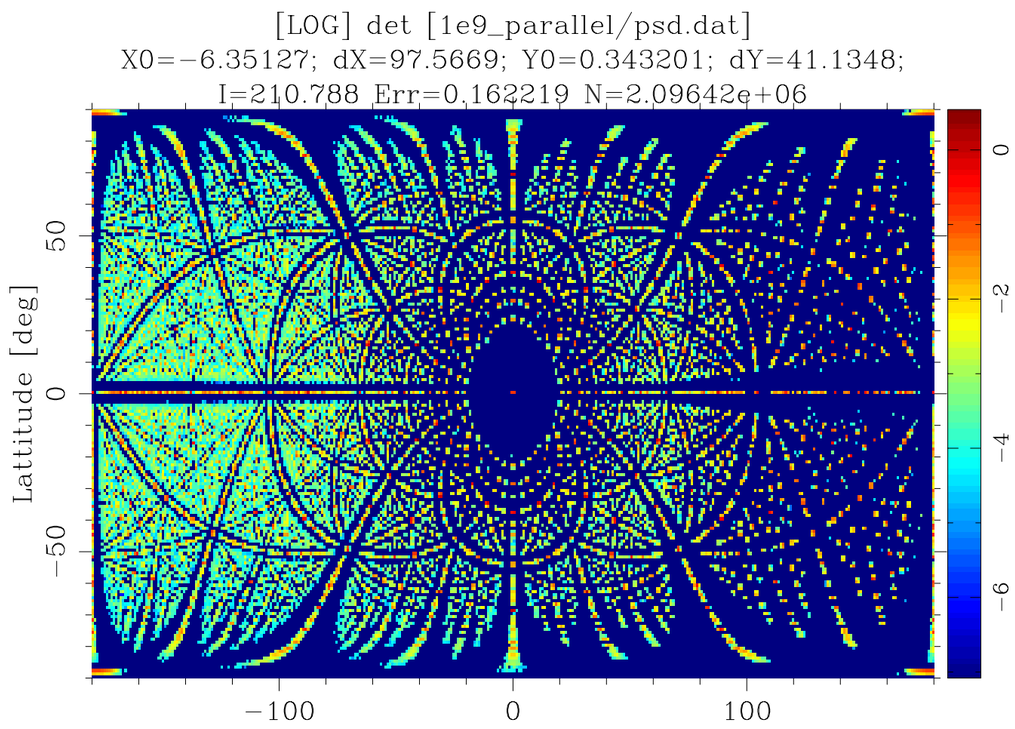
Sim data speak for themselves - 1e9 rays

Old comp

New comp

Rubedoxin
124K reflections





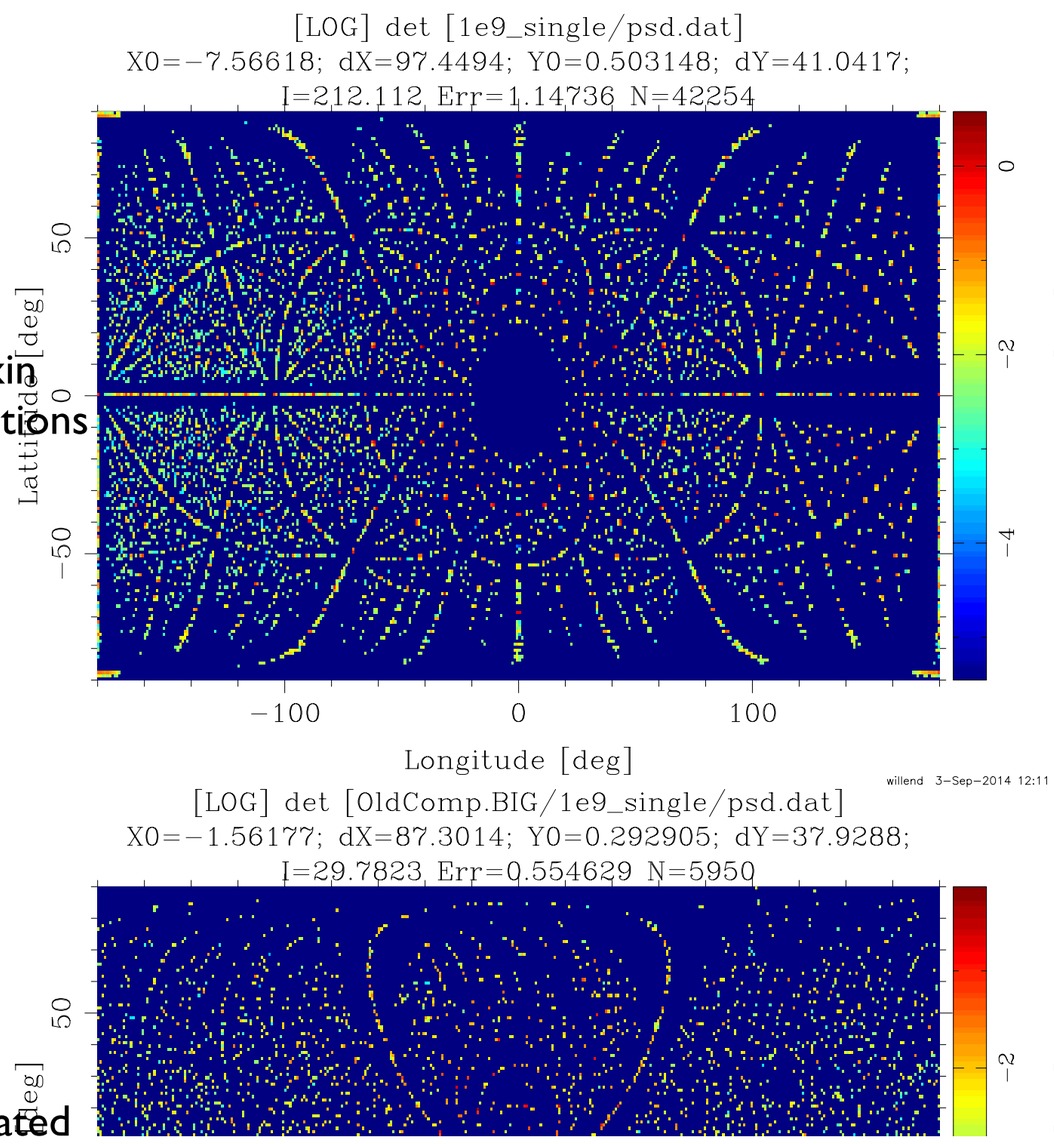
~ Factor **50**
more efficient

Predeuterated
pyrophosphatase
1.7M reflections

~ Factor **500**
more efficient

Sim data speak for themselves - 1e9 rays

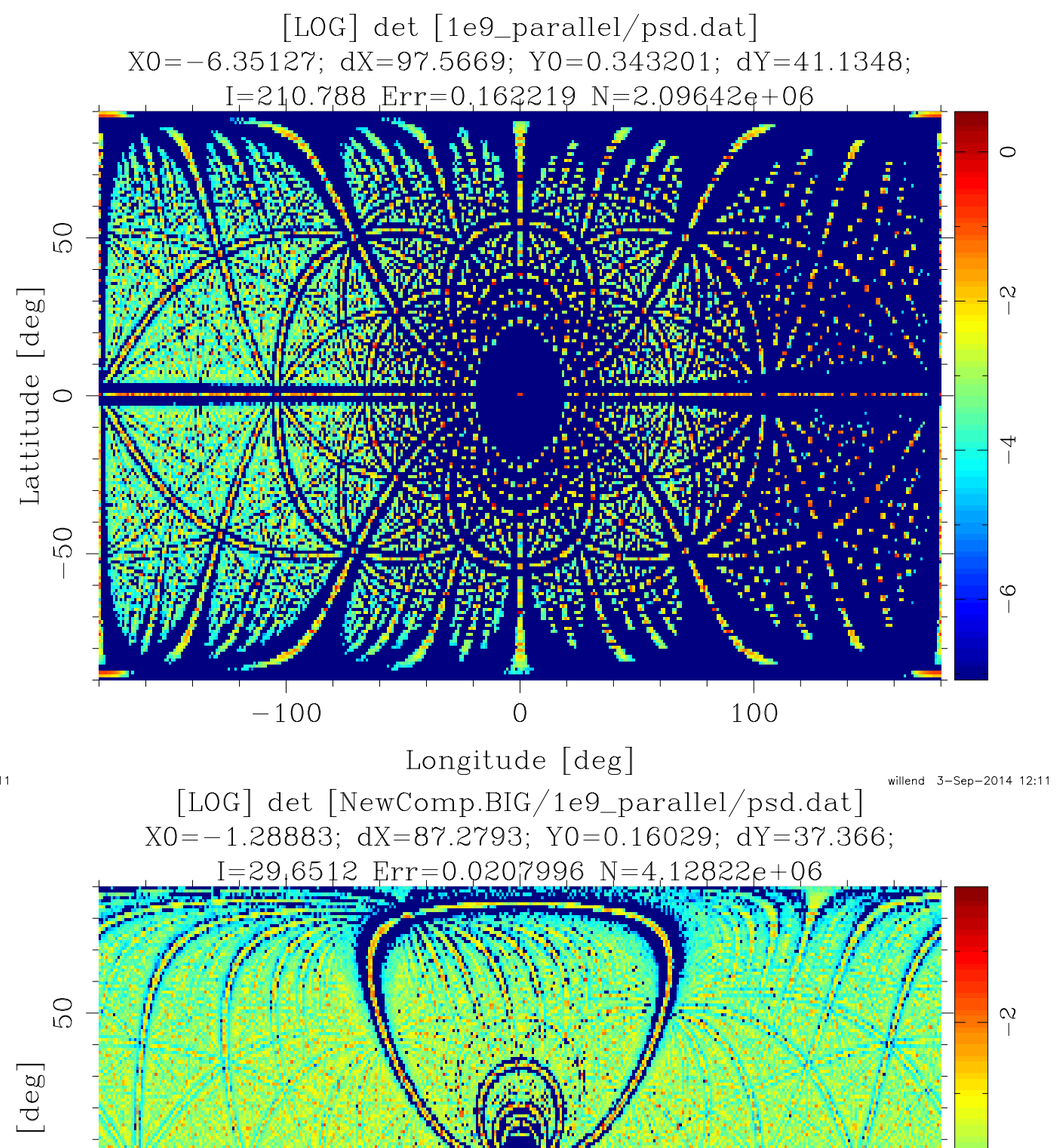
Old comp



Rubedoxin
124K reflections

Predeuterated

New comp



~ Factor **50** more efficient

~ Factor **500** more efficient

Use: Check out template_NMX from the McStas distribution

Similar optimisation of the PowderN component

People

- The success of the project is also about the people:
  - Present McStas team members

- K Lefmann

E Farhi

P Willendrup

E Knudsen

U Filges

T R Nielsen

  - Past McStas team members

- K Nielsen

PO Åstrand

K Lieutenant

P Christiansen

J Brinch