SANS in McStas

2019 CSNS McStas School

Agenda

- A quick discussion of the SANS technique
- Sample models for SANS in McStas

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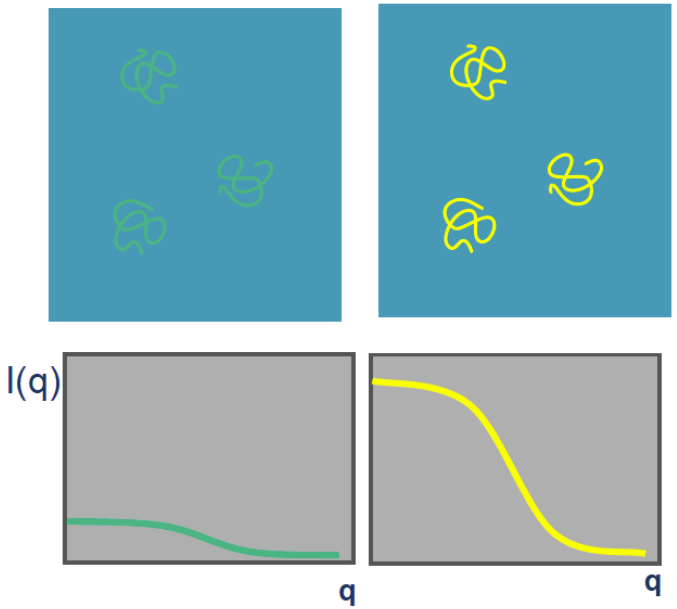
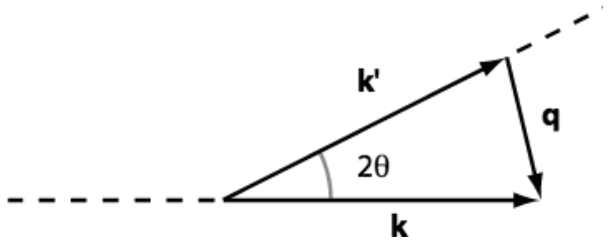
Small angle scattering SANS

- SANS method can be used for many types of material
- Often: Molecule + Liquid (buffer solution)
- Isotropic scattering





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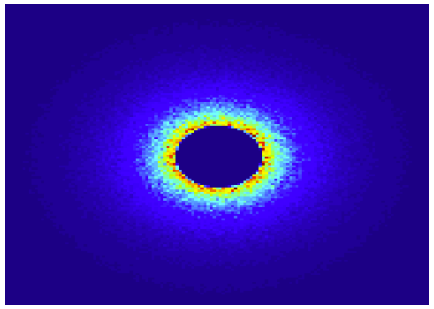
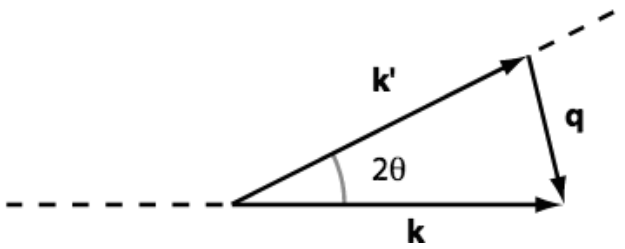
SANS



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

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
- Instrument requirements: good collimation, long flight distance after detector.

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SANS other samples

McStas has a suite of SANS-models:

Try ellipsoidal and

cylindrical particles

-or-

Elliptic cylinders

Go for Nanodiscs and Liposomes

Also – SASmodels from SASview

- 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

SANS spheres

Input parameters

Parameters in **boldface** are required; the others are optional.

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	0.05
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

Dilute, monodisperse, hard spheres in solution, with given contrast and radius

SasView_models

Input parameters

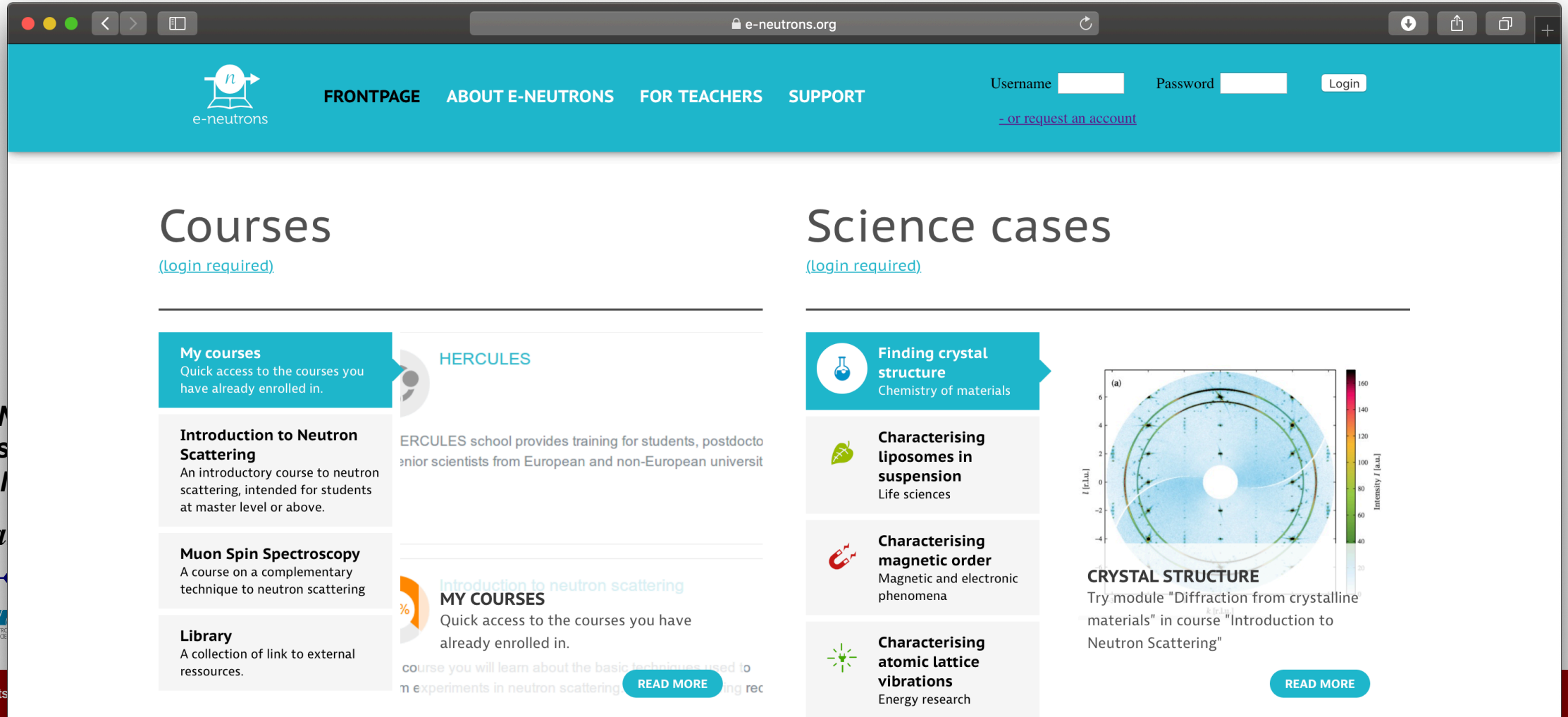
Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
model_index			21
model_scale			1.0
model_pars			{60}
model_abs	1/m	Absorption cross section density at 2200 m/s	0.5
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	m	relative focus target position	0
target_y	m	relative focus target position	0
target_z	m	relative focus target position	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

SasView_models

47	parallelepiped	(sld, solvent_sld, a_side, b_side, c_side)
48	parallelepiped_xy	(sld, solvent_sld, a_side, b_side, c_side, theta, phi, psi)
49	pearl_necklace	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_sld, solvent_sld)
50	pearl_necklace_xy	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_sld, solvent_sld)
51	sphere	(sld, solvent_sld, radius)
52	sphere_xy	(sld, solvent_sld, radius)
53	star_polymer	(radius2, arms)
54	star_polymer_xy	(radius2, arms)
55	stickyhardsphere	(effect_radius, volfraction, perturb, stickiness)
56	stickyhardsphere_xy	(effect_radius, volfraction, perturb, stickiness)
57	triaxial_ellipsoid	(sld, solvent_sld, req_minor, req_major, rpolar)
58	triaxial_ellipsoid_xy	(sld, solvent_sld, req_minor, req_major, rpolar, theta, phi, psi)

Exercise will take place on the e-neutrons.org infrastructure (using a web-simulator)



e-neutrons.org

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e-neutrons

Problem | Discussion | Read | View source | View history | Search

Problem:Fourier transform

Mathematically the scattering amplitude is the Fourier transform of the distribution of scattering centers (nuclei, electrons, spins) within the material. The scattered intensity (the scattering function) is the square of the scattering amplitude.


One-dimensional crystal.

The Fourier transform of a function $\rho(r)$ is written as

$$F(q) = \int \rho(r) \exp(iqr) dr,$$

where $\rho(r)$ is the function in real space given by positions r, and q is a coordinate in Fourier space (which in scattering terms usually is called "reciprocal space"). $\rho(r)$ is in case of scattering theory the position sensitive scattering length density within the sample.

We will consider a one-dimensional space, *i.e.* all particles (scattering centers) are positioned on a line, and correspondingly only calculate the one-dimensional Fourier transform. We assume further that all particles are points (size = 0).

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Question 1

Calculate the Fourier transform and the scattering intensity of a sample with only one particle, and plot the normalized scattered intensity $I(q) = |F(q)|^2/N^2$ versus qR.

Hint [show]

Hint [show]

Solution [show]

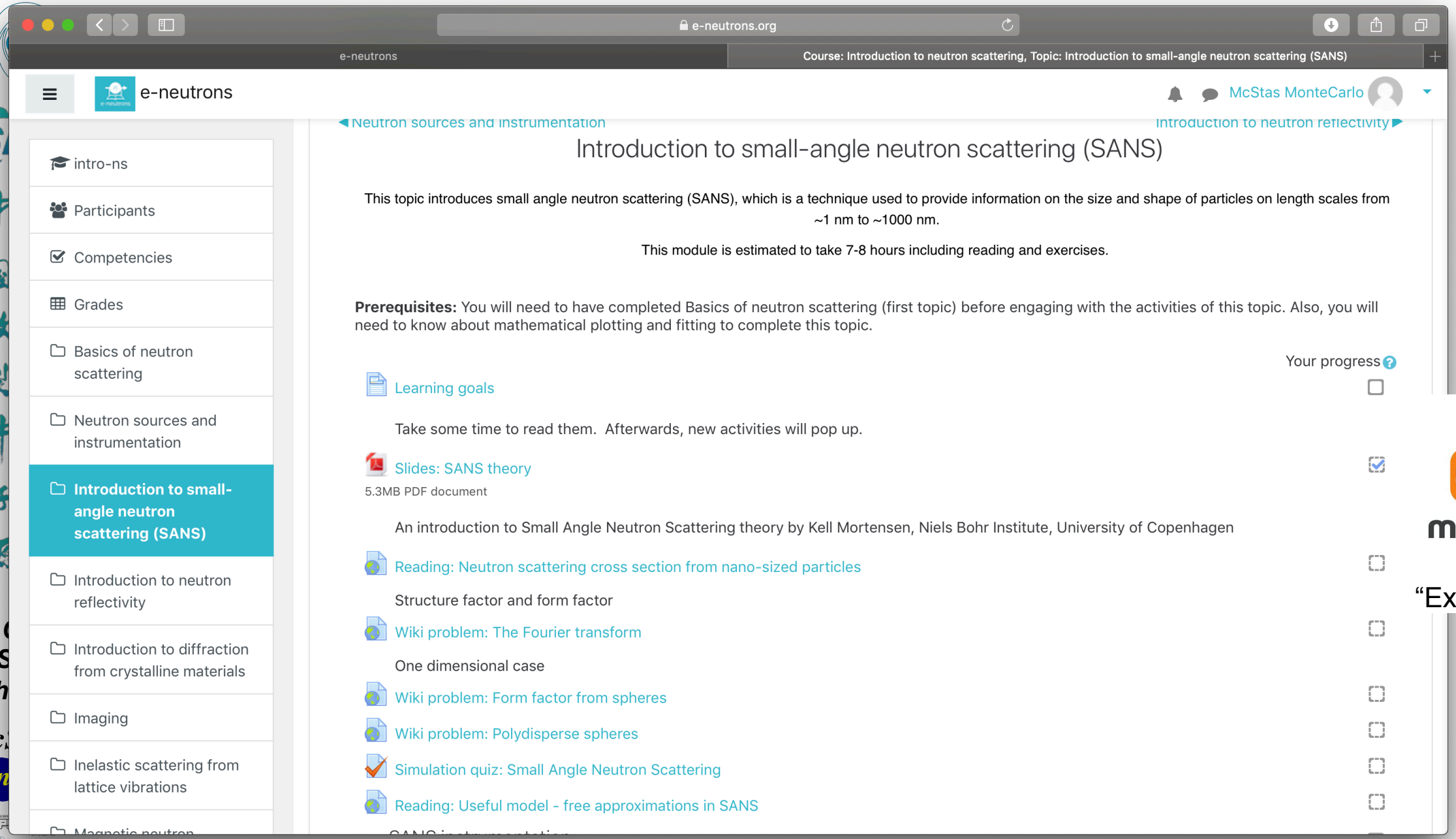
Question 2

Calculate the Fourier transform and the scattering intensity of a one-dimensional crystal with two particles separated with a distance R, and plot the normalized scattered intensity $I(q)$ versus qR.

Hint [show]

MediaWiki

"Textbook"



moodle

"Exercises"

sim.e-neutrons.org

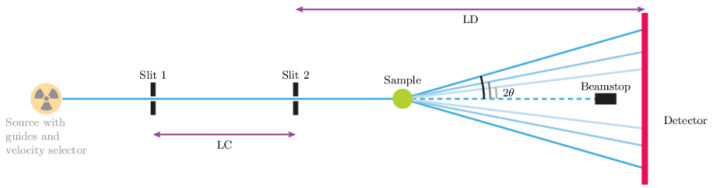
e-neutrons | intro-ns: Simulation quiz: Small Angle Neutron Scattering | Instrument

McStas

Logged in as mcstas (see recent simruns) Logout

Show menu

SANSsimple (click for documentation)



Parameters for SANSsimple

pinhole_rad [m] :	0.004	radius of the collimating pinholes (0.004)
LC [m] :	3	length of the collimator – distance between pinholes (3)
LD [m] :	3	distance between the last pinhole slit and detector (3)
Lambda [AA] :	6	Average wavelength traced from source (6)
DLambda [AA] :	0.6	Wavelength band +/- traced from source (0.6)
R [AA] :	400	radius of the hard, monodisperse spheres in the sample (400)
dR [AA] :	0	Normal variance of Radius (0)
dbilayer [AA] :	35	Thickness of spherical shell, only relevant when SAMPLE==2 (35)
PHI [1] :	0.01	Volumefraction of the hard, monodisperse spheres in the sample (0.01)
Delta_Rho [fm/AA^3] :	0.6	Volume specific scattering length density contrast of the hard, monodisperse spheres in the sample as compared to the solution (0.6)
Qmax [AA^-1] :	0.3	Maximum scattering vector allowed by geometry to hit the detector area (0.3)
BEAMSTOP [0/1] :	1	If set, the beamstop is inserted in front of the detector in order to block the transmitted beam (1)
SAMPLE [0/1/2] :	1	When SAMPLE==0, no sample is used, SAMPLE==1 sample is composed of hard spheres, if SAMPLE==2 sample is composed ofspherical shells. (1)
Sigma_a [barn] :	0	Absorption crossection of the sample (0)

Runtime configuration

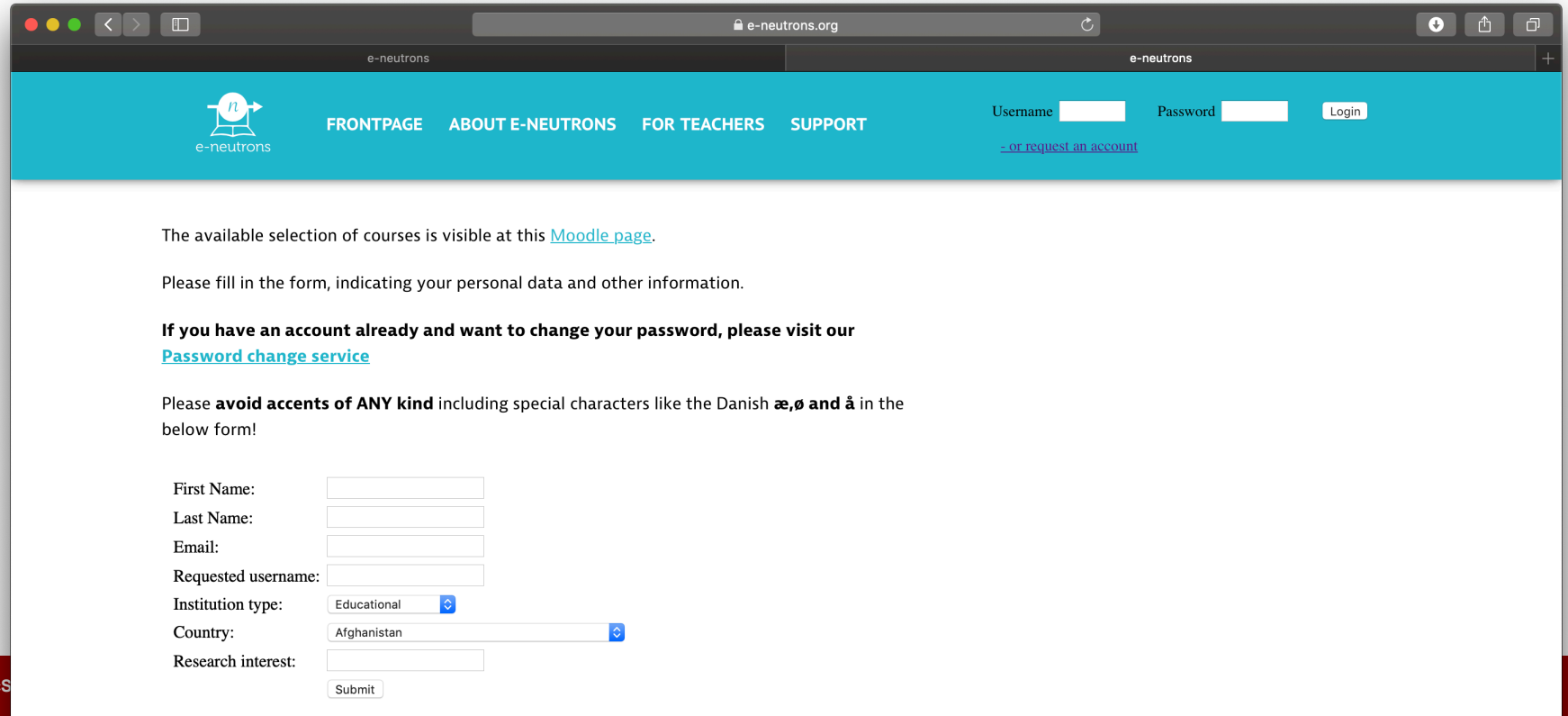
McStas

"Simulator"

Exercise will take place on the e-neutrons.org infrastructure (using a web-simulator)

1. Please fill in the form at https://www.e-neutrons.org/?page_id=423

2. (Once everyone has done this, I will enable the accounts)



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Exercise will take place on the e-neutrons.org infrastructure (using a web-simulator)

1. Please fill in the form at https://www.e-neutrons.org/?page_id=423
2. (Once everyone has done this, I will enable the accounts)
3. You will receive an email with login-credentials
4. Use these credentials to log in to the simulation quiz at https://www.e-neutrons.org/moodle/mod/quiz/view.php?id=4276
5. Follow the instructions in the quiz

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Exercise will take place on the e-neutrons.org infrastructure (using a web-simulator)

Fallback solution:

* Get the PDF and other files from the file ‘fallback.zip’ at

https://github.com/McStasMcXtrace/Schools/tree/master/CSNS_March_2019/4_Thursday_March_28th/4_SANS

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