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# SANS in McStas

2019 CSNS  
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# Agenda

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

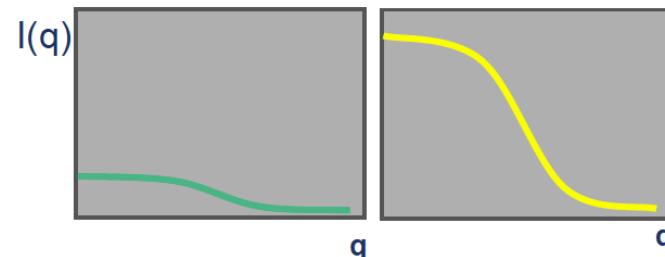
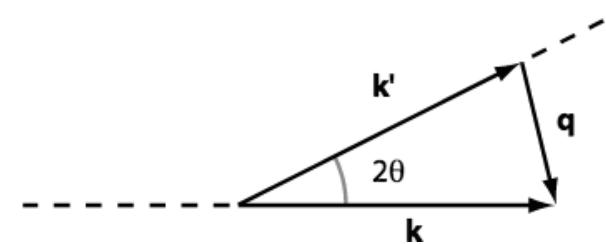
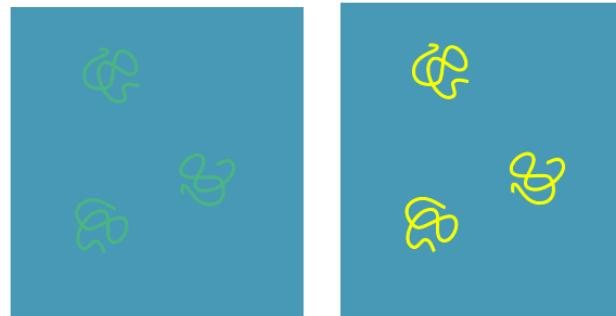
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# Small angle scattering SANS

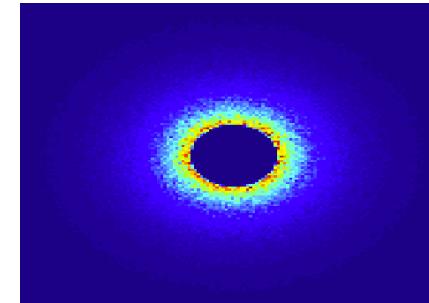
- SANS method can be used for many types of material
- Often: Molecule + Liquid (buffer solution)
- Isotropic scattering



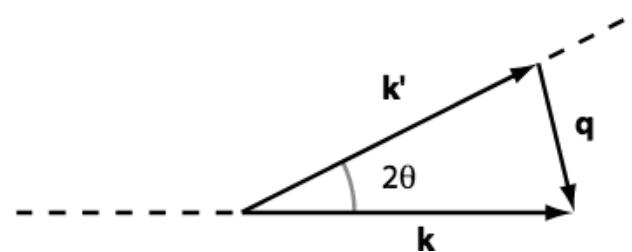
# SANS

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



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



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 other samples

- 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

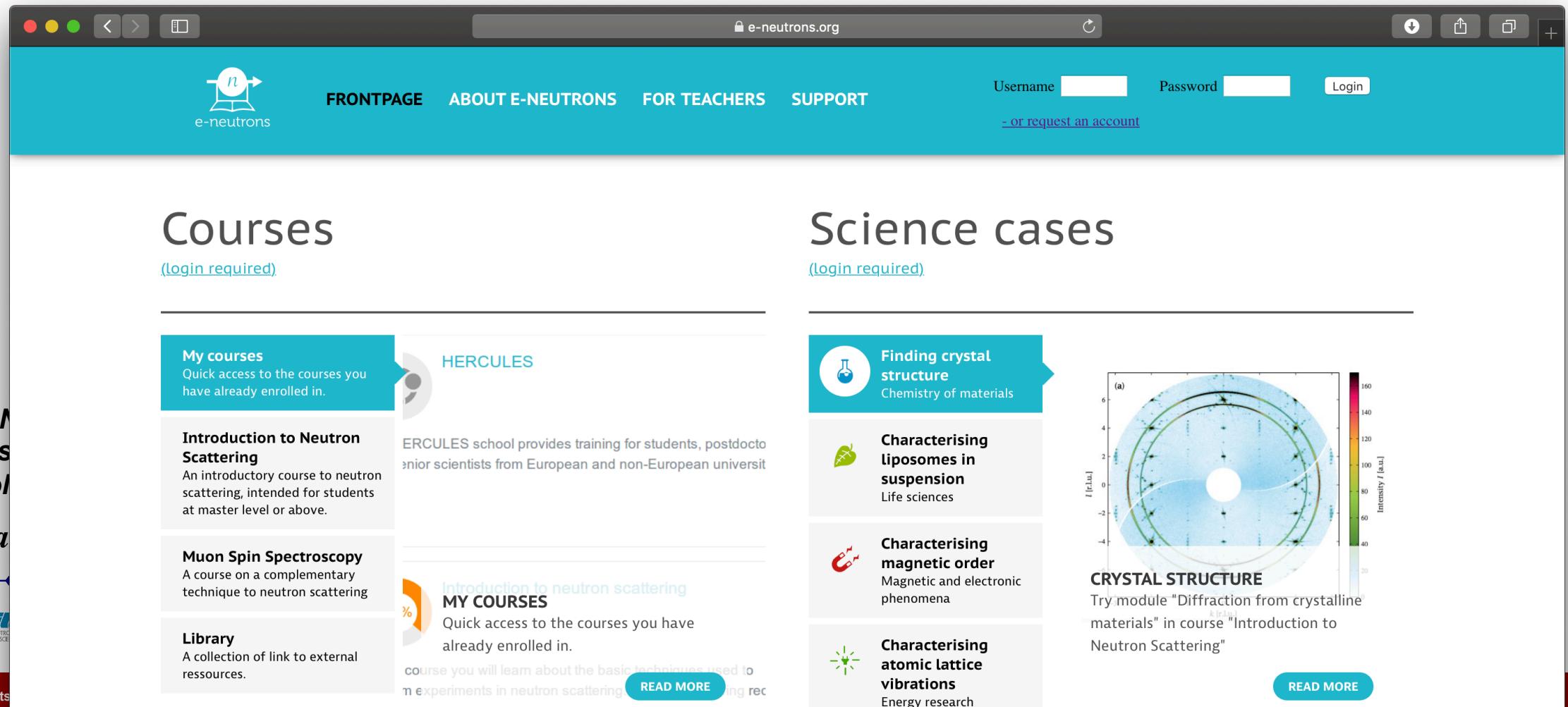
Parameters in **boldface** are required; the others are optional.

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

# Exercise will take place on the [e-neutrons.org](https://e-neutrons.org) infrastructure (using a web-simulator)



The screenshot shows the e-neutrons.org website interface. At the top, there is a navigation bar with links to FRONTPAGE, ABOUT E-NEUTRONS, FOR TEACHERS, and SUPPORT. There are also fields for Username and Password, and a Login button. Below the navigation bar, there are two main sections: "Courses" and "Science cases".

**Courses** (login required):

- My courses**: Quick access to the courses you have already enrolled in.
- Introduction to Neutron Scattering**: An introductory course to neutron scattering, intended for students at master level or above.
- Muon Spin Spectroscopy**: A course on a complementary technique to neutron scattering.
- Library**: A collection of links to external resources.

**HERCULES**: ERCULES school provides training for students, postdoctoral scientists and senior scientists from European and non-European universities.

**Science cases** (login required):

- Finding crystal structure**: Chemistry of materials
- Characterising liposomes in suspension**: Life sciences
- Characterising magnetic order**: Magnetic and electronic phenomena
- Characterising atomic lattice vibrations**: Energy research

**CRYSTAL STRUCTURE**: Try module "Diffraction from crystalline materials" in course "Introduction to Neutron Scattering".

**READ MORE**

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.

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).

**Contents [hide]**

- 1 Question 1
- 2 Question 2
- 3 Question 3
- 4 Question 4
- 5 Question 5

**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]



One-dimensional crystal.

Log in



“Textbook”

6. marts 2019      2019 McStas school @ CSNS

e-neutrons.org

e-neutrons

Course: Introduction to neutron scattering, Topic: Introduction to small-angle neutron scattering (SANS)

McStas MonteCarlo

Neutron sources and instrumentation

## Introduction to small-angle neutron scattering (SANS)

This topic introduces small angle neutron scattering (SANS), which is a technique used to provide information on the size and shape of particles on length scales from ~1 nm to ~1000 nm.

This module is estimated to take 7-8 hours including reading and exercises.

**Prerequisites:** You will need to have completed Basics of neutron scattering (first topic) before engaging with the activities of this topic. Also, you will need to know about mathematical plotting and fitting to complete this topic.

Your progress?

**Learning goals**

Take some time to read them. Afterwards, new activities will pop up.

**Slides: SANS theory**   
5.3MB PDF document  
An introduction to Small Angle Neutron Scattering theory by Kell Mortensen, Niels Bohr Institute, University of Copenhagen

**Reading: Neutron scattering cross section from nano-sized particles**   
Structure factor and form factor

**Wiki problem: The Fourier transform**   
One dimensional case

**Wiki problem: Form factor from spheres**

**Wiki problem: Polydisperse spheres**

**Simulation quiz: Small Angle Neutron Scattering**

**Reading: Useful model - free approximations in SANS**

SANS in practice



“Exercises”

sim.e-neutrons.org

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

**McStas**

Show menu

SANSsimple ([click for documentation](#))

Logged in as mcstas (see recent simruns) [Logout](#)

Parameters for SANSsimple

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

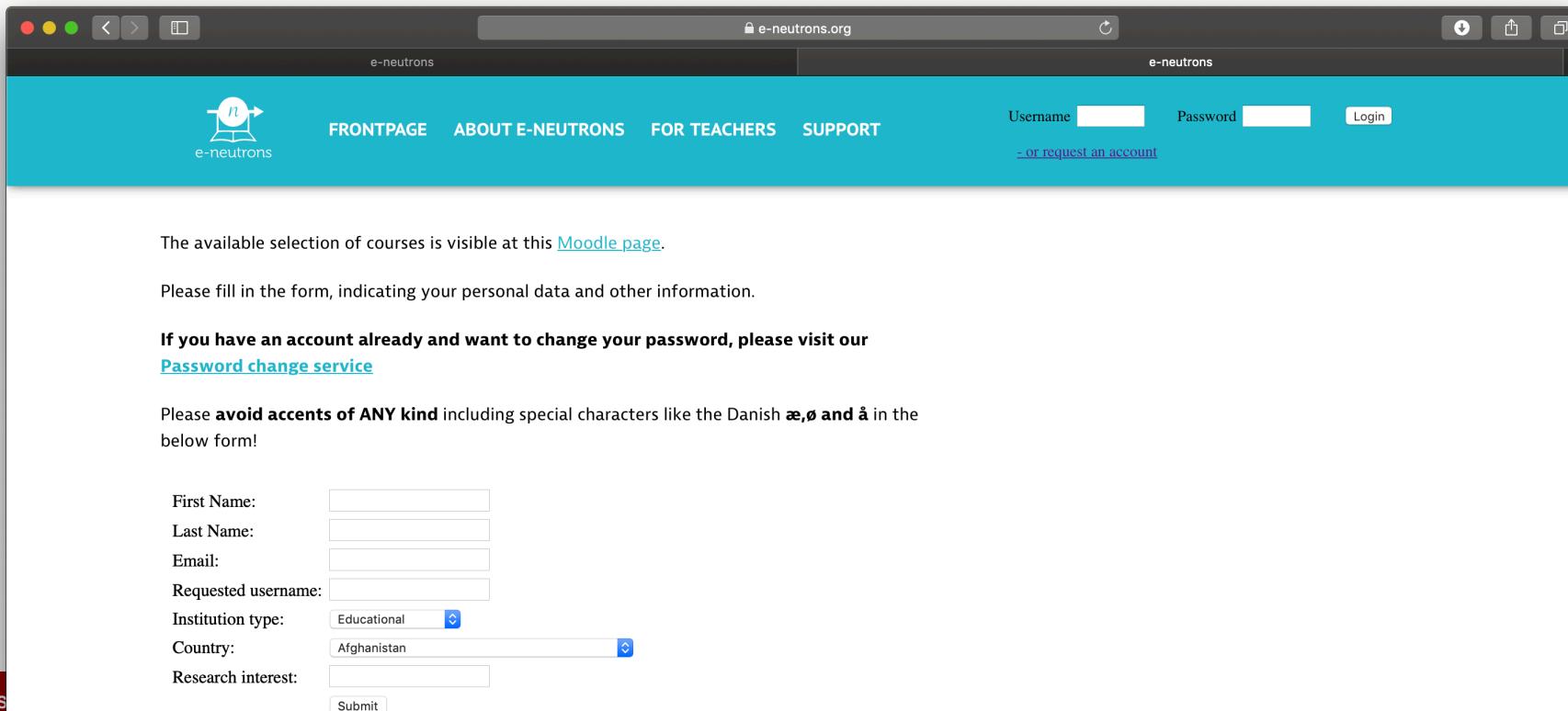
Runtime configuration



“Simulator”

# Exercise will take place on the [e-neutrons.org](https://www.e-neutrons.org/?page_id=423) infrastructure (using a web-simulator)

1. Please fill in the form at [https://www.e-neutrons.org/?page\\_id=423](https://www.e-neutrons.org/?page_id=423)
2. (Once everyone has done this, I will enable the accounts)



The screenshot shows a web browser window for the e-neutrons.org website. The header bar includes the URL 'e-neutrons.org' and a search bar. Below the header is a navigation bar with links for 'FRONTPAGE', 'ABOUT E-NEUTRONS', 'FOR TEACHERS', 'SUPPORT', 'Username' (input field), 'Password' (input field), and a 'Login' button. A link 'or request an account' is also present. The main content area contains instructions: 'The available selection of courses is visible at this [Moodle page](#). Please fill in the form, indicating your personal data and other information.' It also includes a note about avoiding accents and a form for entering personal data. The form fields include 'First Name', 'Last Name', 'Email', 'Requested username', 'Institution type' (dropdown: 'Educational'), 'Country' (dropdown: 'Afghanistan'), 'Research interest', and a 'Submit' button.

The available selection of courses is visible at this [Moodle page](#).

Please fill in the form, indicating your personal data and other information.

If you have an account already and want to change your password, please visit our [Password change service](#)

Please avoid accents of ANY kind including special characters like the Danish æ,ø and å in the below form!

First Name:

Last Name:

Email:

Requested username:

Institution type:

Country:

Research interest:

# Exercise will take place on the [e-neutrons.org](https://www.e-neutrons.org) infrastructure (using a web-simulator)

1. Please fill in the form at [https://www.e-neutrons.org/?page\\_id=423](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

**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](https://github.com/McStasMcXtrace/Schools/tree/master/CSNS_March_2019/4_Thursday_March_28th/4_SANS)