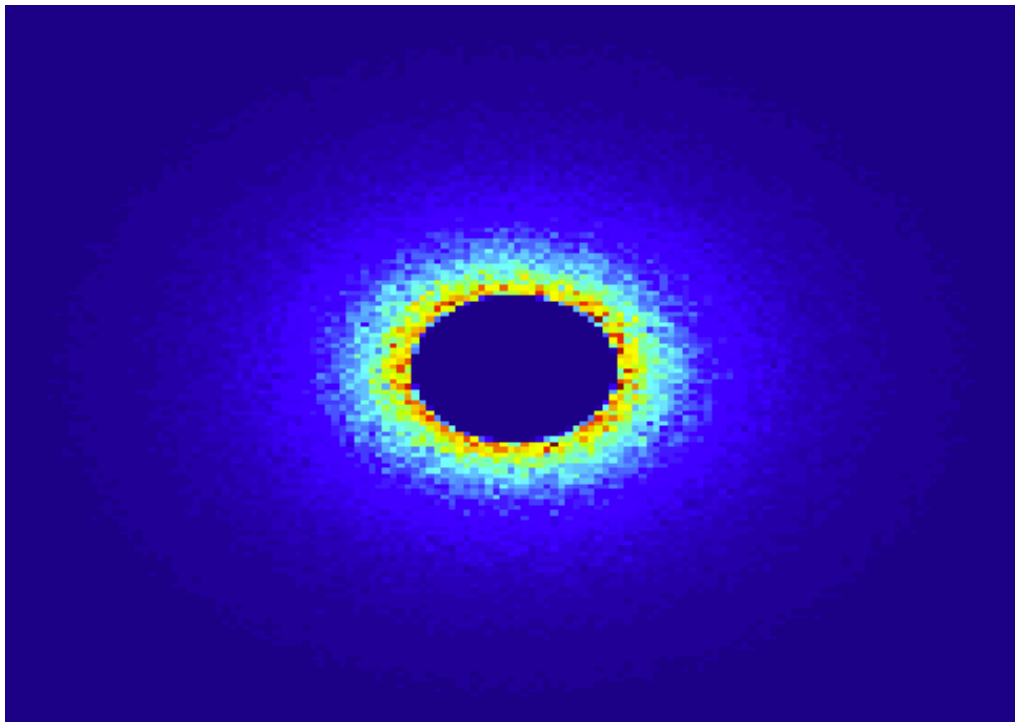
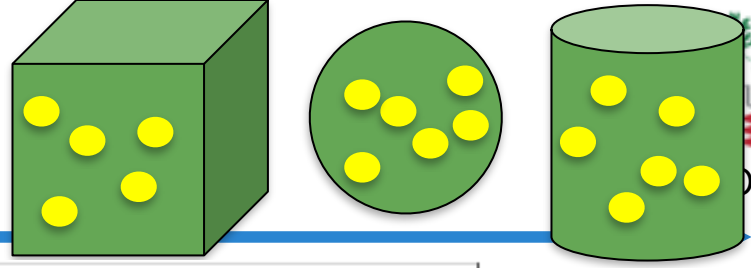
Small Angle Neutron Scattering



Sans_Spheres.comp



October 2018

Name	Unit	Description	Default
R	AA	Radius of scattering hard spheres	100
Phi	1	Particle volume fraction	1e-3
Delta_rho	fm/AA^3	Excess scattering length density	0.6
sigma_abs	m^-1	Absorption cross section density at 2200 m/s	0.50
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert . dimension of sample, as a height for cylinder/box	0
zdepth	m	depth of sample	0
radius	m	Outer radius of sample in (x,z) plane for cylinder/sphere	0
target_x	-		0
target_y	m	position of target to focus at	0
target_z	-		6
target_index	1	Relative index of component to focus at, e.g. next is +1	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
focus_r	m	Detector (disk-shaped) radius	0

MORE SANS SAMPLES

October 2018

Try ellipsoidal and cylindrical particles
-or-
Elliptic cylinders
Go for Nanodiscs and Liposomes

Sample form: Box only
Particle concentration: MOLAR

- *SANS_AnySamp.comp*
- *SANS_DebyeS.comp*
- *SANSCylinders.comp*
- *SANSEllipticCylinders.comp*
- *SANSGuinier.comp*
- *SANSLiposomes.comp*
- *SANSNanodiscs.comp*
- *SASview.comp*
- *SANSNanodiscsFast.comp*
- *SANSNanodiscsWithTags.*
- *SANSNanodiscsWithTagsFast*
- *SANSPDB.comp*
- *SANSPDBFAST.comp*
- *SANSShells.comp*
- *SANSSpheres.comp*

As always, more info at
http://mcstas.org/download/components

MORE SANS SAMPLES

October 2018

file:///Applications/McStas-2.5miguel.app/Contents/Resources/mcs

DTU R12 Pro...tion NYPROD | Move MS offi...mors Forums | How To: Inst...umors Forums | How to install...on dell d610? | Trådløst netværk | My current n...oogle Groups

[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:**(Unknown)

… Or use one of many SASmodels Definitions directly from SASview…

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
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

MDOC
```

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)

DTU ESS EUROPEAN SPALLATION SOURCE

SANSCurve.comp

- *Mimick the behaviour of a sample: Feed I(q) curve*

Name	Unit	Description
DeltaRho	cm/AA^3	Excess scattering length density of the particles.
Volume	AA^3	Volume of the particles.
Concentration	mM	Concentration of sample.
AbsorptionCrosssection	1/m	Absorption cross section of the sample.
xwidth	m	Dimension of component in the x-direction.
yheight	m	Dimension of component in the y-direction.
zdepth	m	Dimension of component in the z-direction.
SampleToDetectorDistance	m	Distance from sample to detector (for focusing the scattered neutrons).
DetectorRadius	m	Radius of the detector (for focusing the scattered neutrons).
FileWithCurve		

Revisit Monitors: PSD_monitor_rad.comp

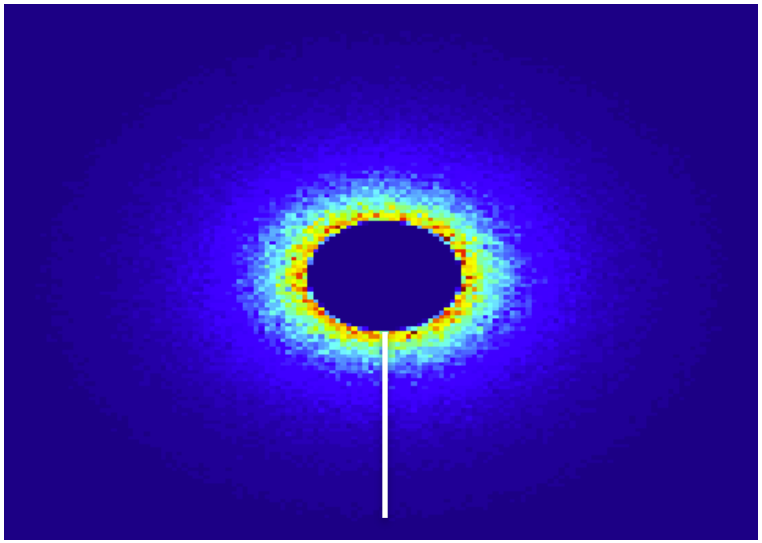
October 2018

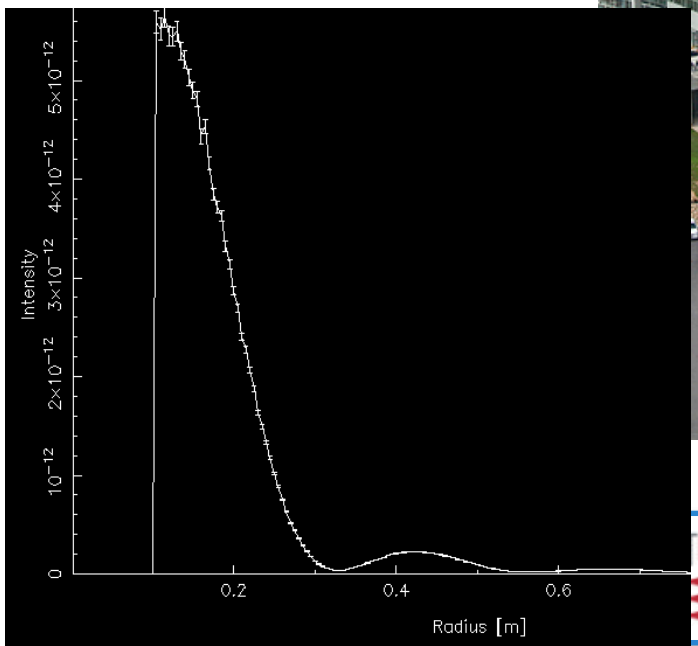
Name	Unit	Description	Default
nr	1	Number of concentric circles	100
filename	text	Name of file in which to store the detector image	0
filename_av	text	Name of file in which to store the averaged detector image	0
rmax	m	Outer radius of detector	0.2

r_rad(

filename_av="radial_averag.dat", max=1)

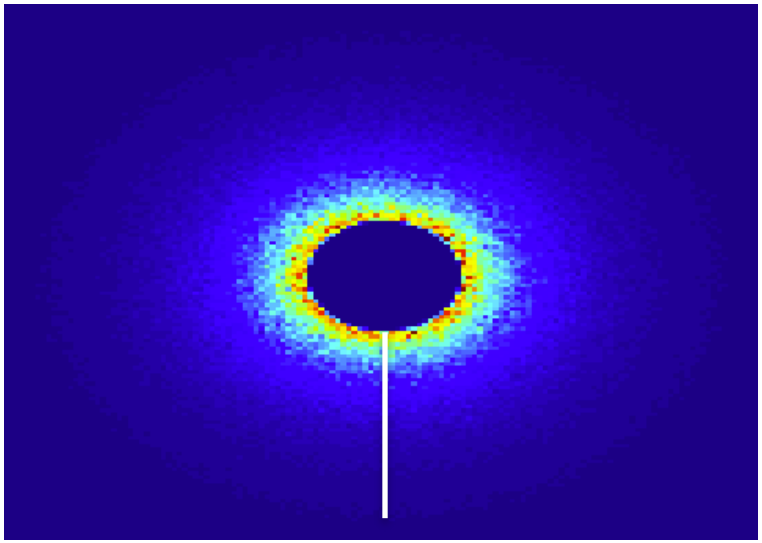
AT (0, 0, 12) RELATIVE Sample





SANS Q MONITOR

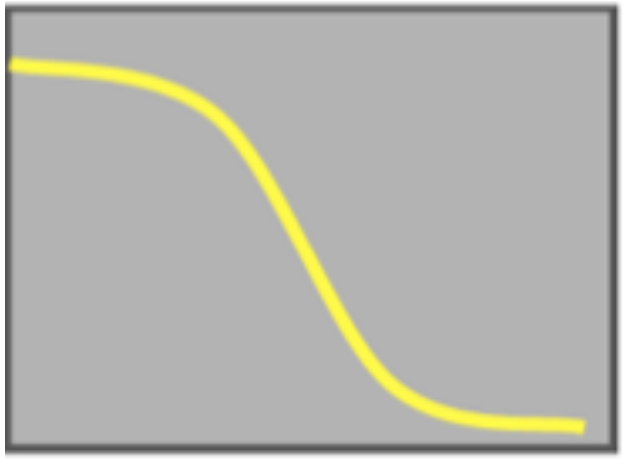
October 2018



I(r) and I(q) profiles

Input Parameters

RadiusDetector	[m]
DistanceFromSample	[m]
NumberOfBins	
LambdaMin	[AA]
Rfilename	string
qFilename	string
Restore_neutron	



EXERCISE

Open the file Ex_5_5_SANS.instr given to you.

Study the file. Notice the two instrument parameters

- Insert a Sans_spheres_sample
  (R = 100, Phi = 1e-3, Delta_rho = 0.6, sigma_abs = 0,
  xwidth=0.01, yheight=0.01, zdepth=0.01, focus_r=?, target_z=?)

- Insert a PSD_monitor_rad 0.0001m behind the beamstop
  (rmax=0.2, nr=200, give filenames)
- Use the instrument parameters to complete the components

- Run a simulation with 1e7 neutrons
- Plot the I(r) curve.

- Change the sample-detector distance.
  What do you observe?

Curious? Lost? Need help?
Try $ mcdoc or visit http://mcstas.org/download/components

October 2018

SANS models

- *Get a new instrument: We'll use the ISIS_SANS2d*
- *We'll explore some of the SANS-options that exist in McStas.*
- *The SANS2D-model does not include a sample, nor detector at present, so we'll add that in. Add Ls2d and RR to your* **DEFINE INSTRUMENT** *line in the top of the file to be able to scan them.*

  1) *Add a PSD_monitor to replicate the detector:*

```
COMPONENT detector_front = PSD_monitor(
  nx = 200, ny = 200, filename = "PSD.dat",
  xwidth = 1, yheight=1, restore_neutron=1)
AT(0,0,Ls2d) RELATIVE sample.
```

  2) *Add a sample – First we'll use the the standard SANS_spheres comp:*

-
```
COMPONENT sample = SANS_spheres(
  xwidth=0.01, yheight=0.01, zdepth=0.001,
  focus_xw=1, focus_yh=1, target_z=Ls2d,
  R=RR, Delta_rho=0.6)
AT (0, 0, 0.2) RELATIVE psd4
```

Now run a simulation to see what you get.

SASmodels

- *Now we shall explore the possibilities that SasView_models can give us. Change the sample to a SasView_models.comp. Keep the target parameters but change the last line to:*
  `model_index=51, model_pars={1,7,50}`
- *The model_index indeicates which of a large number of models scatterung fucntions) the sample is using. You can use mcdoc to find out which, and what the parameters mean. Try to generate a picture similar to the one before.*
- *Try a couple of the other SasView_models.*
- `ex. model_index=23, model_pars={50,0.2}`

SANS models

- *2D SANS images are all fine – but wouldn't it be better if we could let the computer do the radial integration for us?*
- *recipe: Insert another monitor – for instance a* **`Monitor_nD`** *with* **`options="radius ..."`**
- *or an instance of* **`SANSQ_monitor`**
- *Remember to use* **`mcdoc`** *– it's your friend!*

RESOURCES

October 2018

- *Need more information?*
- *Plan on doing a SANS experiment?*
- *Visit the SANS world directory*

- *Neutron scattering length densities*
- *https://www.ncnr.nist.gov/resources/activation/*
- *http://sld-calculator.appspot.com/*

- *SASview*