

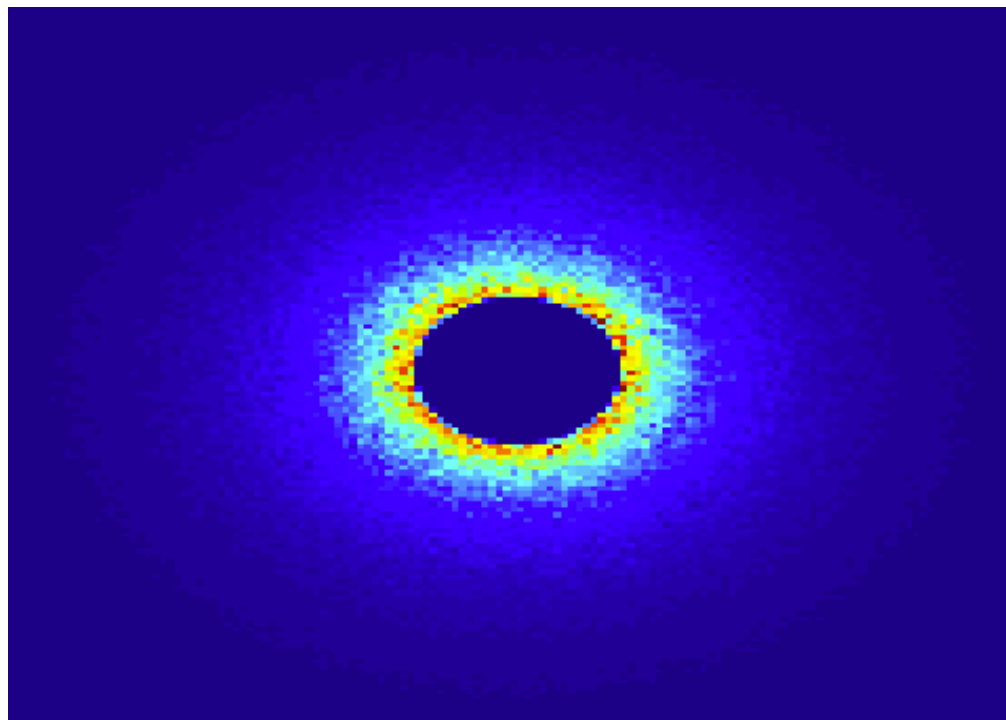
McStas



McStas School
Bariloche - Argentina

15th-19th
FEBRUARY
2016

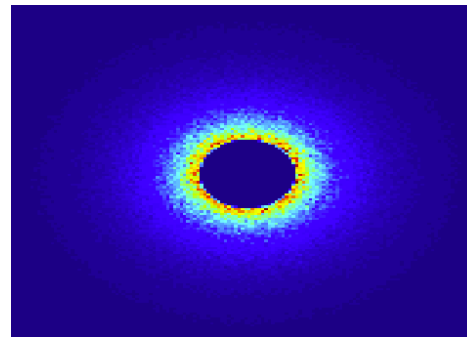
9.5 Small Angle Neutron Scattering



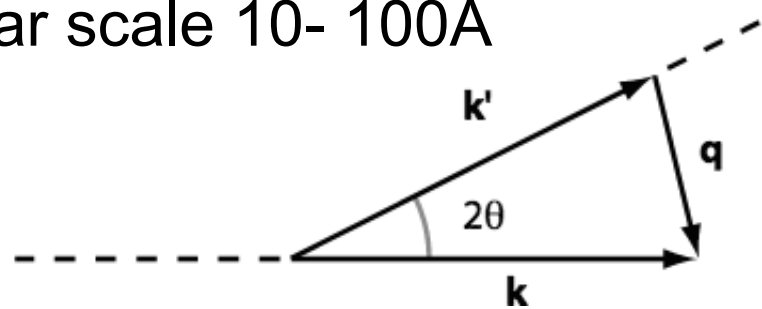
WHAT IS SANS?

Small Angle Neutron Scattering

- Elastic Scattering
- Small angle -> small q -> big r
- Gain information on the molecular scale 10-100Å
- Low signal to noise
- Contrast method



$$q = \frac{4\pi}{\lambda} \sin(\theta)$$



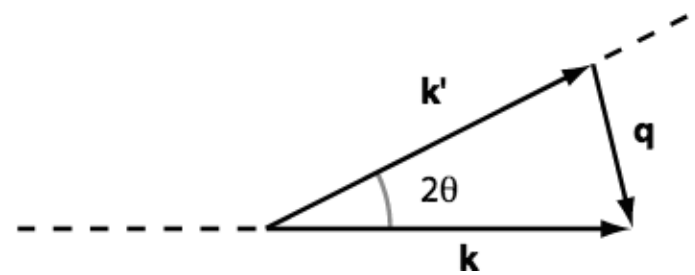
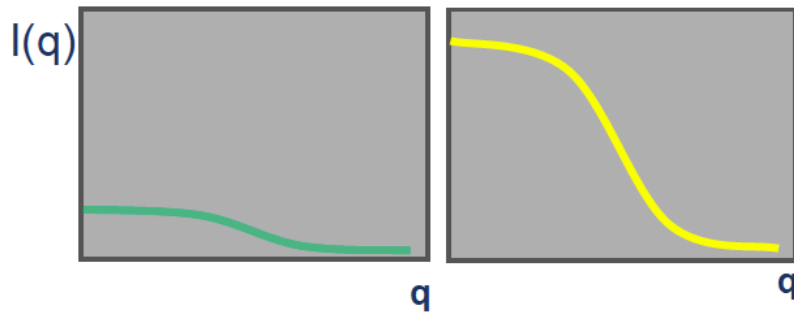
Want to learn more about SANS instruments?
-> Session by Emmanuel tomorrow

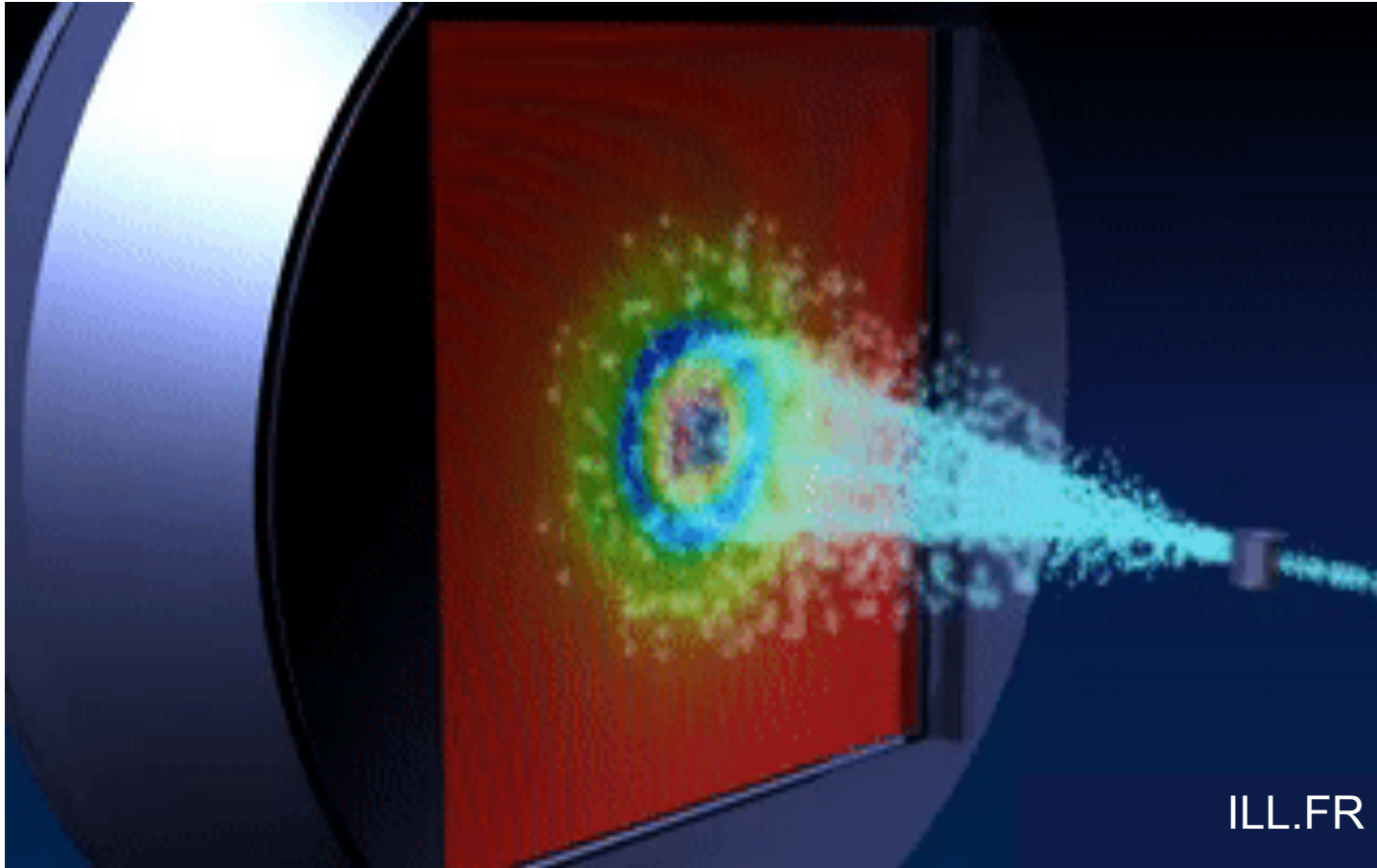
Still not enough? Check out
<http://smallangle.org/content/Learning-About-SAS>



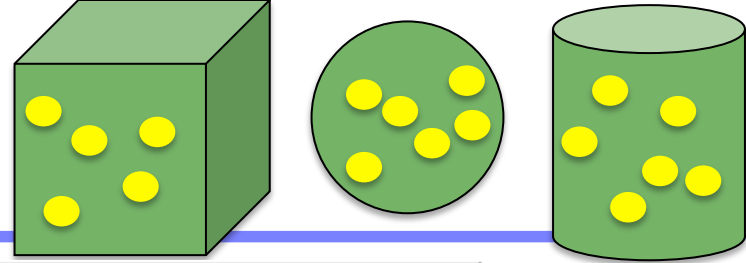
SANS Sample

- SANS method can be used for many samples
- Specific sample: Molecule + Liquid (buffer solution)
- Isotropic scattering





Sans_Spheres.comp



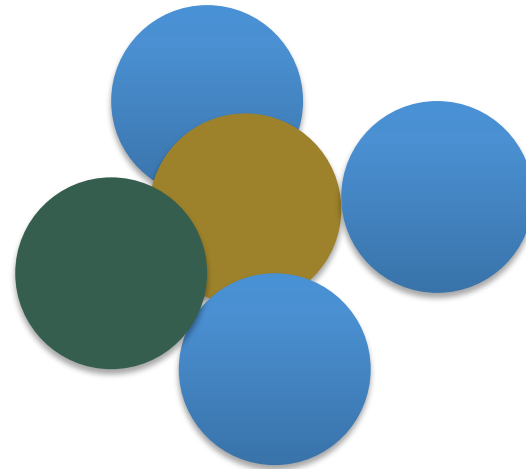
Name	Unit	Description	Default
R	AA	Radius of scattering hard spheres	100
Phi	1	Particle volume fraction	1e-3
Delta_rho	fm/AA ³	Excess scattering length density	0.6
sigma_abs	m ⁻¹	Absorption cross section density at 2200 m/s	0.50
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert. dimension 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



SCATTERING LENGTH DENSITY

Model the scattering power of a material (e.g. molecule)
Length scale larger than atomic dimension

$$\rho = \frac{1}{V} \sum_V b_i$$



Look up Scattering Length Densities at:

<http://sld-calculator.appspot.com/>

<https://www.ncnr.nist.gov/resources/activation/>

In McStas: Monodisperse samples





So you don't like spheres



MORE SANS SAMPLES

Try ellipsoidal and
cylindrical particles

-or-

Elliptic cylinders

Go for Nanodiscs and
Liposomes

Sample form: Box only
Particle concentration: MOLAR

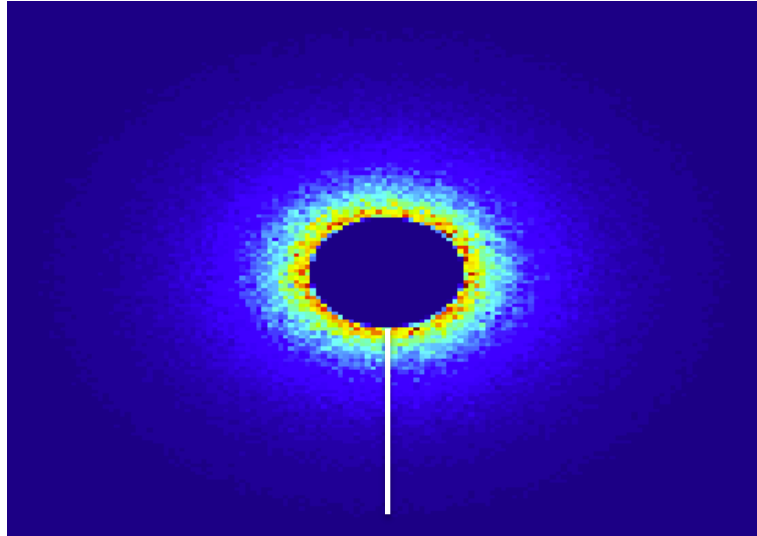
- SANS_AnySamp.comp
- SANS_DebyeS.comp
- SANSCylinders.comp
- SANSEllipticCylinders.comp
- SANSGuinier.comp
- SANSLiposomes.comp
- SANSNanodiscs.comp
- SANSNanodiscsFast.comp

- SANSNanodiscsWithTags.
- SANSNanodiscsWithTagsFast
- SANSPDB.comp
- SANSPDBFAST.comp
- SANSShells.comp
- SANSSpheres.comp

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



SANS Q MONITOR

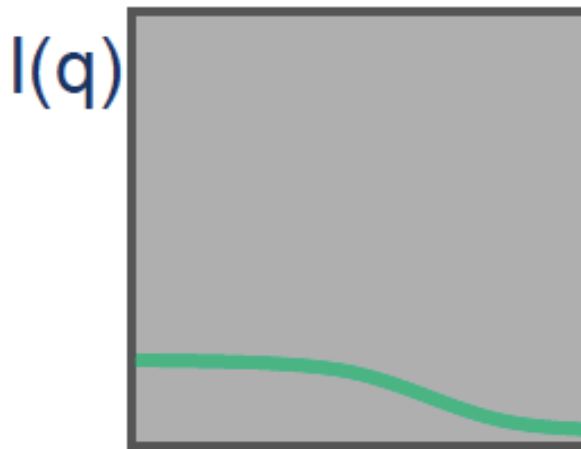


I(r) and I(q) profiles

Input Parameters

RadiusDetector [m]
DistanceFromSample [m]
NumberOfBins
LambdaMin [AA]

Rfilename string
qFilename string
Restore_neutron



EXERCICE 9.5

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

Open the file Ex_9_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?



RESOURCES

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/>

Small angle scattering, various resources, animations and tutorials

<http://smallangle.org/>

