11'TH NOBUGS|2016
Copenhagen, Denmark, 17th to 19th October
NEW OPPORTUNITIES FOR BETTER USER GROUP SOFTWARE

Integrating software: SASview, McStas and Mantid for powerful virtual SANS experiments

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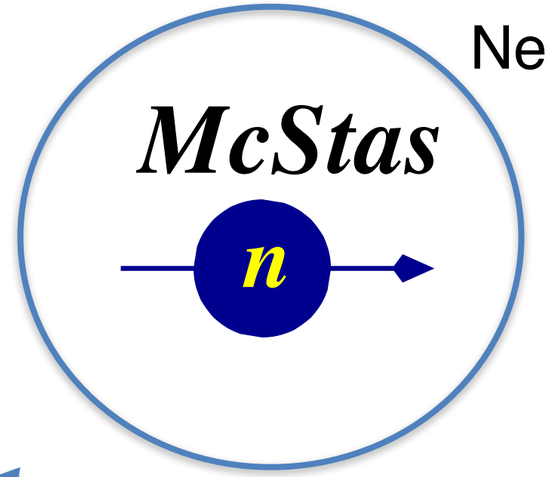
Agenda

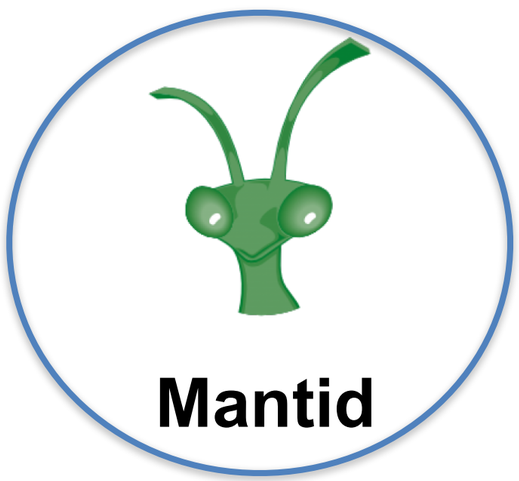
- A brief introduction to the softwares
  - **McStas** - *A neutron Monte Carlo ray-trace simulation package*
  - **SASview** - *Small Angle Scattering Analysis Software Package*
  - **Mantid** - *Manipulation and Analysis Toolkit for Instrument Data*
- The integration
  - Why did we do it?
  - How was it done?
- Future

"Full-circle" virtual experiment software integration

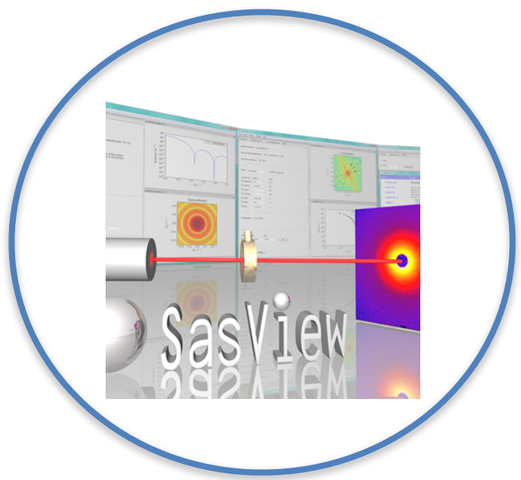
Neutron transport



Reduction



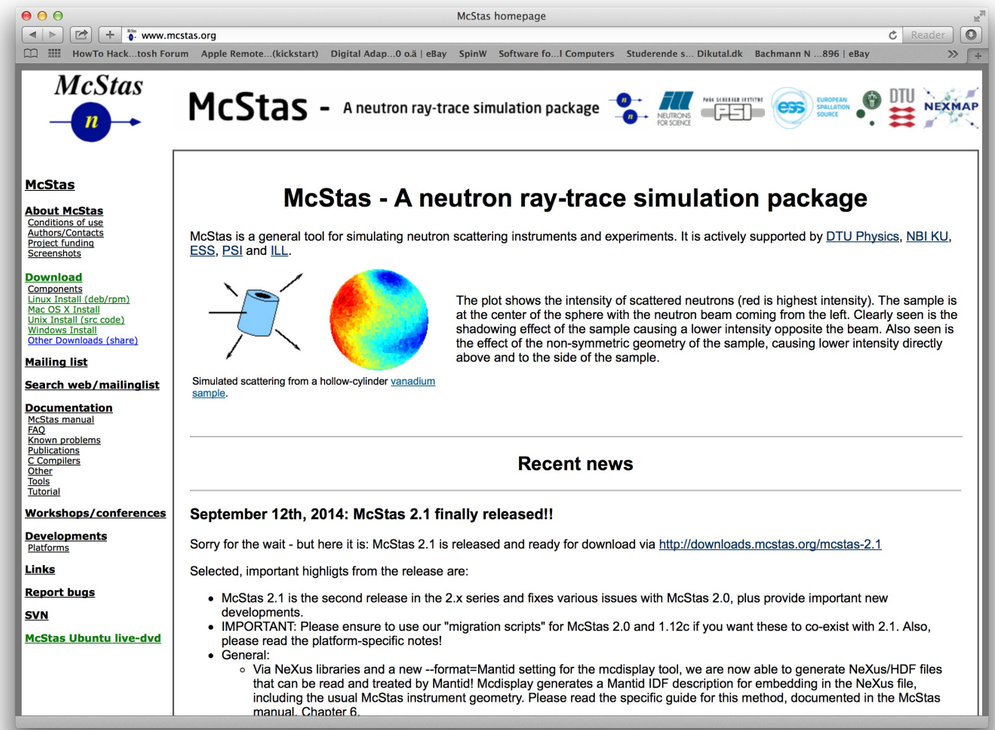
Data analysis



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

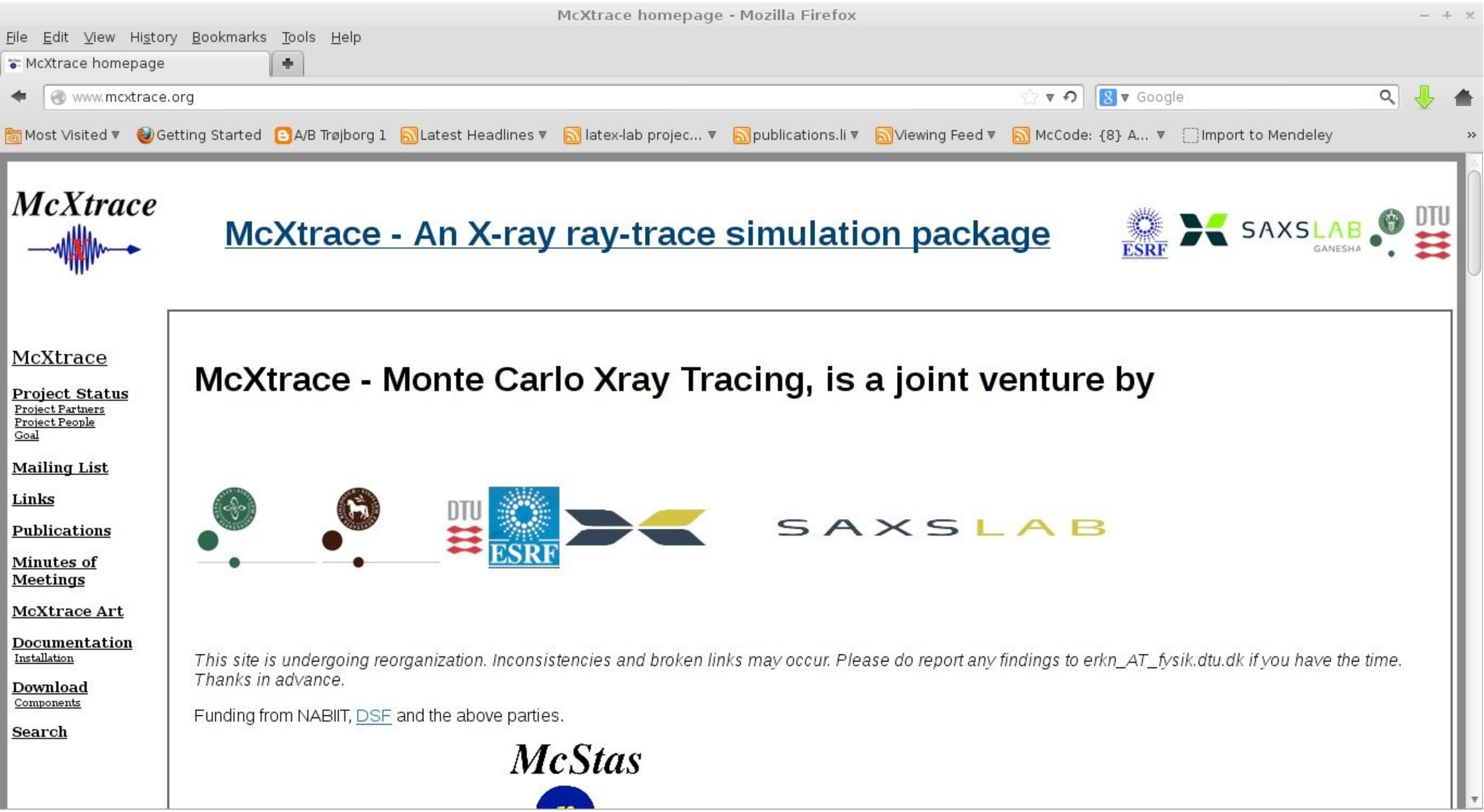
GNU GPL license
Open Source



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

mcstas-users@mcstas.org mailinglist

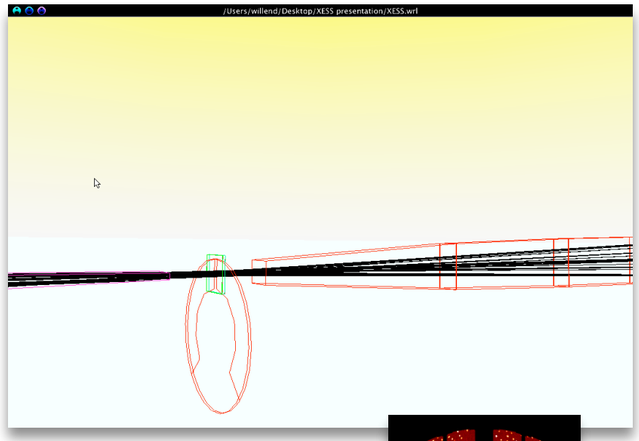
- Not only neutrons, there is also McXtrace...

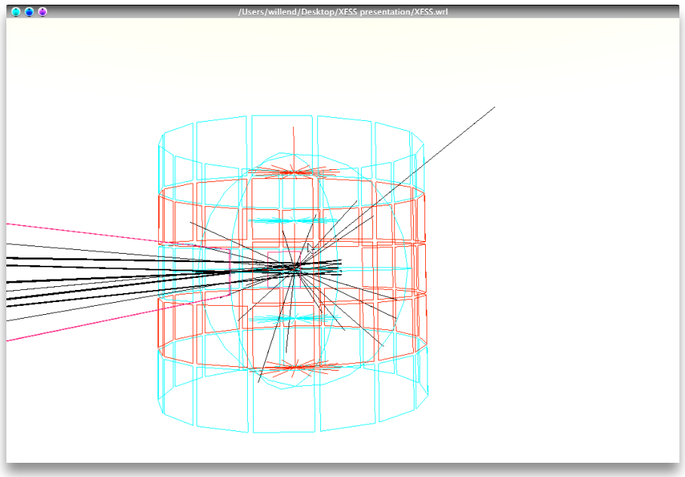


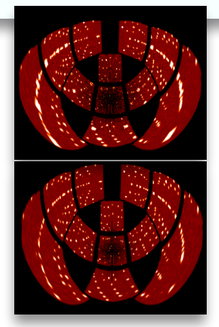
What is McStas used for?

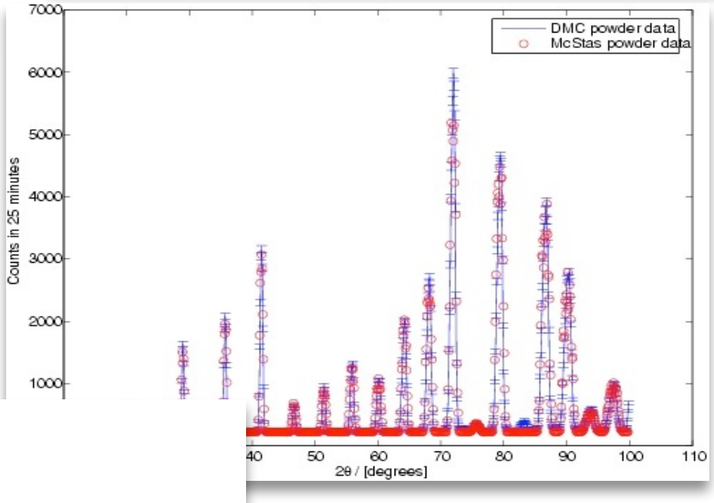
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

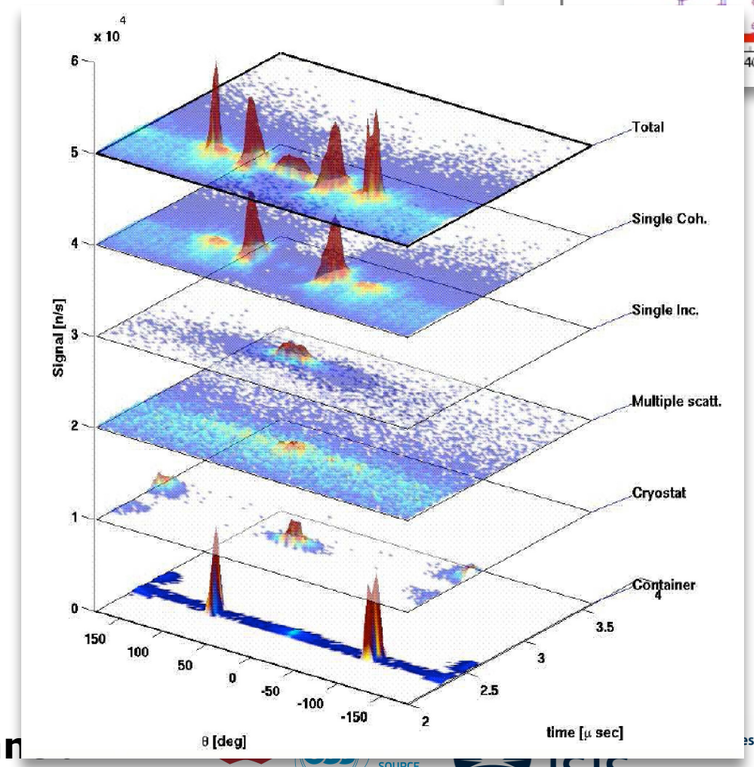
(KU, DTU, e-Learning…)

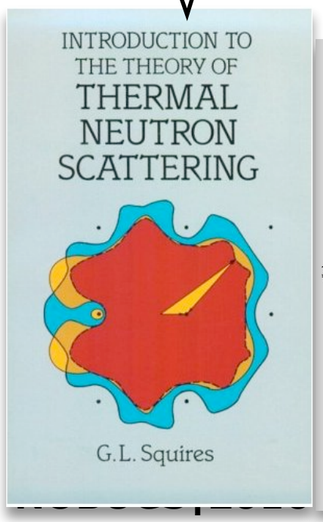


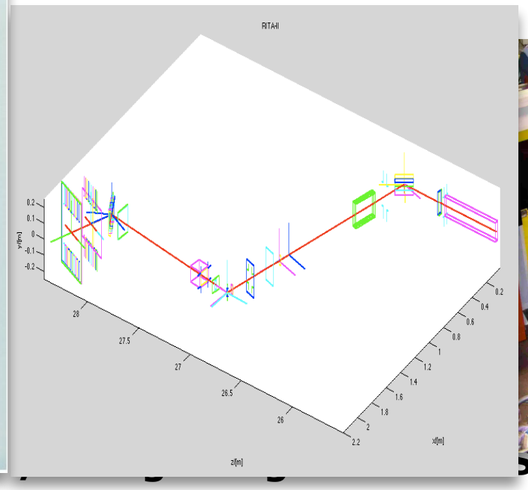










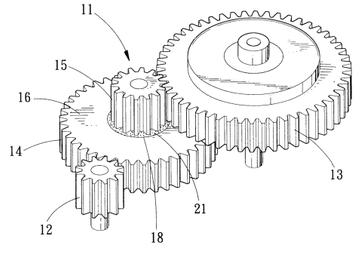


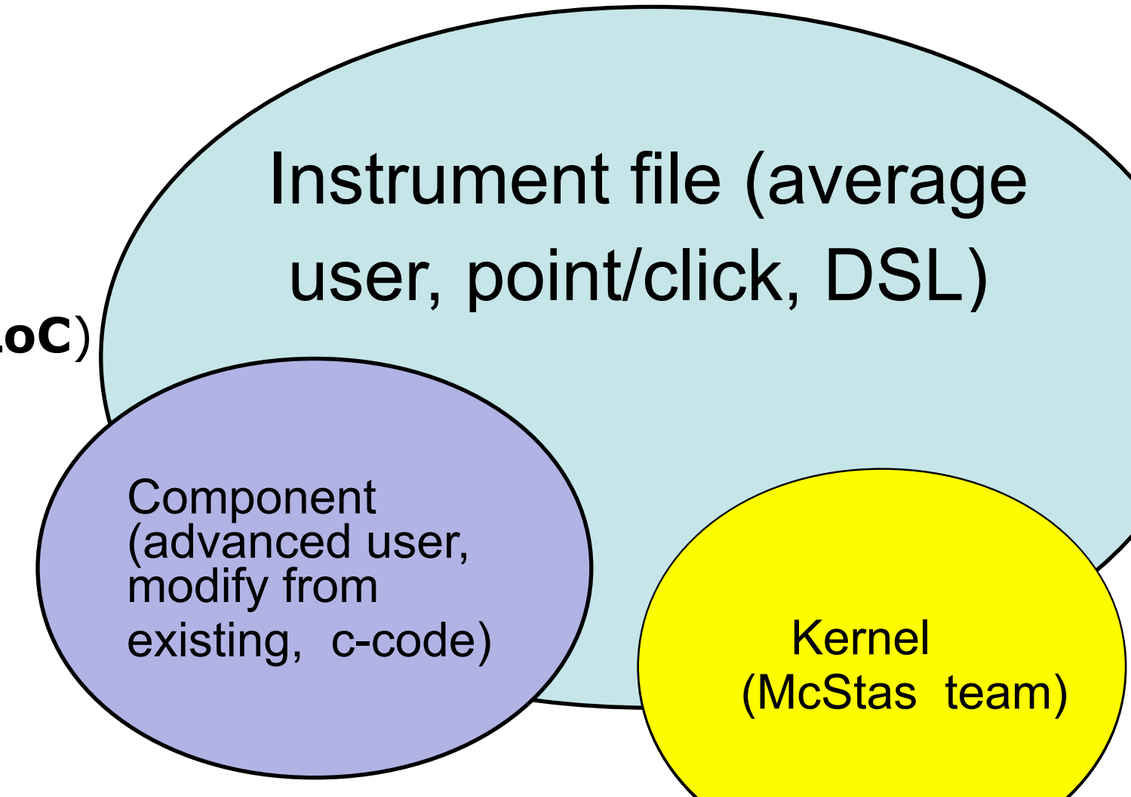
SASview, McStas and Man

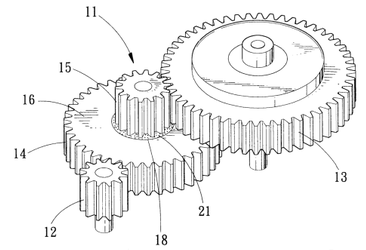
McStas overview

- 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 (**short ~200 LoC**)
- DSL + **ISO-C** code gen.







DSL + **ISO-C** code gen.

Relevant new feature: automatic C-lib dependency linking

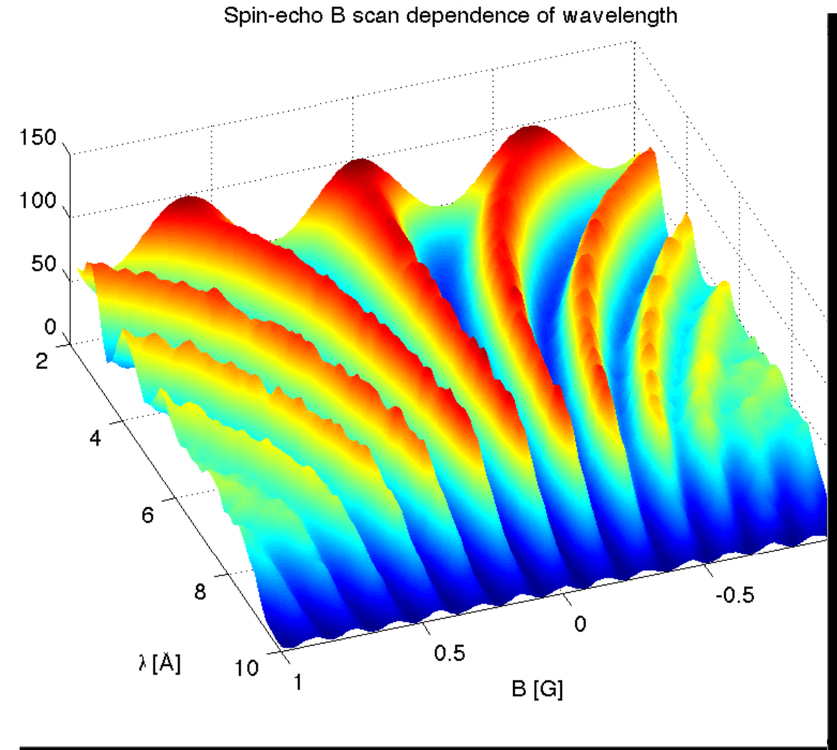
- Automatic generation of c-lib dependencies

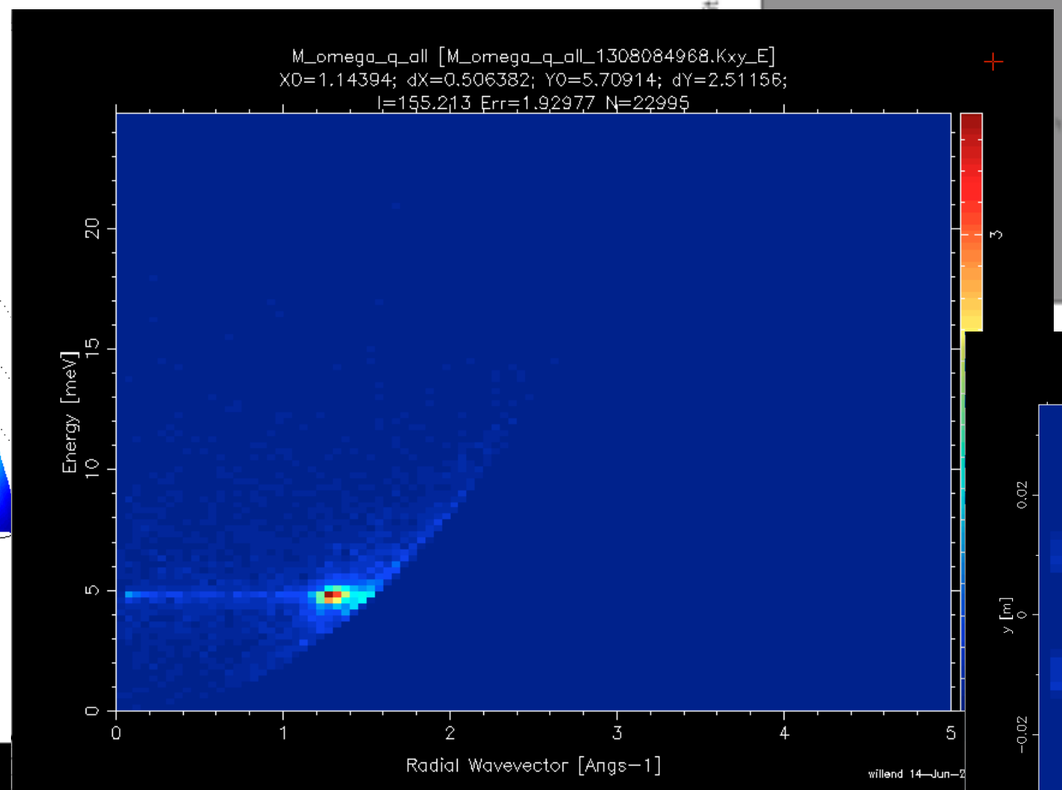
```
mcstas -t -o ISIS_CRISP.c ISIS_CRISP.instr
Info:    'ISIS_moderator' is a contributed component.
Warning: Using DEFINITION parameter of component Multilayer_Sample() (potential syntax error) at line
ISIS_CRISP.instr:148
  sldPar={ 0.0 , 6.35e-6 }
Warning: Using DEFINITION parameter of component Multilayer_Sample() (potential syntax error) at line
ISIS_CRISP.instr:148
  dPar={ 0.0 }
Warning: Using DEFINITION parameter of component Multilayer_Sample() (potential syntax error) at line
ISIS_CRISP.instr:148
  sigmaPar={ 5.0 }
Warning: Using DEFINITION parameter of component Multilayer_Sample() (potential syntax error) at line
ISIS_CRISP.instr:148
  focus_xw=2 * tend
Warning: Component isis_source=ISIS_moderator(string Face) definition parameter
         may be changed into a setting parameter to avoid
         warnings at compile time.
CFLAGS=-lgsl -lgslcblas
```

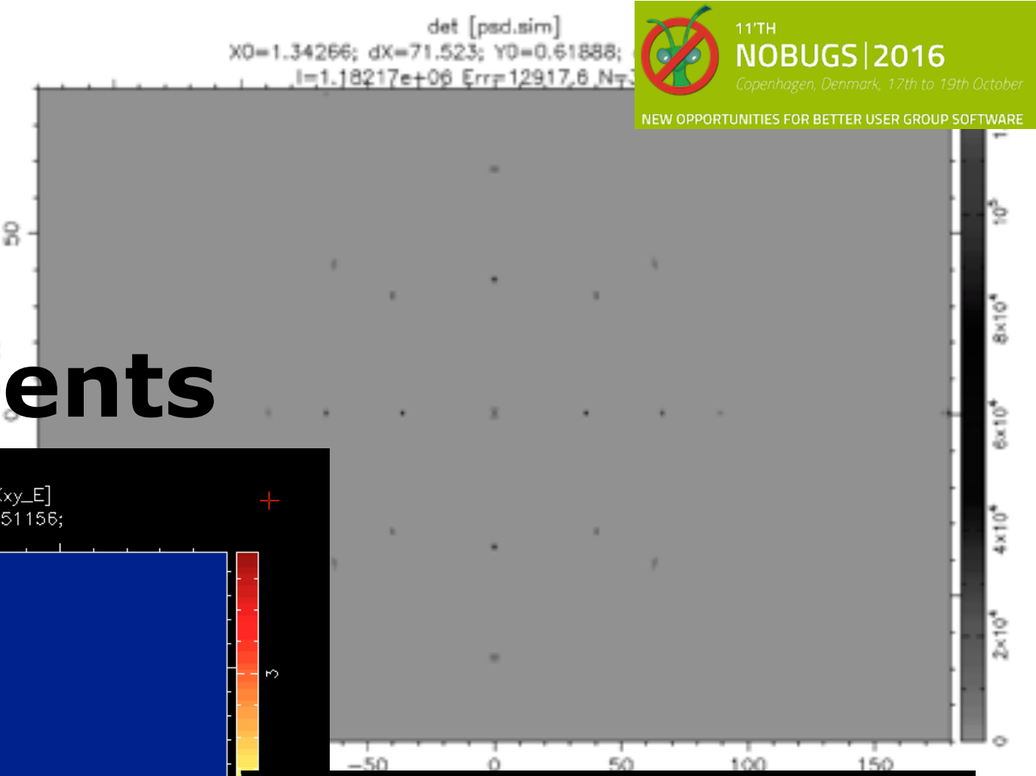
- For allowing components and instruments relying on external libs to link these automatically - ease of use
  - SASview sample comp: DEPENDENCY "-std=c99"
  - NeXus could be done with DEPENDENCY "-DUSE_NEXUS -lNeXus" (so far avoided because of need to distribute libs…
- Will be picked up by mcrun / mcgui on the fly and passed to the compiler

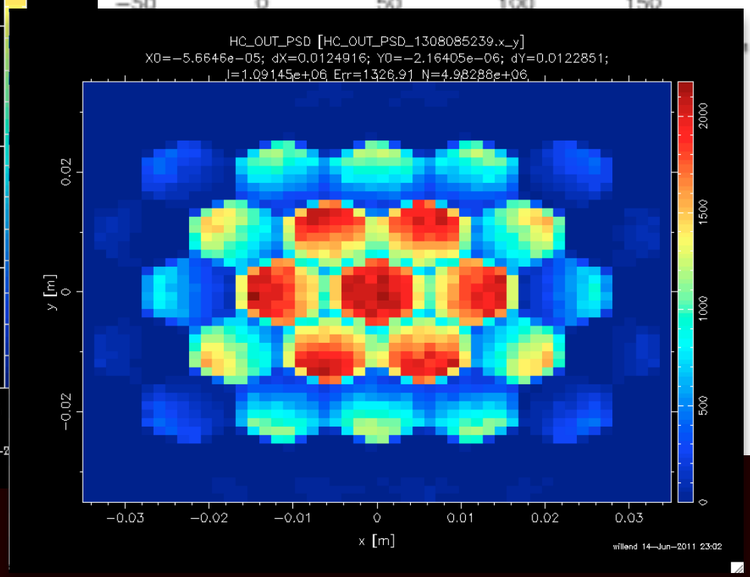
McStas

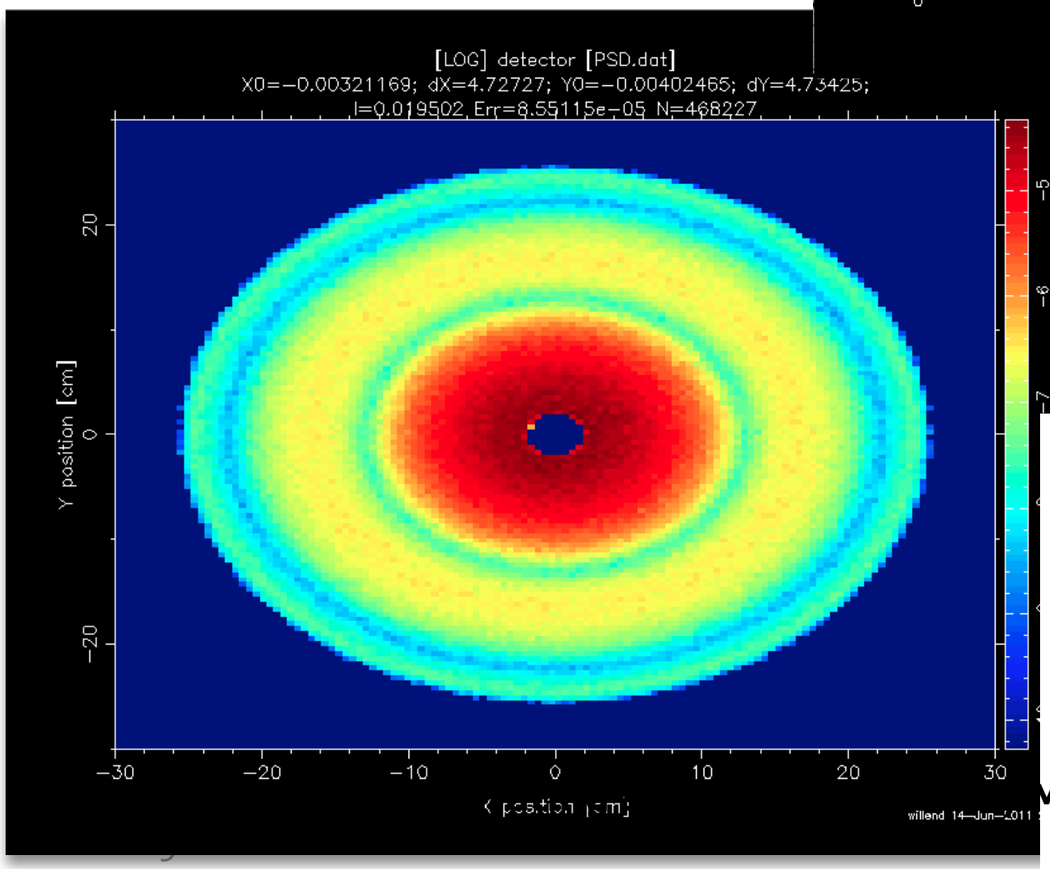
Example suite: 123 instruments

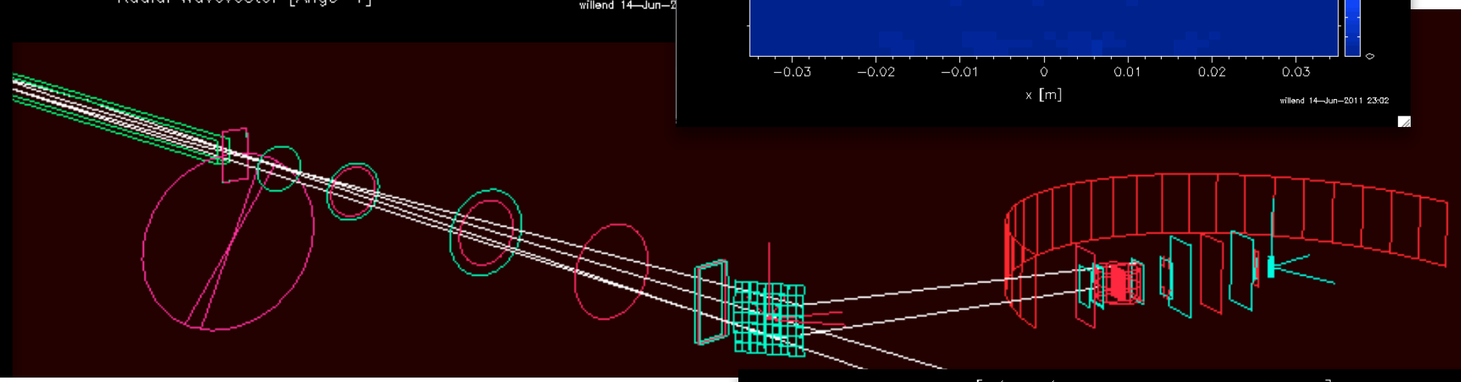












McStas and Mantid

DTU ess EUROPEAN SPALLATION SOURCE

Science & Technology Facilities Council ISIS

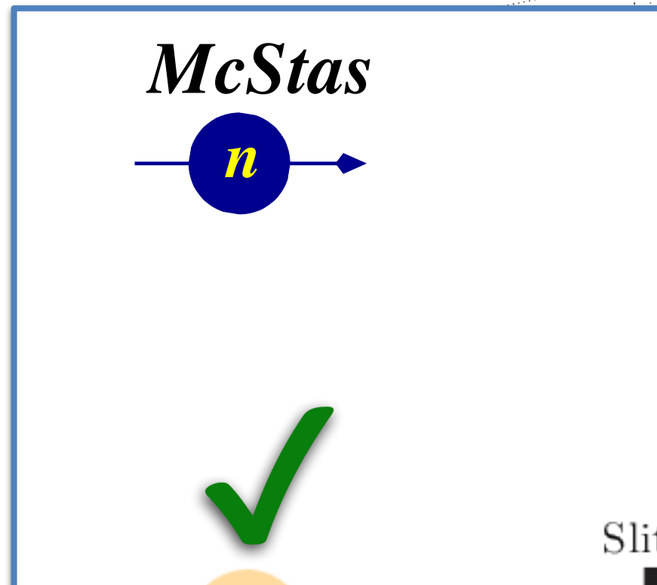
Sas View

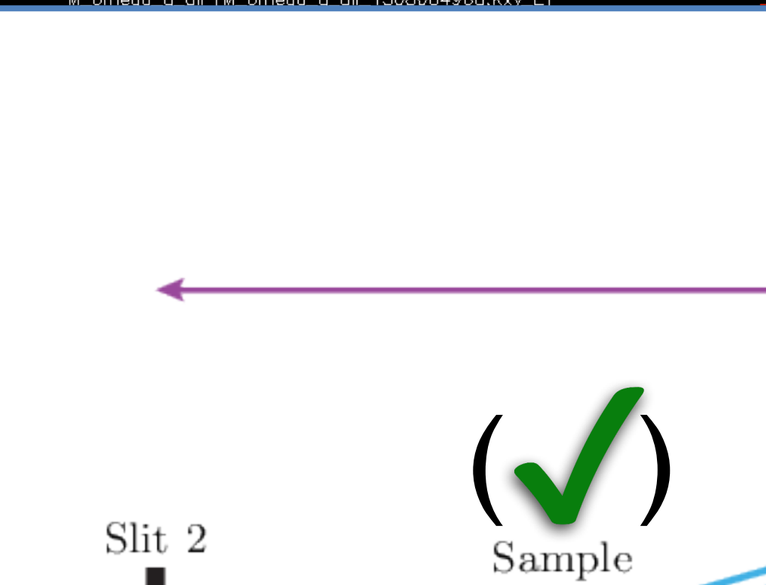
McStas

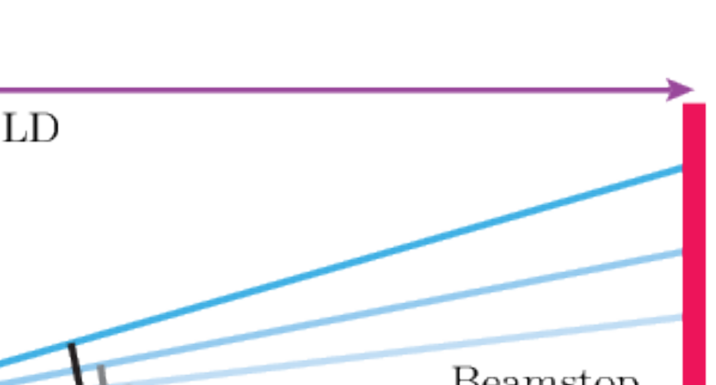
MANTID

Example suite: 123 instruments

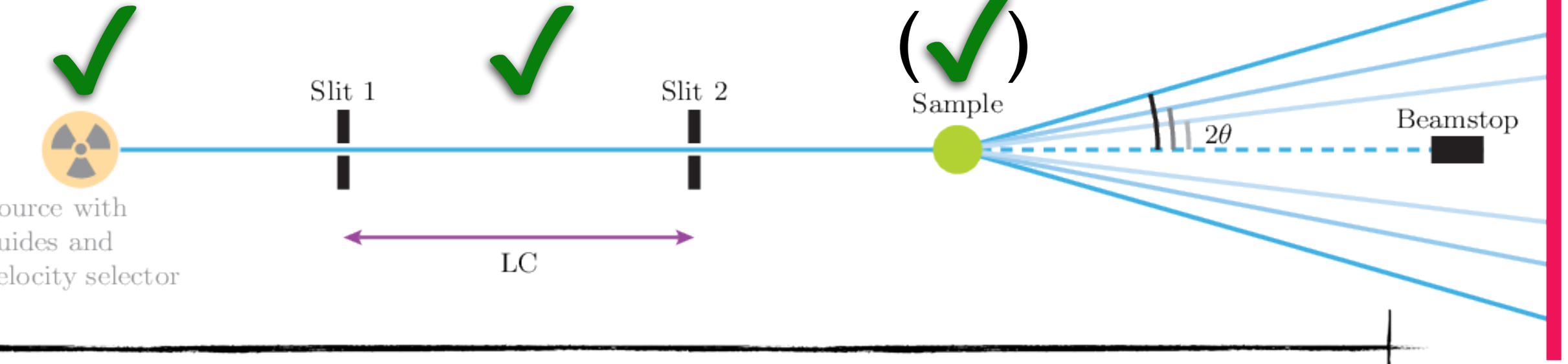
Spin-echo B scan dependence of wavelength







McStas and Mantid

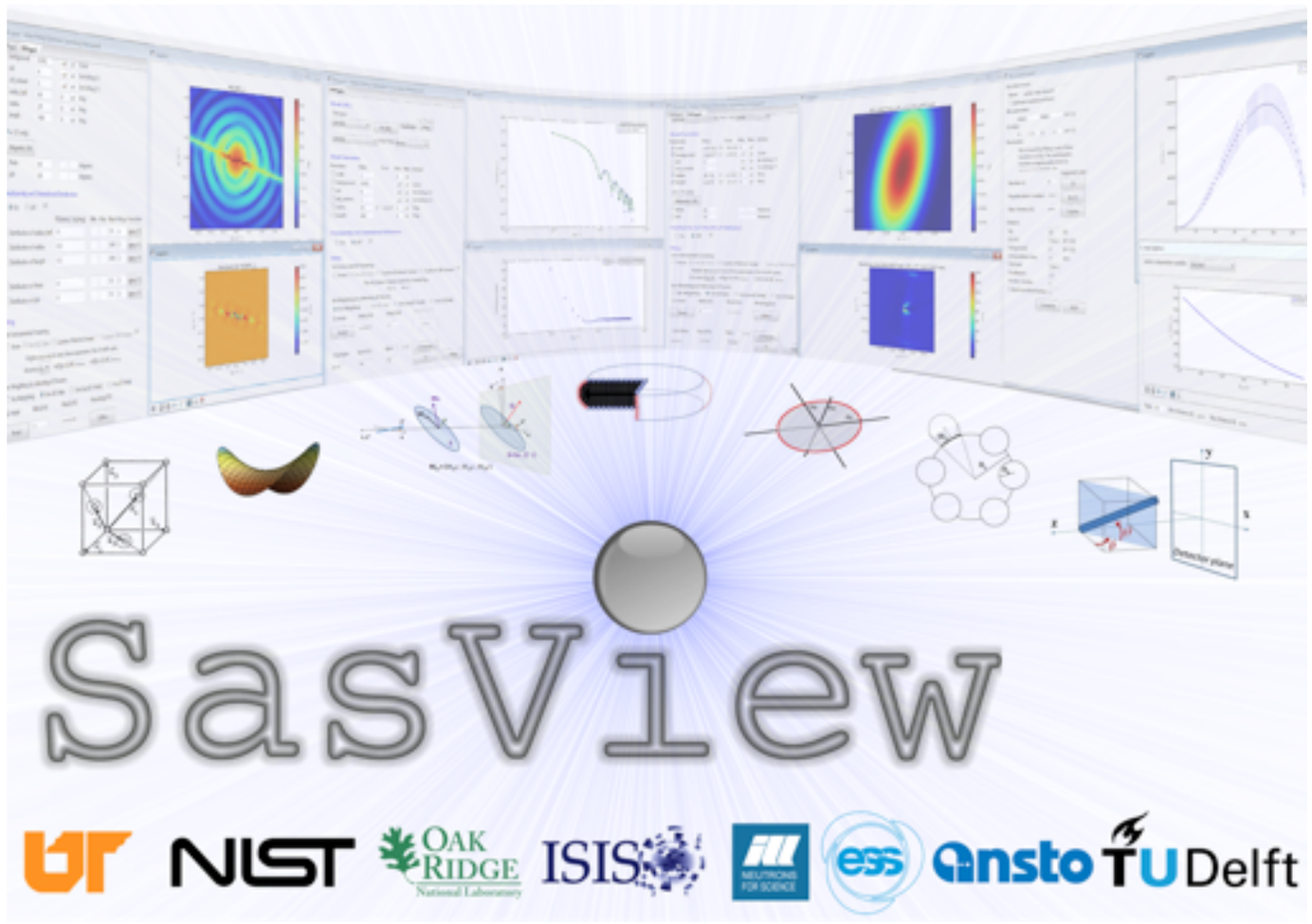


McStas includes “everything” to simulate “anything” at a neutron scattering instrument

SasView - Small Angle Scattering Analysis Software Package

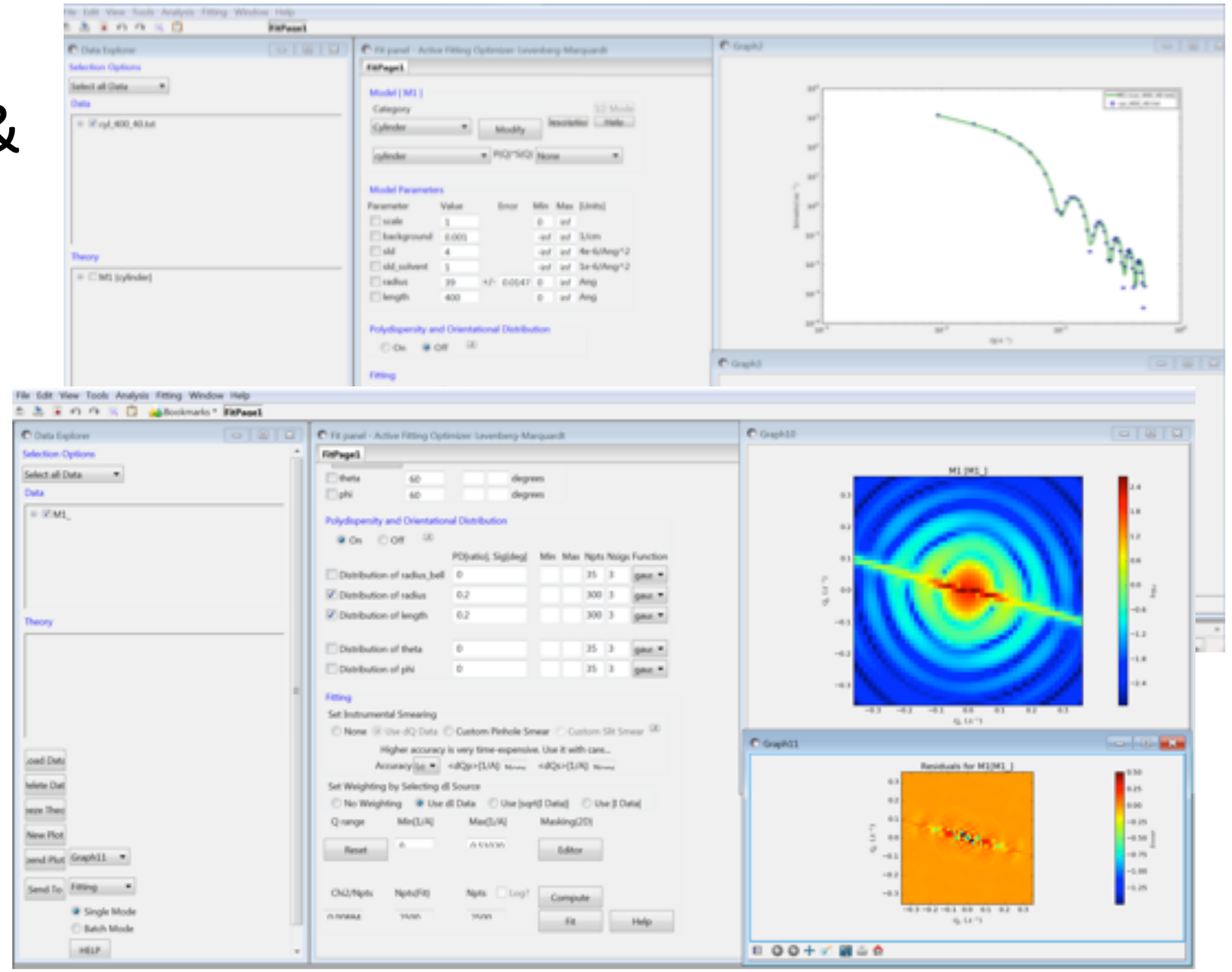
EUROPEAN SPALLATION SOURCE

- Operates on reduced scattering data
- **Performs modeling in inverse space**
- Data analysis toolbox:
  - Fitting **models** to data
  - P(r) inversion
  - Model-independent analysis
- Other useful tools



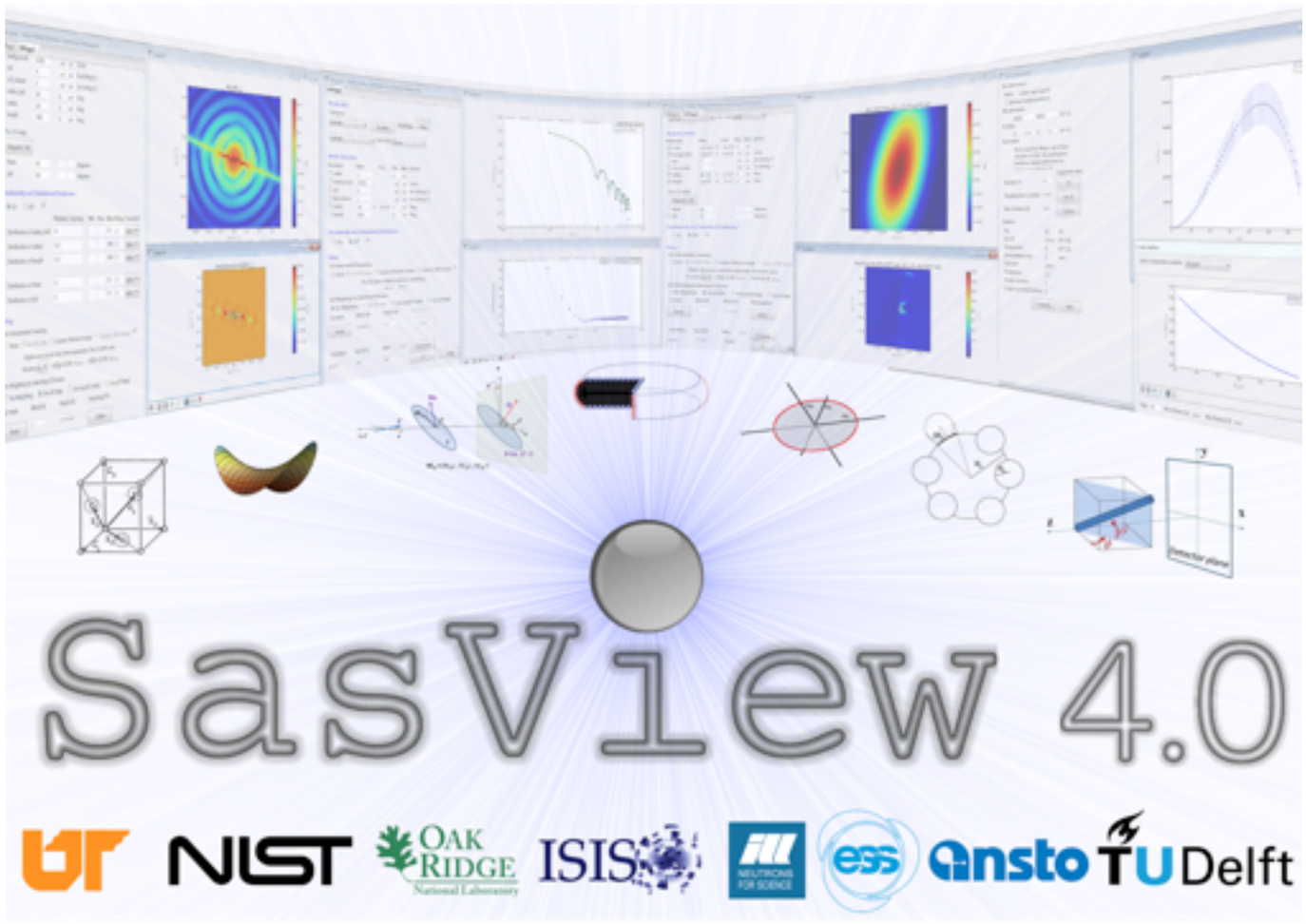
SasView - Fitting

- Handles 1D and 2D data
- support for canSAS XML & NXcanSAS formats
- **Form and structure factors for various particle shapes**
- Different optimizers (Bayesian Statistics)
- Allows polydispersity
- Simultaneous and batch fitting



SasView 4.0 is out

- SasView "built-in" models have been separated out into an **independent package (aka SASmodels)**
- Easy to add custom user models (including advanced)
- Support for OpenCL
- All model documentation has been reviewed and updated
- Number of minor bugs fixed

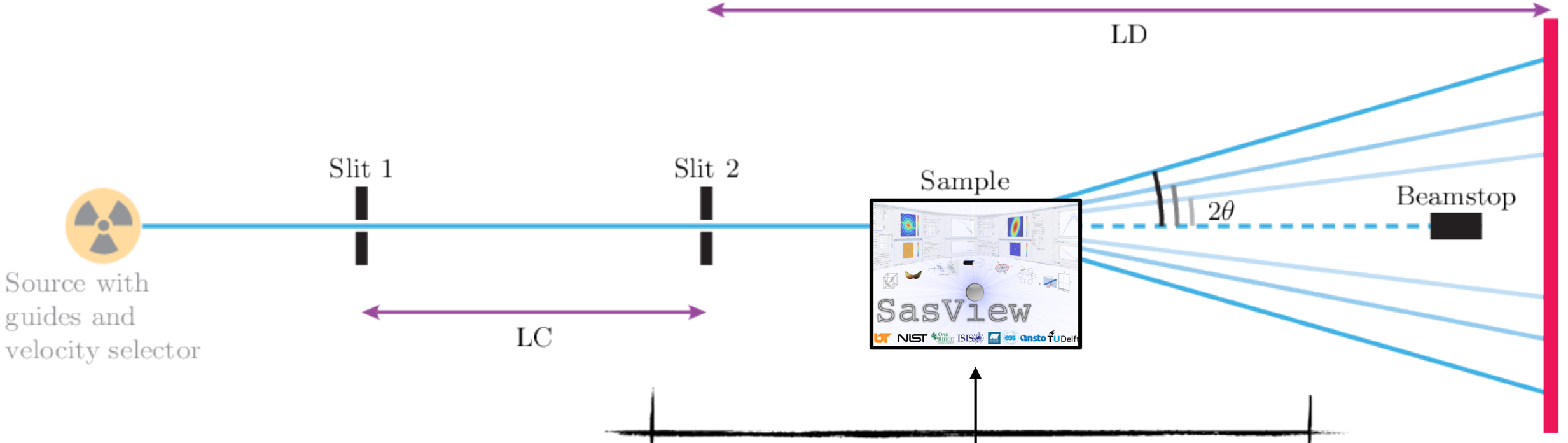


Available from:
https://github.com/SasView/sasview/releases/tag/v4.0

SasView 4.0 is out

McStas

What will access to SASview give McStas?



Models of $S(\vec{q},\omega)$ - i.e. science

(and lots of them…!)

What is Mantid?

- A Framework for Reduction and Analysis of Neutron and Muon Data
  - Can Be accessed by
    - MantidPlot
    - Python Interface
    - C++ API
  - Has a set of data objects, methods and Algorithms well suited towards scattering science

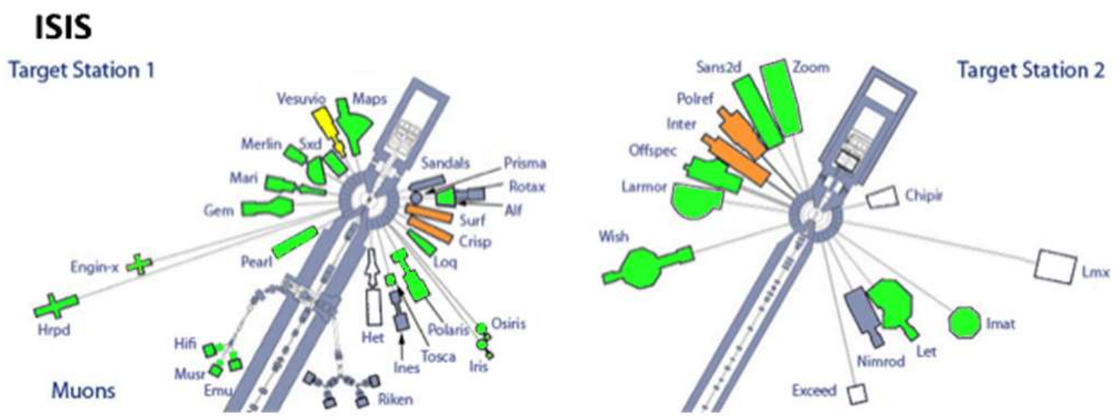
Partners and Contributors

- Partners

- Contributors

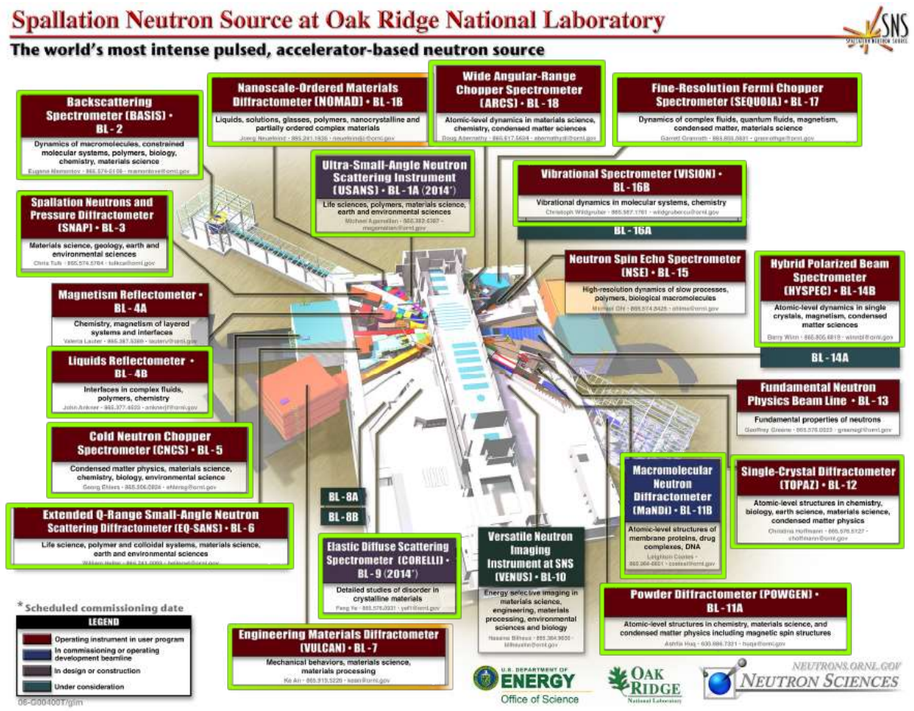
5 Presentation_name

Deployment at ISIS



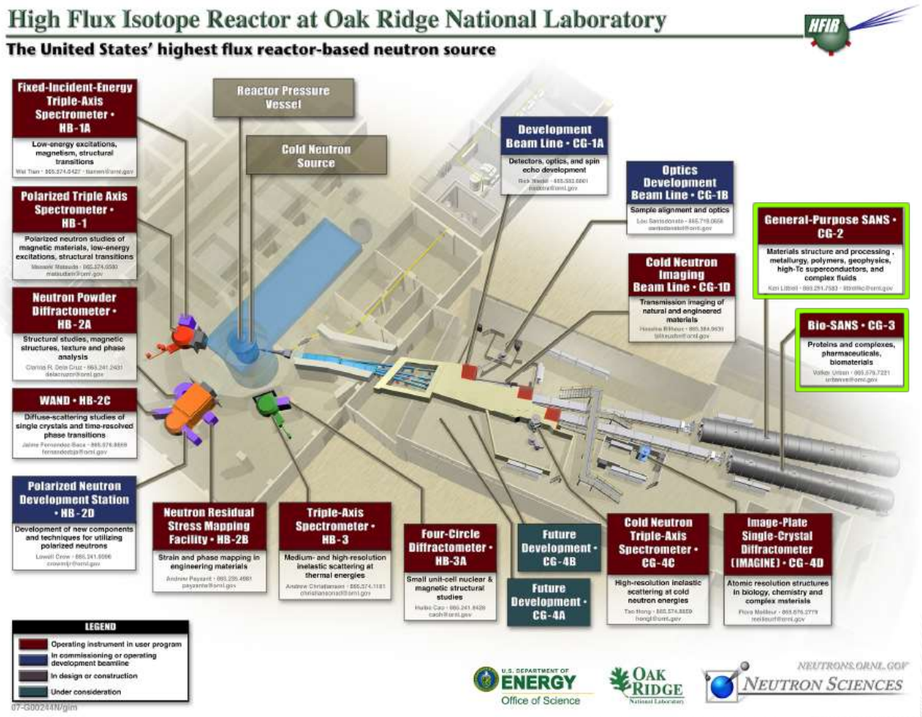
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Deployment at SNS



OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Deployment at HFIR



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Other instruments

NEUTRONS FOR SCIENCE®

- NMI3 supported evaluation
- IN4,5 & 6
- D33

PAUL SCHERRER INSTITUT PSI

- Focus
- Poldi

Orphée Laboratoire Léon Brillouin

- Mibemol

FRM II
Forschungs-Neutronenquell Heinz Maier-Leibnitz

- TofTof

ansto

- Pelican
- Bilby

ess EUROPEAN SPALLATION SOURCE

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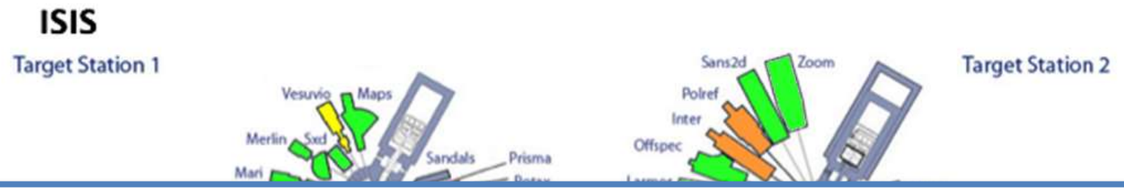
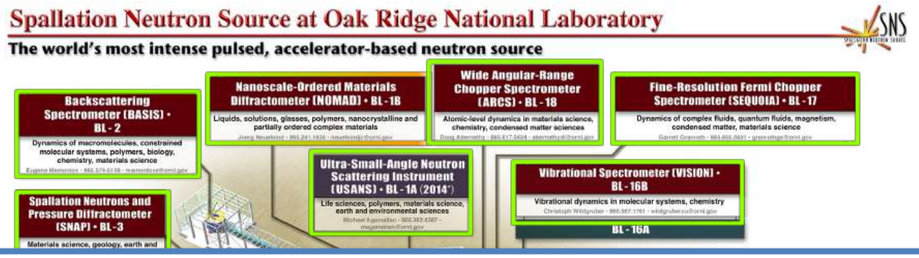
Deployment at ISIS



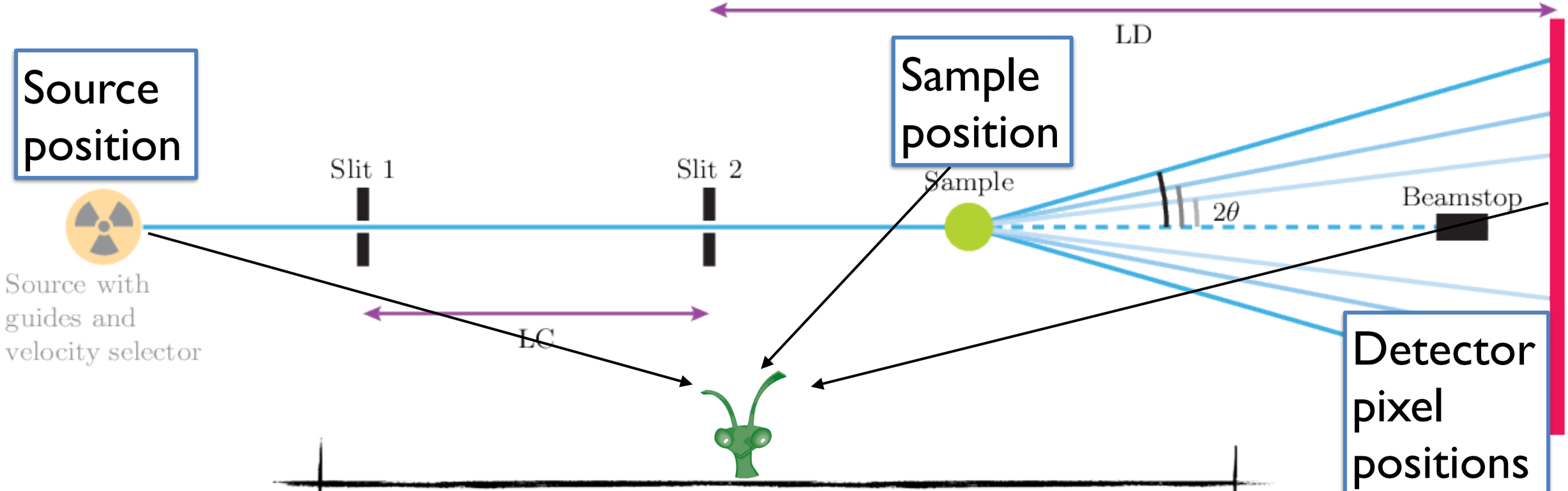
Deployment at SNS



McStas

What will access to Mantid give McStas?

EUROPEAN SPALLATION SOURCE

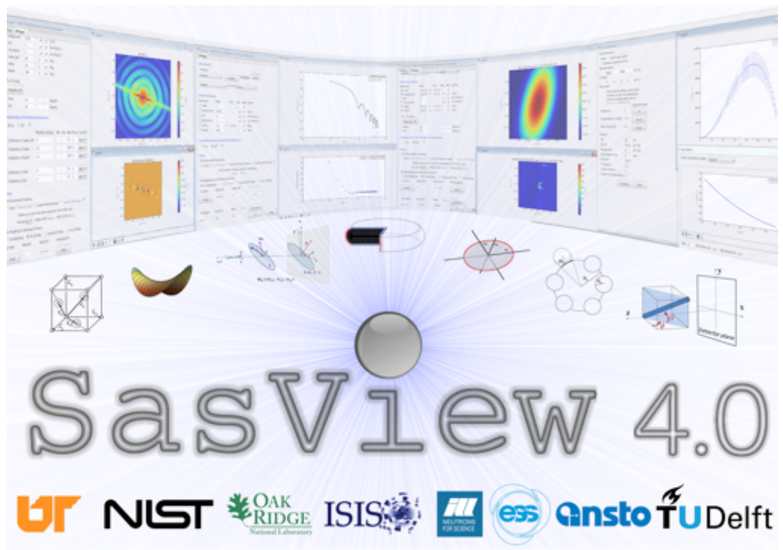


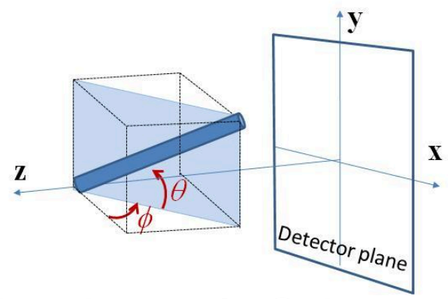
$$+\mathrm{ToF}_n \rightarrow \vec{k_i}, \vec{k_f}, \vec{q}, \hbar\omega, \rightarrow S(\vec{q},\omega) \rightarrow \text{science}$$

(Presentation and handling of simulation data ala non-virtual ToF instruments…)

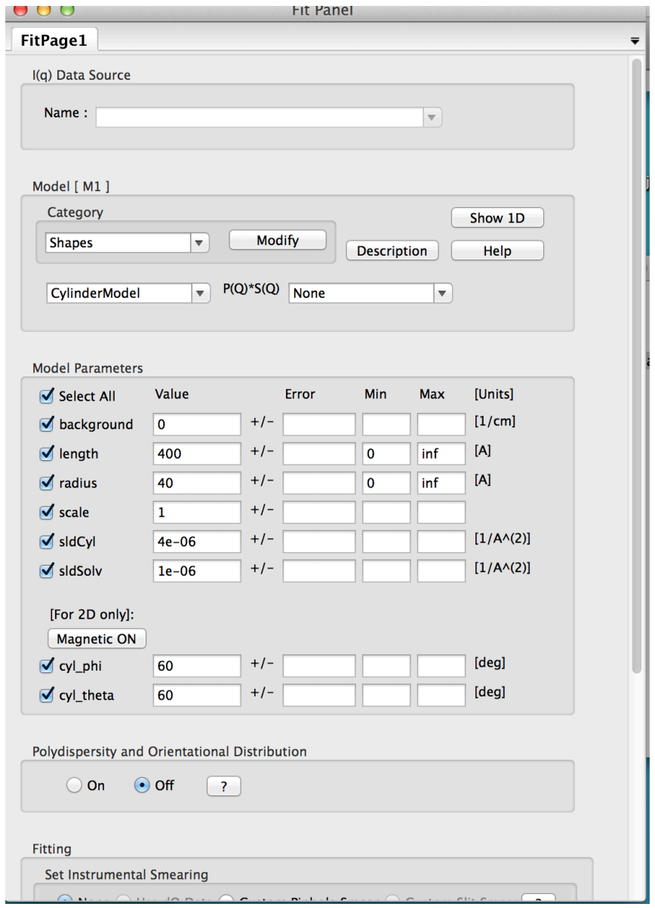
Why? Driver is development of instruments

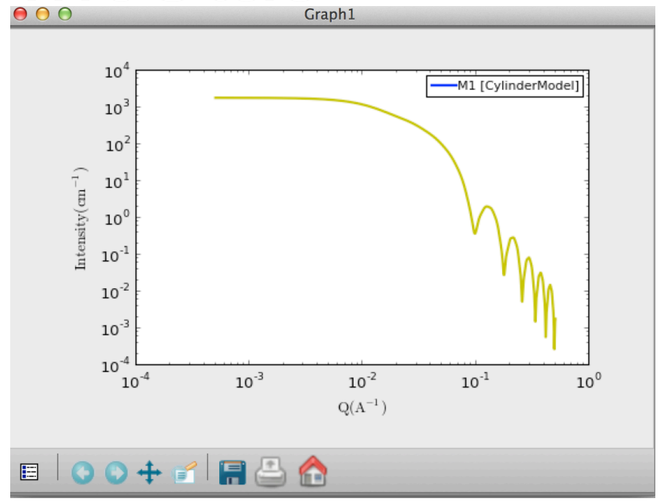
- ✓ McStas used for instrument design work at
- ✓ LoKI team needed 2D scattering kernels in McStas
- ✓ Use SasView scattering kernels in McStas

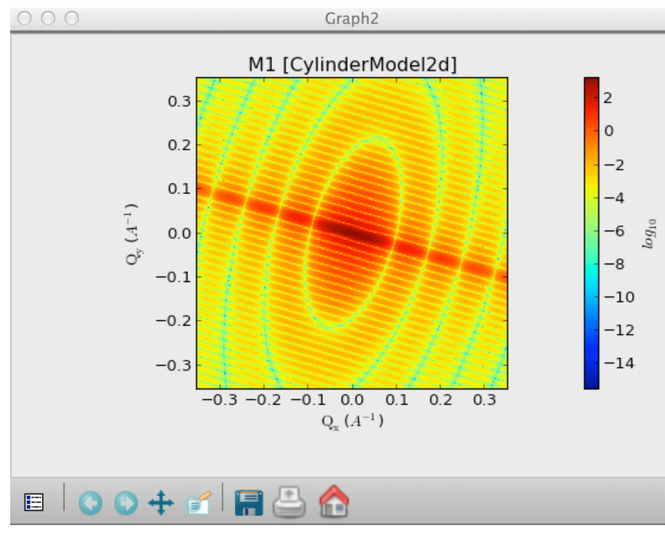




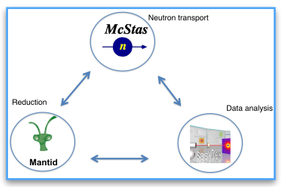
SasView scattering kernel: Orientated cylinder







- ✓ Mantid is reduction software for
- → Make solution with all 3 for bootstrapping the analysis pipeline!



How?

McSt

The `SasView_m`

This SANS sample exposes Sas

Identification

- **Author:** Jakob Garde, To
- **Origin:** SasView, DTU, I
- **Date:** 03.02.2016
- **Version:** 0.5

Description

```
Sample for use in SANS ins                                                    he shape:

Shape:        - A filled b
              - A cylinder
              - A filled s

These parameters are mutua

Example using spheres in t
     SasView_model(model_i
                   x


The algorithm of this comp                                                    9 -g -O2 -lm.
Or, add the flag "-std=c99

The list of scattering mod                                                    ble below.

A few models may require m

McStas does currently not

The 2D scattering scatteri                                                    index=10 to use cylinder_xy.
```

Generator .py scripts.

Input:

Folder with SASmodels

Output:

c-code snippets

McStas component interface

Linked documentation

Result distributed with McStas

User has tools to (re-)generate

McStas mcdoc: SasView_model

[Identification | Description | Input parameters | Output parameters | Links]

The `SasView_model` Component

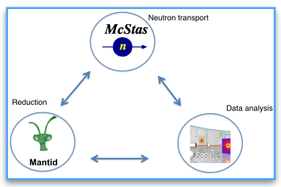
This SANS sample exposes SasView's scattering kernels to McStas. In this way SasView's monodisperse scattering kernels can be call from McStas.

Identification

- **Author:** Jakob Garde, Torben Nielsen, Peter Willendrup
- **Origin:** SasView, DTU, European Spallation Source ERIC
- **Date:** 03.02.2016
- **Version:** 0.5

Description

```
Sample for use in SANS instruments. The models describe mono disperse particles in thin solution. The sample geometry may have the shape:

Shape:          - A filled box with dimensions xwidth, yheight and zdepth.
                - A cylinder with dimensions radius and yheight.
                - A filled sphere given by radius.

These parameters are mutually exclusive.

Example using spheres in thin solution, with radius=200 AA and a delta_sld=0.6 fm/AA^3:
     SasView_model(model_index=47, model_scale=1.0, model_pars={1, 7, 200}, model_abs=0.0,
                           xwidth=0.01, yheight=0.01, zdepth=0.005,)


The algorithm of this component requires use of the ISO C standard c99. You could use MCSTAS_CFLAGS like MCSTAS_CFLAGS = -std=c99 -g -O2 -lm.
Or, add the flag "-std=c99" to "C flags" in the mcgui or mcgui-py config.

The list of scattering models in SasView is called sasmodels. The list of McStas available SasView sasmodels are found in the table below.

A few models may require manual documentation lookup using the above link to the SasView site.

McStas does currently not support multiplication of formfactor models with structure factor models.

The 2D scattering scattering kernels are denoted by modelname_xy. I.e. to evalulate scattering from aligned cylinders use model_index=10 to use cylinder_xy.
```



Slides from Torben Nielsen, ESS McStas school May-June 2016

EUROPEAN SPALLATION SOURCE

How?

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McStas mcdoc: SasView_model

Model no.	SasView name	Parameters
0	None	None
1	barbell	(sld, solvent_sld, bell_radius, radius, length)
2	barbell_xy	(sld, solvent_sld, bell_radius, radius, length, theta, phi)
3	bcc_paracrystal	(dnn, d_factor, radius, sld, solvent_sld)
4	bcc_paracrystal_xy	(dnn, d_factor, radius, sld, solvent_sld, theta, phi, psi)
5	capped_cylinder	(sld, solvent_sld, radius, cap_radius, length)
6	capped_cylinder_xy	(sld, solvent_sld, radius, cap_radius, length, theta, phi)
7	core_shell_cylinder	(core_sld, shell_sld, solvent_sld, radius, thickness, length)
8	core_shell_cylinder_xy	(core_sld, shell_sld, solvent_sld, radius, thickness, length, theta, phi)
9	cylinder	(sld, solvent_sld, radius, length)
10	cylinder_xy	(sld, solvent_sld, radius, length, theta, phi)
...	...	...
58	triaxial_ellipsoid_xy	(sld, solvent_sld, req_minor, req_major, rpolar, theta, phi, psi)

McStas

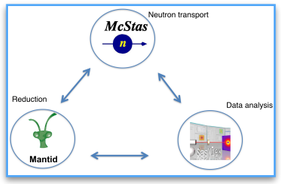
Normal McStas interface

...

Available SasView sasmodels - Extended paramet

sasmodels name	Parameters	Units	Range
barbell	{ 4, 1, 40, 20, 400 }		
barbell_xy	{ 4, 1, 40, 20, 400, 60, 60 }		
	Parameters:		
	Barbell scattering length density	4e-6/Ang^2	[-inf, inf]
	Solvent scattering length density	1e-6/Ang^2	[-inf, inf]
	Spherical bell radius	Ang	[0, inf]
	Cylindrical bar radius	Ang	[0, inf]
	Cylinder bar length	Ang	[0, inf]
	In plane angle	degrees	[-inf, inf]
	Out of plane angle	degrees	[-inf, inf]

...
with access to SASview models and their docs



McStas mcdoc: SasView_model

- Links to SasView documentation

2.1.14. CylinderModel

This model provides the form factor for a right circular cylinder with uniform scattering length density. The form factor is normalized by the particle volume.

For information about polarised and magnetic scattering, click here.

2.1.14.1. Definition

The output of the 2D scattering intensity function for oriented cylinders is given by (Guinier, 1955)

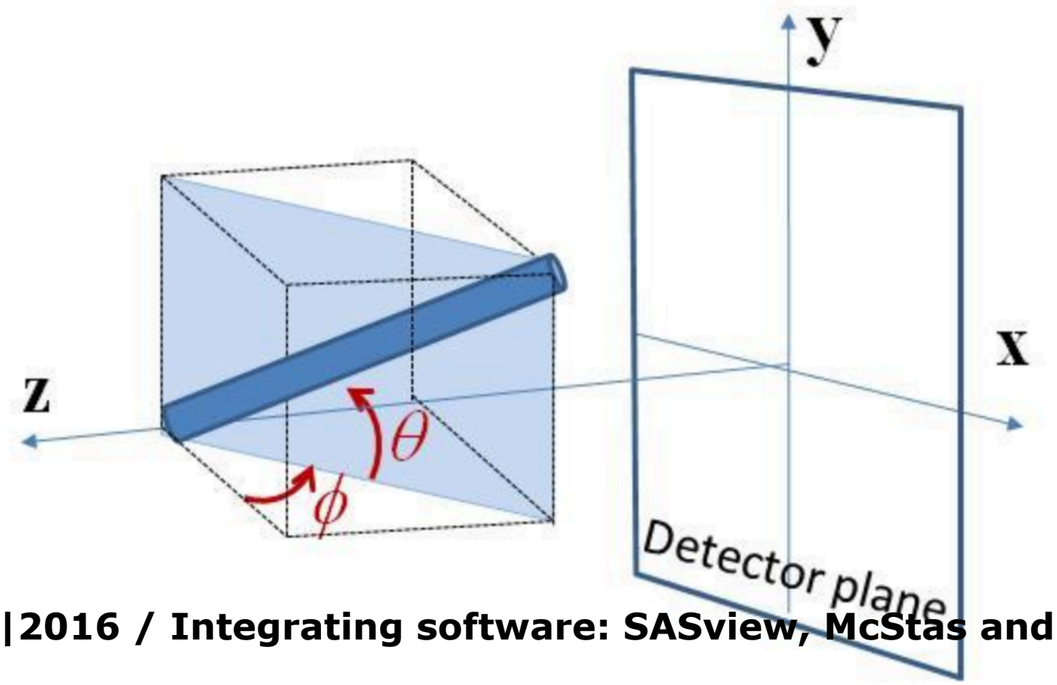
$$P(q,\alpha) = \frac{scale}{V} f^2(q) + bkg$$

where

$$f(q) = 2(\Delta\rho)V \sin(qL\cos\alpha/2)/(qL\cos\alpha/2)\frac{J_1(qr\sin\alpha)}{(qr\sin\alpha)}$$

and α is the angle between the axis of the cylinder and the *q*-vector, *V* is the volume of the cylinder, *L* is the length of the cylinder, *r* is the radius of the cylinder, and Δρ (contrast) is the scattering length density difference between the scatterer and the solvent. *J1* is the first order Bessel function.

To provide easy access to the orientation of the cylinder, we define the axis of the cylinder using two angles θ and ϕ. Those angles are defined in Figure 1.

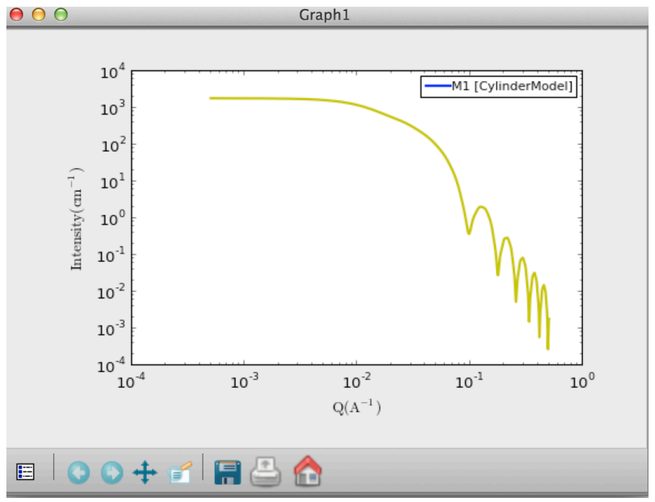


SASview model docs

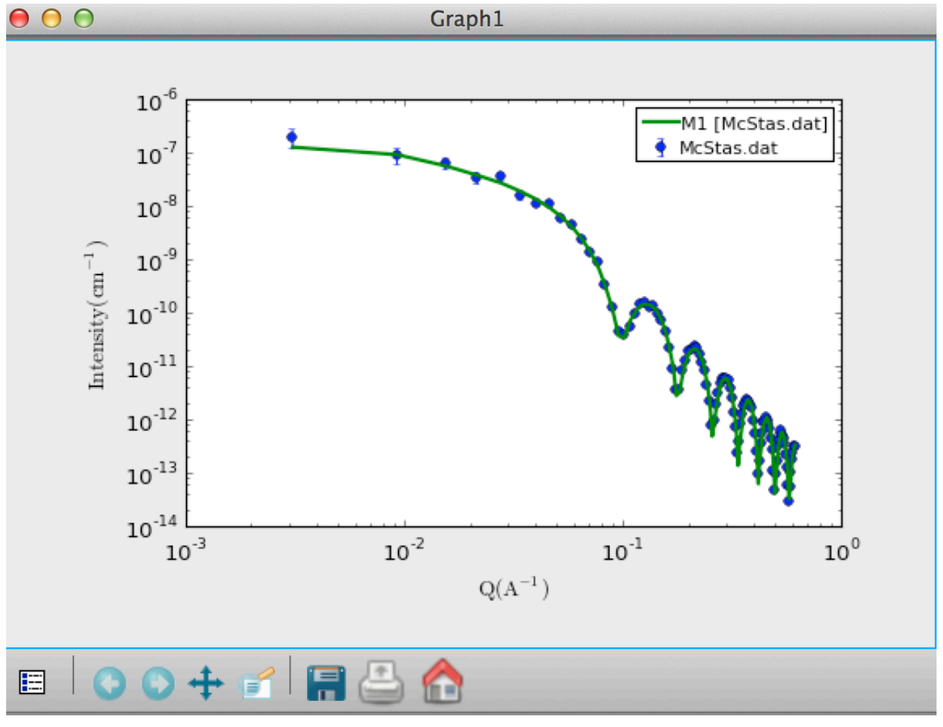
Works?

SasView -> McStas -> SasView

- SasView cylinder model (1D) scattering kernel used in McStas
- radius = 40 Å, length = 400 Å

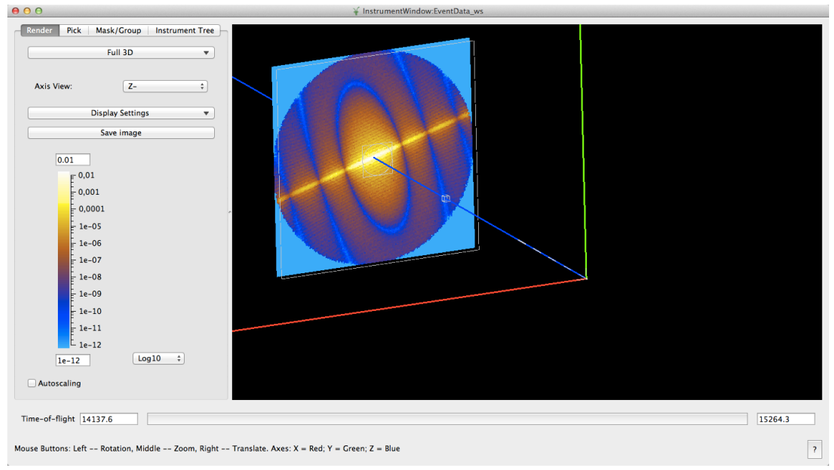


- McStas event data saved as I(q)
- SasView reads McStas I(q) data
- SasView fit engine gives:
- radius = 40 Å
- Length = 401 Å

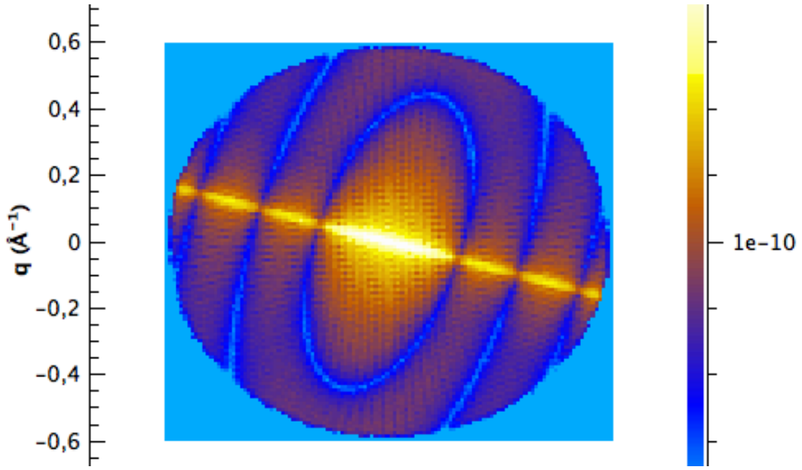


SasView -> McStas -> Mantid -> SasView

McStas -> event data

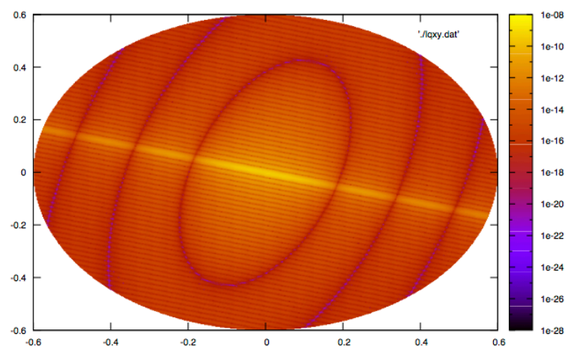


Mantid -> I(qx,qy)

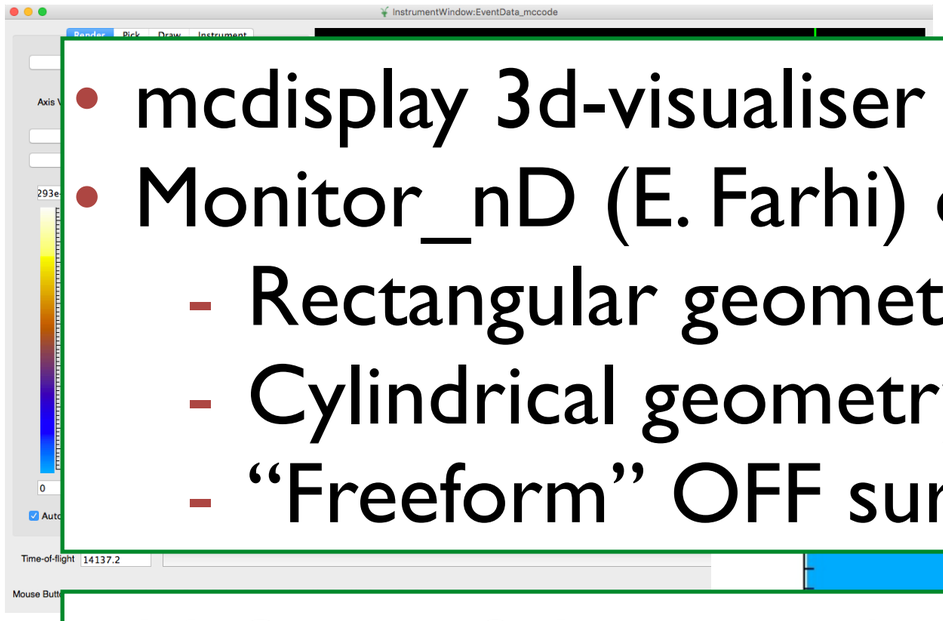


SasView -> model parameters

2D scattering kernel: Orientated cylinder

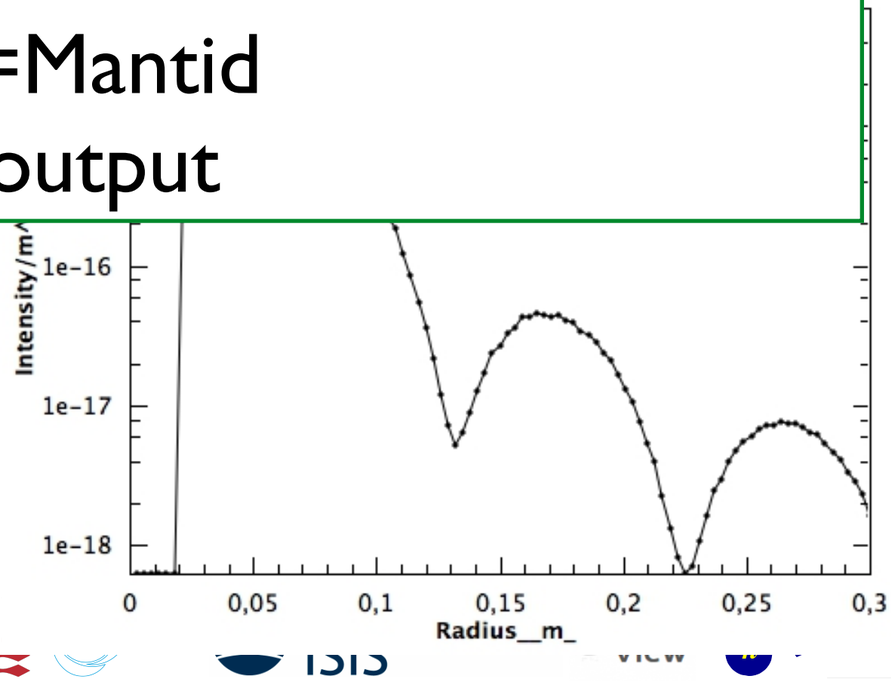


McStas data in Mantid

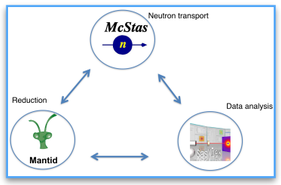


- mcdisplay 3d-visualiser modified to generate Mantid IDF xml file
- Monitor_nD (E. Farhi) output event data with "Pixel ID" and ToF
  - Rectangular geometry
  - Cylindrical geometry
  - "Freeform" OFF surface geometry

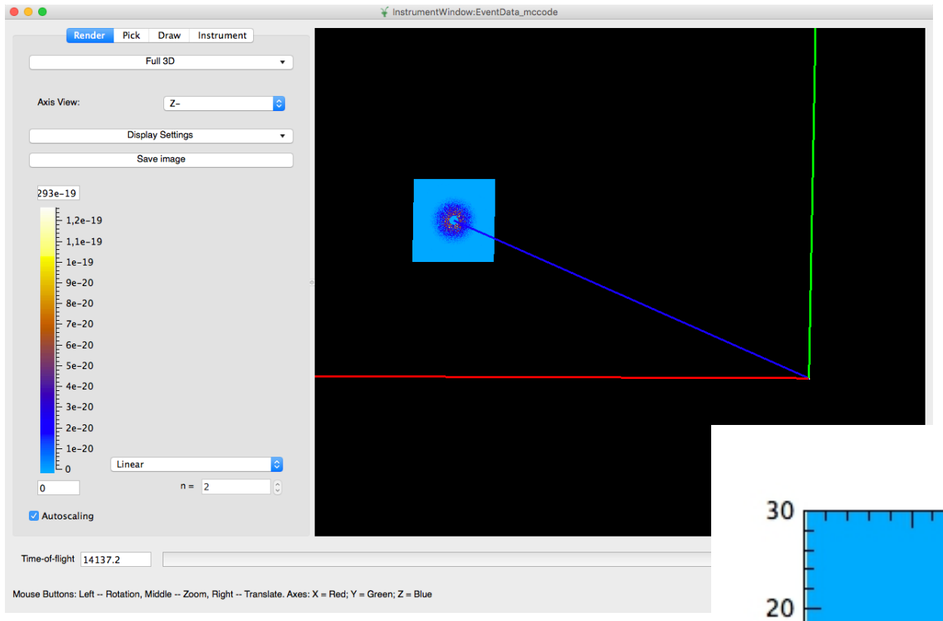
- McStas > 2.1 on machine, NeXus libs, Mantid
- Special component naming, defines source, sample and detectors for Mantid geometry
- Generate XML using mcdisplay --format=Mantid
- Run with mcrun/mcgui selecting NeXus output



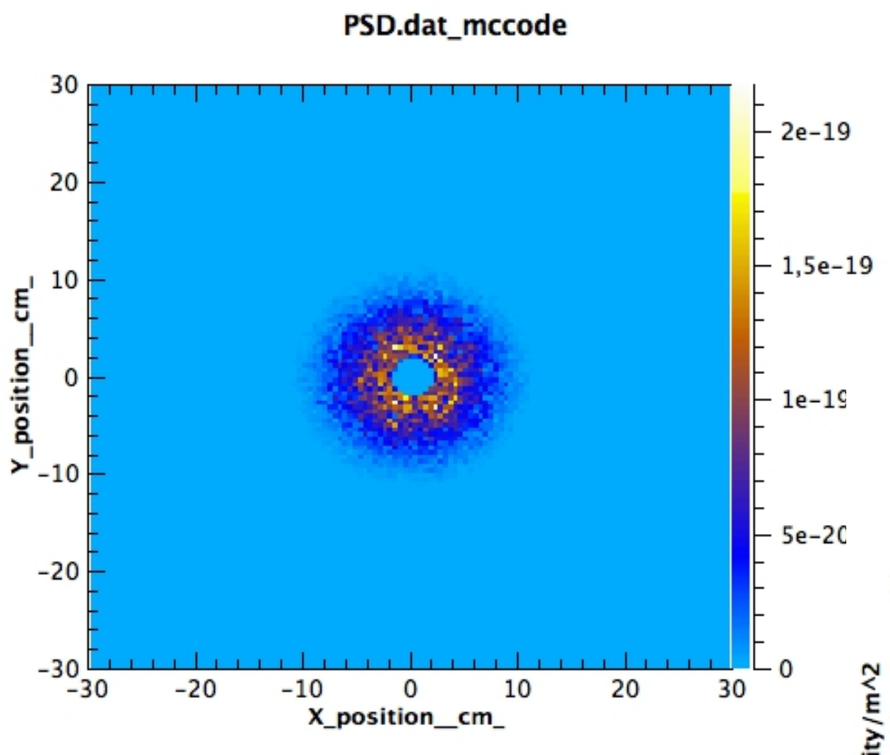
Nielsen, T.R.; Markvardsen, A.J.; Willendrup, P.: *McStas and Mantid integration*
Journal of Neutron Research, vol. 18, no. 2-3, pp. 61-77, 2015
DOI: 10.3233/JNR-16002

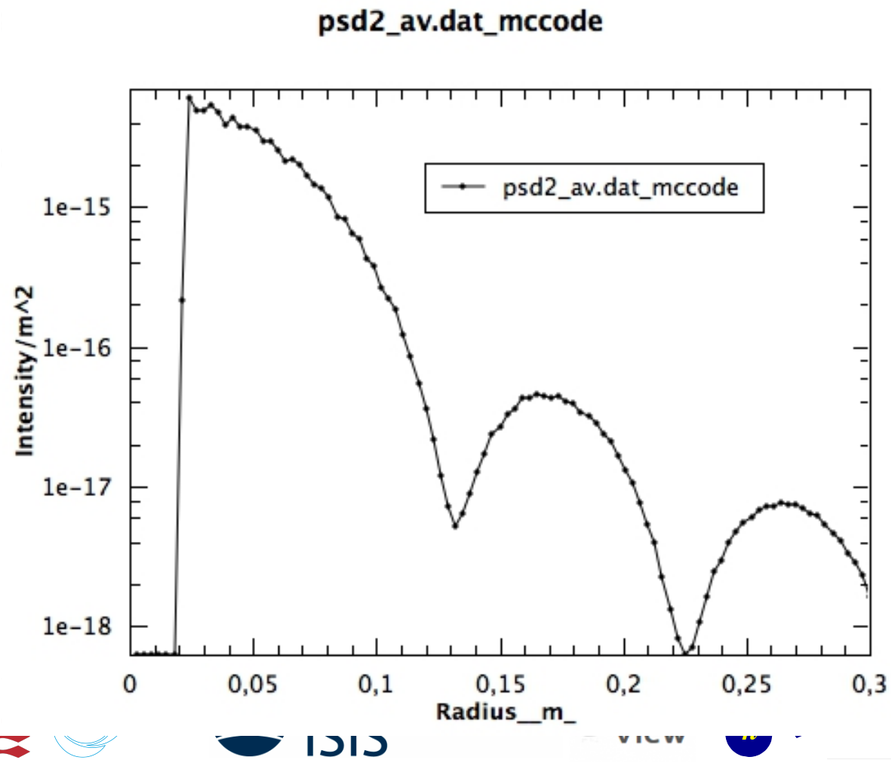


McStas data in Mantid



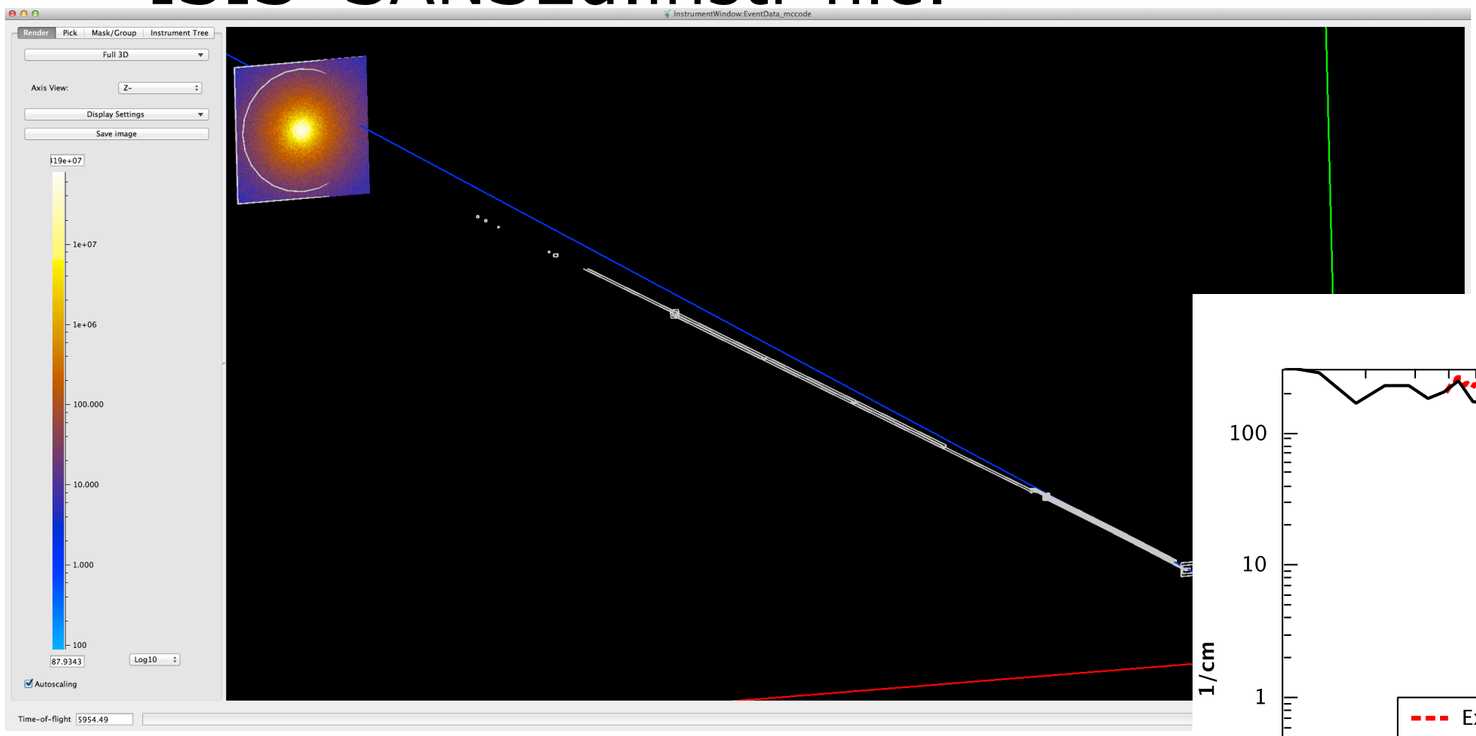
templateSANS_Mantid.instr

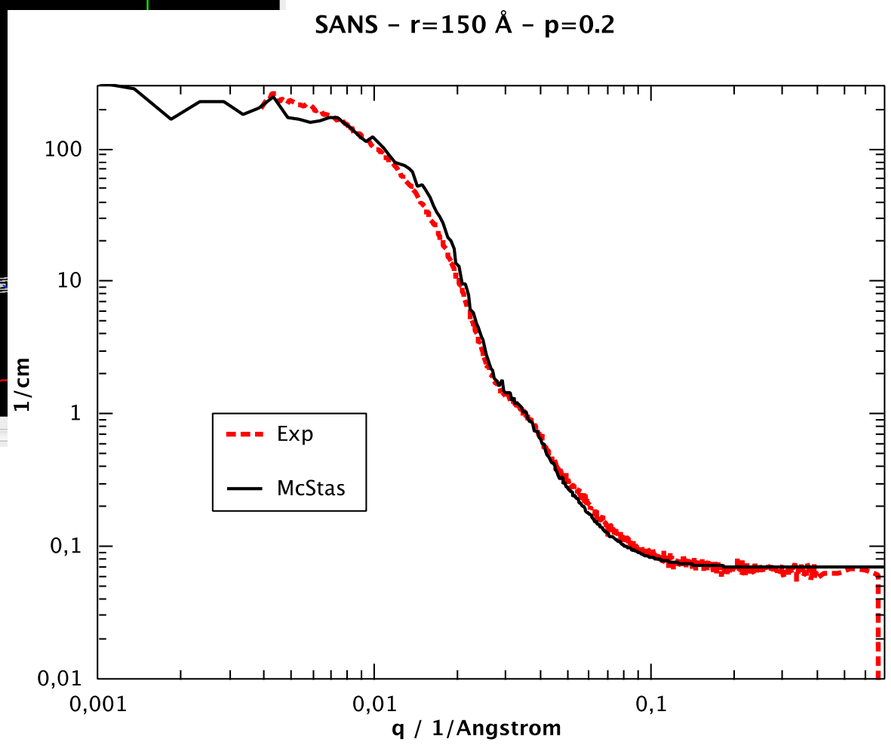




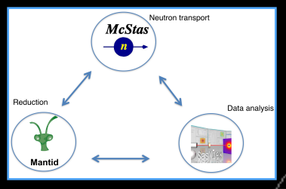
Data reduction and analysis

Mantid view of the McStas event data generated for the ISIS SANS2d.instr file.





Comparison of rescaled scatting intensity I(q) derived from the experimental data and a McStas simulation.



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LoKI detector in OFF file

McStas

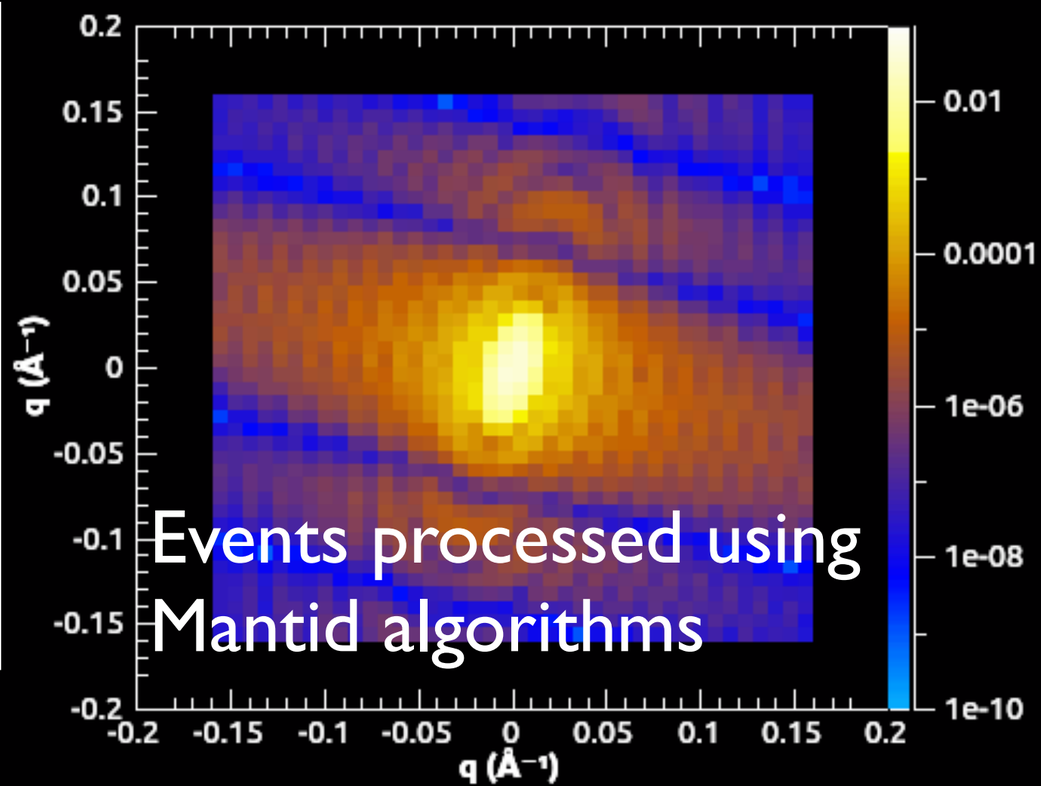
McStas simulation

2D scattering kernel from

SasView

Events visualised in Mantid instrument 3D view

Iqxqy_delta=0.008



Events processed using Mantid algorithms

Future:

- Reduction uses McStas, e.g. for multiple scattering corrections
- Modeling & analysis includes instrument resolution effects from McStas
- Links to other "sample" oriented codes

This work was supported in part by the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000 (the SINE2020 project)

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Want to know more?

Nielsen, T.R.; Markvardsen, A.J.; Willendrup, P.: *McStas and Mantid integration*
Journal of Neutron Research, vol. 18, no. 2-3, pp. 61-77, 2015
DOI: 10.3233/JNR-16002

New developments in the McStas neutron Monte Carlo ray-tracing package

Type: Poster **Session:** Posters
Board #: 29

The [McStas][1] neutron ray-tracing simulation package is a versatile tool for producing accurate simulations of neutron scattering instruments at reactors, short- and long-pulsed spallation sources such as the European Spallation Source. McStas It is extensively used for design and optimization of instruments, virtual experiments, data analysis and user training. McStas was founded as an scientif ... More

Presented by **Mr. Peter WILLENDRUP** on **17 Oct 2016** at **17:00**

Latest results and features with McXtrace 1.3

Type: Poster **Session:** Posters
Board #: 28

[McXtrace][1] [1][2] is a Monte Carlo Ray tracing package for performing simulations of any kind of X-ray optical instrumentation or scattering experiment. We present the latest results obtained using the new release McXtrace version 1.3. Some highlights of simulations using McXtrace include: 1. McXtrace in space - simulations of an X-ray telescope satellite ATHENA [3]. (See image) McXt ... More

Presented by **Dr. Erik KNUDSEN** on **17 Oct 2016** at **17:00**

McStas Says - but we'll do a little also if you want :)

Abstract: The McStas Monte Carlo ray-trace simulation package is a well established tool for simulation of neutron optics, instrument and scattering experiments. McStas is an open source (GPL) code, developed in collaboration between DTU Physics, Institut Laue-Langevin, Paul Scherrer Institute, Niels Bohr Institute and the ESS Data Management and Software Centre.

At the 2016 McStas school held in connection with NOBUGS in Copenhagen, a group of McStas developers and expert users will lead your way through carefully chosen lecture material and hands-on exercises, thereby introducing you to the most important aspects of the package and its use. The covered topics range from basic installation and use of the code to advanced language features and possibilities for self-development of McStas components, all with the aim of allowing you to work independently with the package in the future.

A rough plan for the event includes the following stages:

* Thursday morning: McStas for "absolute beginners" - including intro talk and basic use of the package.
* Thursday afternoon: Overview of the most important optical components
* Friday morning: Samples and "complete instruments
* Friday afternoon: Advanced McStas grammar, interfacing with other codes.

McStas: Thursday 20 October (09:00 - 17:00)

McStas: Friday 21 October (09:00 - 17:00)