McStas SasView

ESS McStas Training 2016
May 30th - June 1st

Agenda

- Intro:
  - McStas interoperability
  - McStas scattering kernels
  - Data Analysis software // scattering kernels
- First example
  - SasView
- Exercise

McStas – key features

- Does one well defined job: Neutron transport
- Output of McStas is well defined: p, x, v, s, t

- Easy to add and define new transport and scattering properties (c-code)

McStas interoperbility

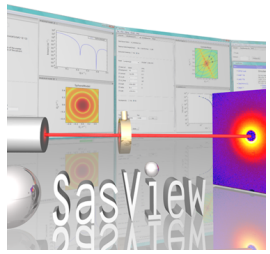
Neutron transport

McStas

Reduction

Mantid

Data analysis



McStas interoperbility

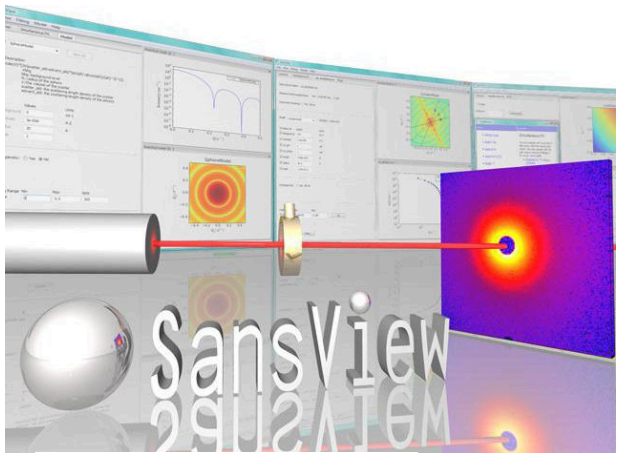
- Try to link different simulation tools as much as possible
- McStas -> Neutron transport
- Mantid -> Data reduction
- Data analysis -> Your own preferred fit engine of choice

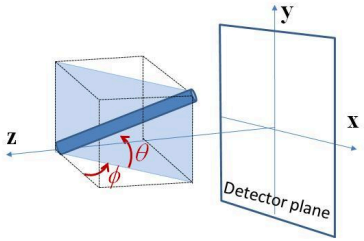
- E.g. SANS
- Use same scattering kernels in the neutron transport simulations = McStas
- Use same scattering kernels in the analysis tool = SasView

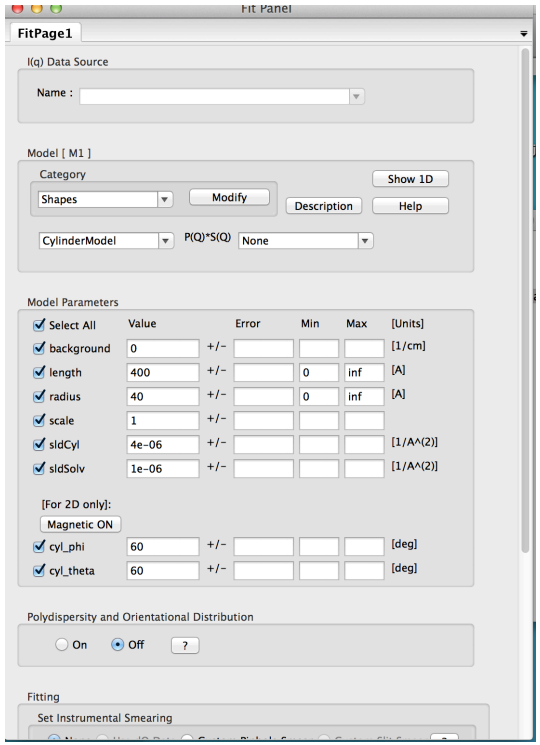
- Prototype: SasView models available in McStas

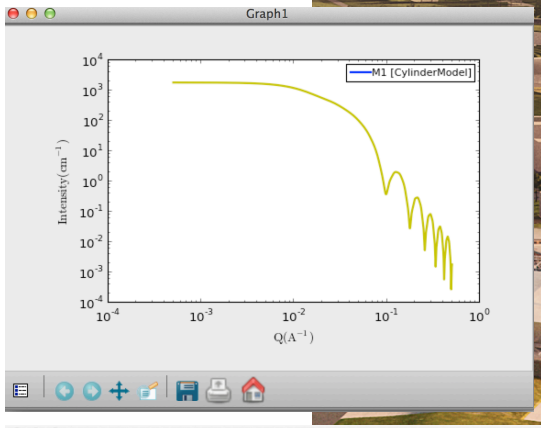
SANS - SasView

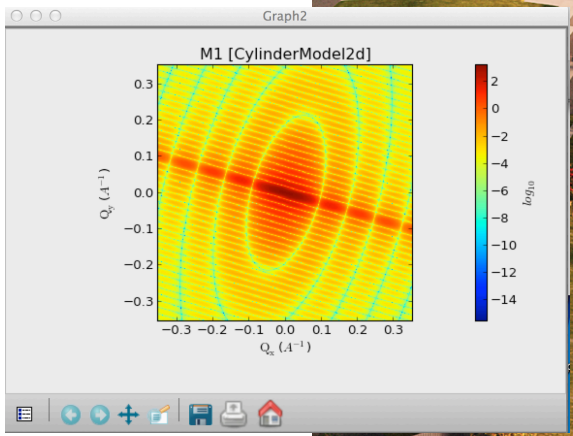
- LoKI team needed 2D scattering kernels in McStas
- Use SasView scattering kernels in McStas











SasView scattering kernel: Orientated cylinder

McStas mcdoc: SasView_model

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

The `sasview_model` Component

This sample component applies sasview models as scattering kernels. NOTE: add the flag "-std=c99" to "C flags" in the mcgui or mcgui-py config.

Identification

- **Author:** Jakob Garde
- **Origin:** SasView, ESS, DTU
- **Date:** 14.07.2015
- **Version:** 0.4

Description

```
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 (spheres in thin solution:
     SANS_sasview_model(model_index=31, model_pars={1, 2, 60},
                        xwidth=0.01, yheight=0.01, zdepth=0.005)

Available SasView models are found in the table below
(A few models may require manual documentation lookup using the above link to the SasView site)

MDOC
```

Model no.	Model 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)

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)

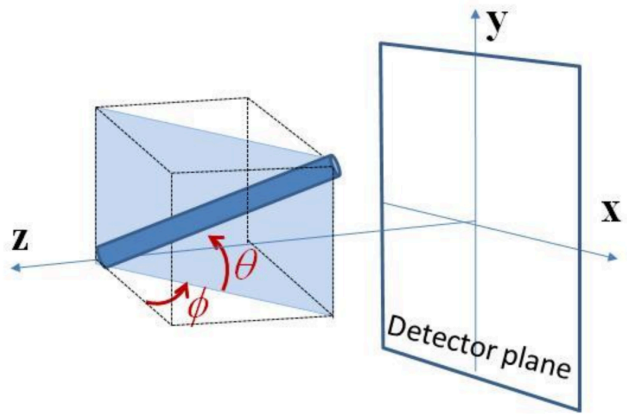
$$P(q,\alpha) = \frac{scale}{V} f^2(\boldsymbol{q}) + bkg$$

where

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

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.



McStas interoperbility

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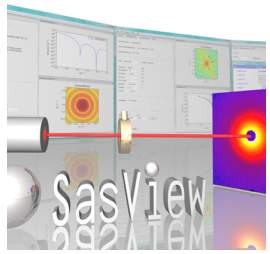
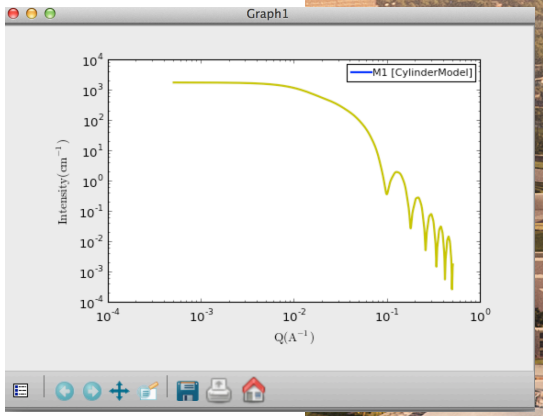


SasView -> McStas -> SasView

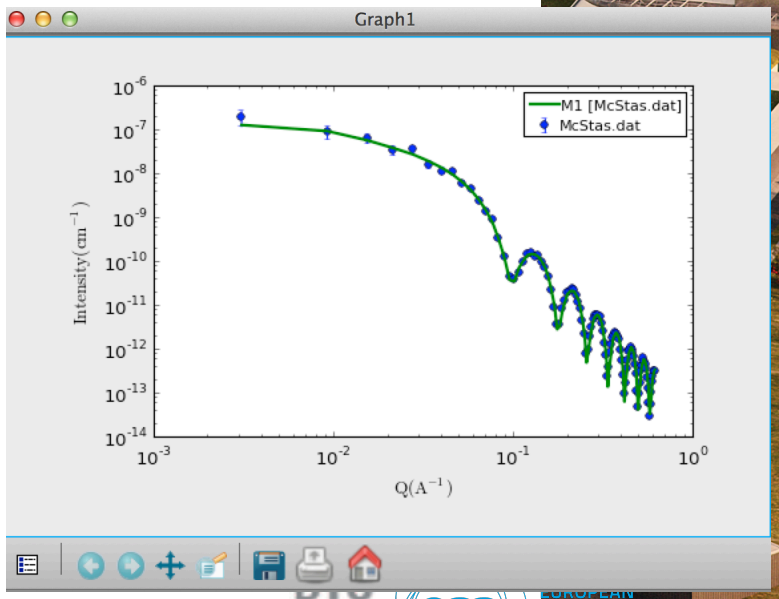
- SasView cylinder model (1D) scattering kernel used in McStas
- radius = 40 Å, length = 400 Å



- McStas event data saved as I(q)

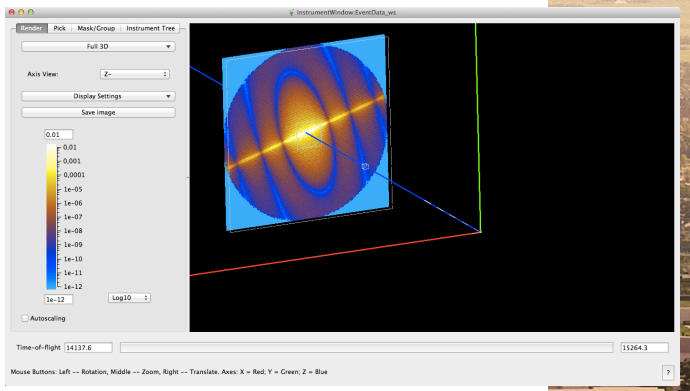
- SasView reads McStas I(q) data

- SasView fit engine gives:
- radius = 40 Å
- Length = 401 Å

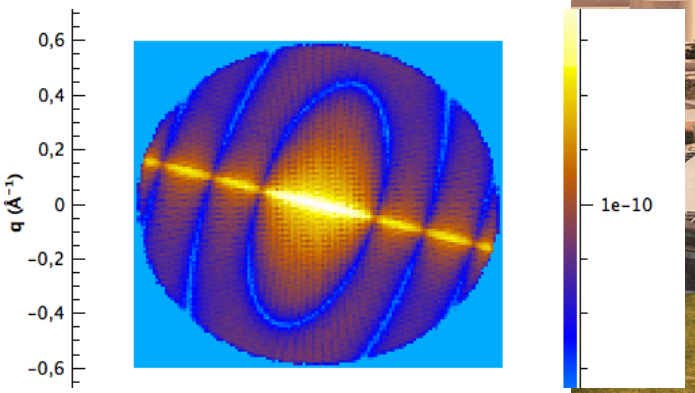


SasView -> McStas -> Mantid -> SasView

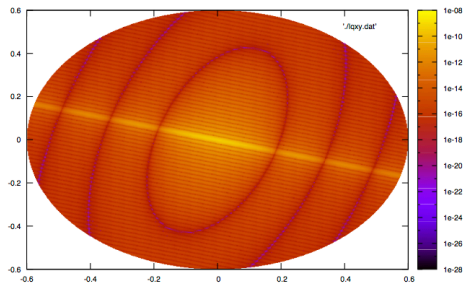
McStas -> event data



Mantid -> I(qx,qy)



SasView -> model parameters



2D scattering kernel: Orientated cylinder

Summary

- Straight forward to add scattering kernels to McStas from other c-code
- Consider if your favorite analysis tool can be linked to McStas

Exercise

- Load templateSasView_Mantid.instr
- Try 2 or 3 different models

- Try to write your own SANS scattering component
- Use Sans_spheres.comp as template
- Try e.g. the broad_peak.py model from SasView
- See https://github.com/SasView/sasmodels/blob/master/sasmodels/models/broad_peak.py