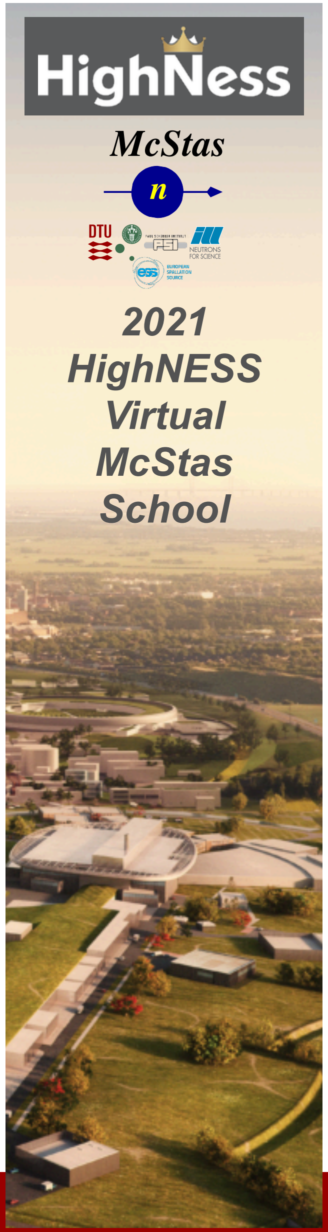
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Peter Willendrup

Further samples…

SANS, reflectometry, inelastic scattering

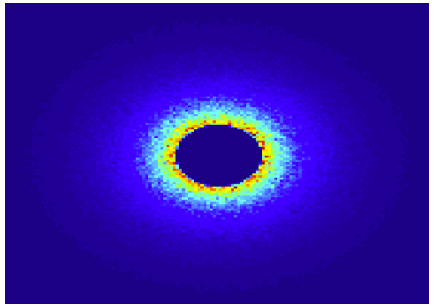


Further samples in McStas

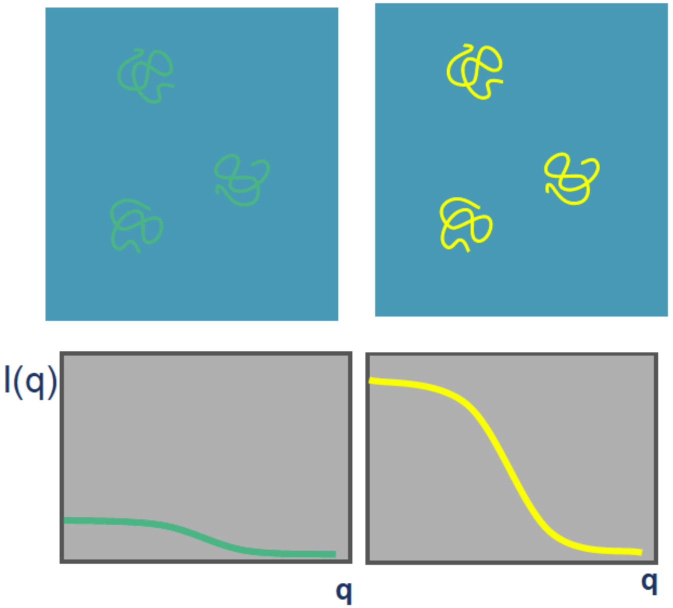
- A look at the “Sample functionality matrix”
- Models for SANS
- Inelastic scattering, examples:
  - Phonon_simple
  - Isotropic_sqw
- McStas performance, TAS / Chopper

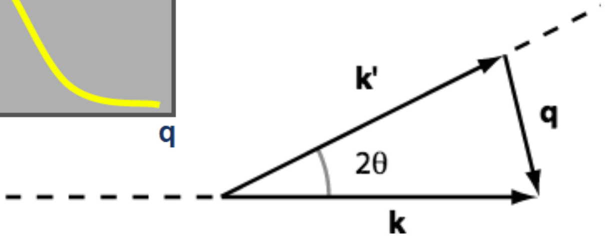
Small angle scattering SANS

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



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



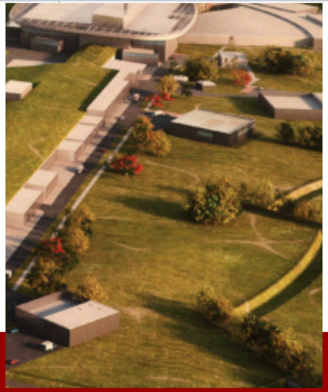


Small Angle Neutron Scattering

- 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.

SANS models in McStas

6	Sans_spheres (and other similar) *McStas team* and *Martin Cramer Pedersen, KU*	Hard spheres in thin solution and other models, defined per-component...	SANS	✓	✓	"✓" - SANS	✗	✗	✗
7	SANS_benchmark2 (and a few other stand-alone models) *Heinrich Frielinghaus, FZJ/JCNS*	Experimentally-benchmarked model set for SANS	SANS	✓	✓	"✓" - SANS	✗	✓ up to 10 orders	✗
8	SASview_models *McStas team*	"Any" model from SASview / SASmodels	SANS	✓	✓	"✓" - SANS	✗	✗ at this point	✗



DTU
EUROPEAN SPALLATION SOURCE

HighNess

HighNess
McStas
2021 HighNESS Virtual McStas School

Example: SANS spheres

Input parameters

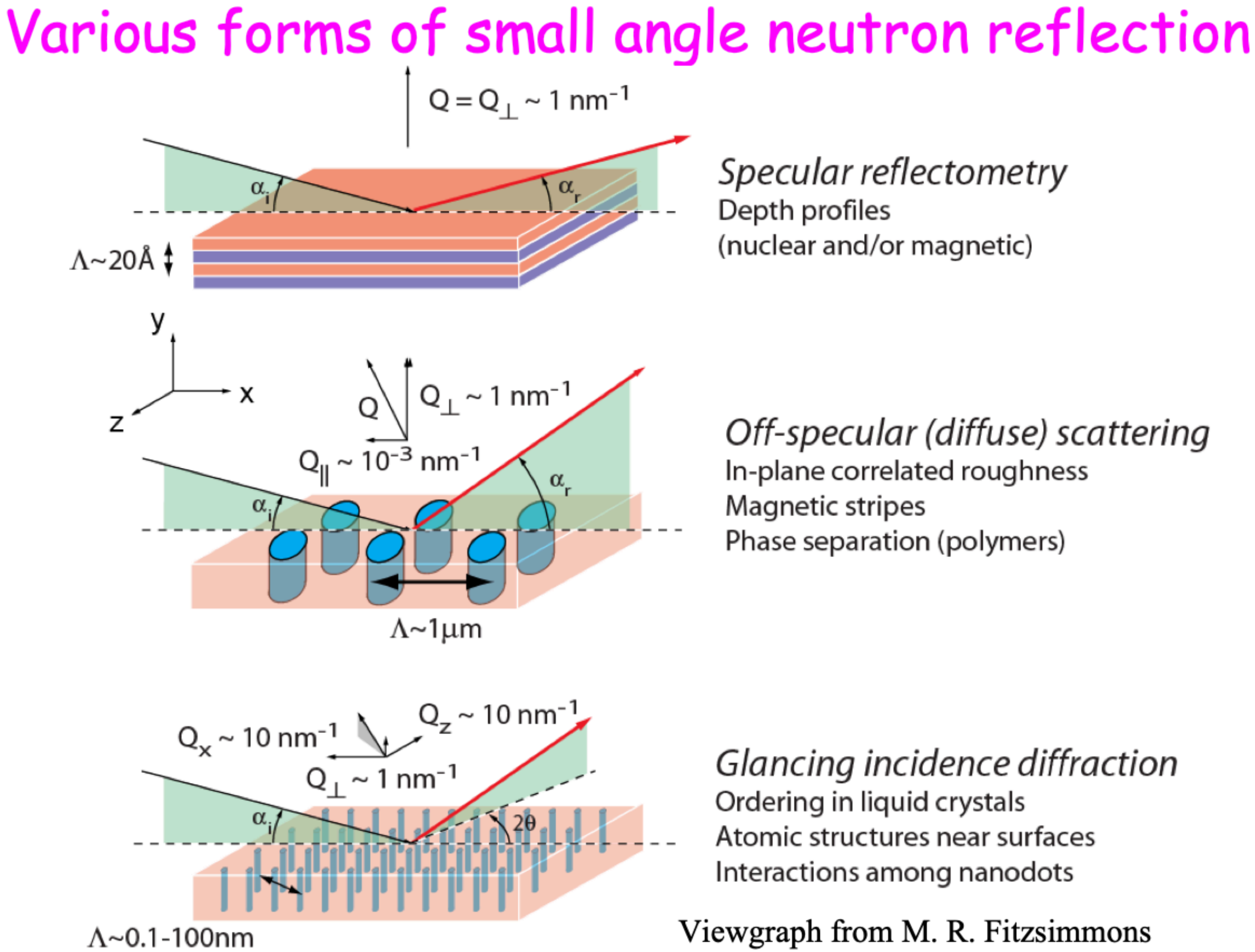
Parameters in **boldface** are required; the others are optional.

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

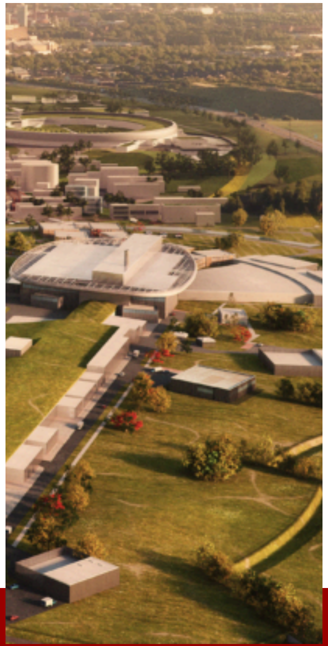
Reflectometry

- Used to probe properties of surfaces and interfaces - solids and liquids



Reflectometry samples in McStas

9	Multilayer_sample *Rob Dalgliesh, ISIS STFC*	Multilayer-sample (additions of phase via matrix-formalism) with incoherent background	Reflectometry	✓	✓	"✓" - Reflectivity curve	✗	✗	✗
22	"Specular reflectometry"	Use a reflectivity-curve with e.g. Mirror.comp	Reflectometry	✓	✓	"✓" - Reflectivity curve	✗	✗	✗



Example: Multilayer_sample

Description

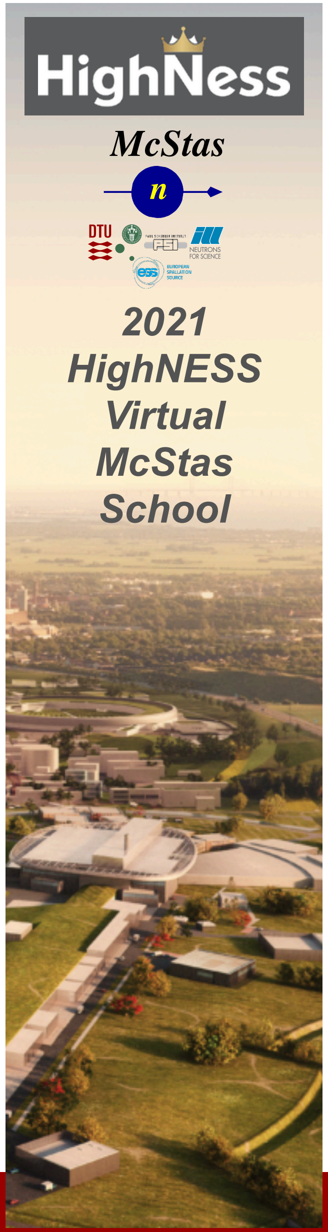
```
in order to get this to compile you need to link against
the gsl and gslcblas libraries.

to do this automatically edit
/usr/local/lib/mcstas/tools/perl/mcstas_config.perl

add -lgsl and -lgslcblas to the CFLAGS line

Horizontal reflecting substrate defined by SLDs,Thicknesses, roughnesses
The superphase may also be determined

Example: Multilayer_Sample(xmin=-0.1, xmax=0.1,zmin=-0.1, zmax=0.1, nlayer=1,sldPar={0.0,2.0e-6,0.0e-6},dPar={20.0}, sigmaPar={5.0,5.0})

Example: d1 500: sld1 (air) 0.0: sld2 (Si) 2.07e-6: sldf1(film Ni) 9.1e-6
```

WARNING: **This is a contributed Component.**

Input parameters

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

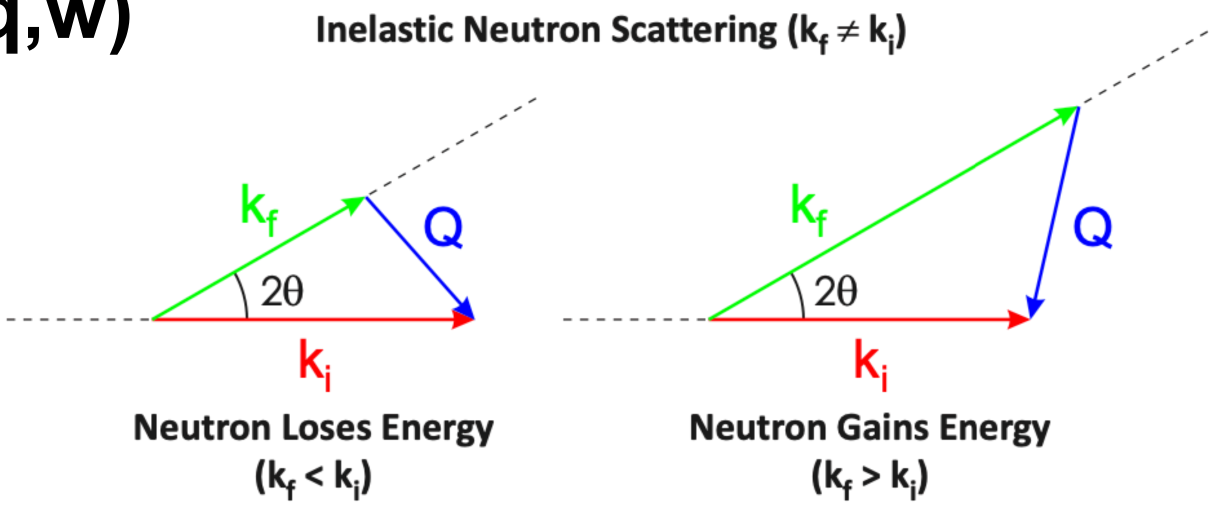
Name	Unit	Description	Default
sldPar	1	(Angstoms ^-2) Scattering length Density's of layers	{0.0
dPar	1	(Angstroms) Thicknesses of film layers	{20.0}
sigmaPar	1	(Angstroms) r.m.s roughnesses of the interfaces	{5.0
xwidth	m	Width of substrate	0.2
zlength	m	Length of substrate	0.2
nlayer	1	Number of film layers	1
frac_inc	1	Fraction of statistics to assign to incoherent scattering	0
ythick	m	Thickness of substrate	0
mu_inc	m^-1	Incoherent scattering length	5.62
target_index	1	relative index of component to focus at, e.g. next is +1.	0
focus_xw	m	Width of target	0
focus_yh	m	Height of target	0



Inelastic scattering S(q,w)

- Partial differential cross section
- Scattering function

- Phonons, Spin waves, …



$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E_f}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k_f}{k_i} N S(\mathbf{q},\omega)$$

$$S(\mathbf{q},\omega)_{coh} = \frac{1}{2\pi\hbar}\int \frac{1}{N}\sum_{jj'}\left\langle e^{-i\mathbf{q}\cdot\mathbf{R}_{j'}(0)} e^{-i\mathbf{q}\cdot\mathbf{R}_j(t)}\right\rangle e^{-i\omega t}\mathrm{d}t$$

McStas samples with inelastic options

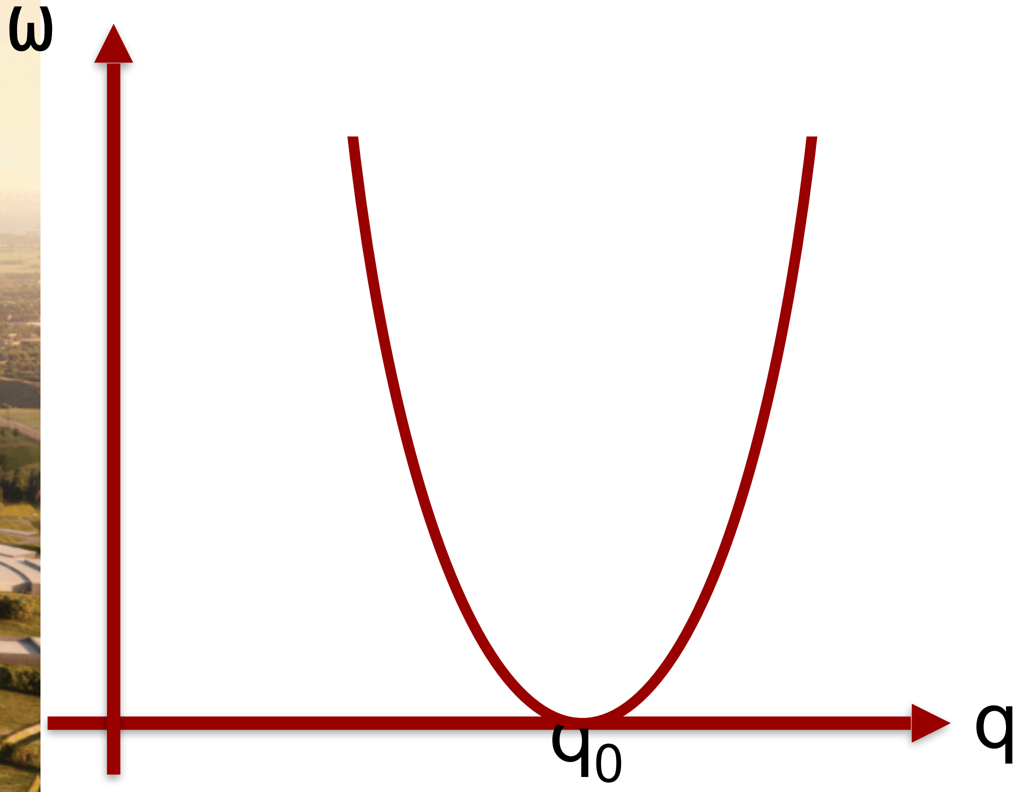
2	Tunelling_sample *McStas team / Kim Lefmann*	Idem 1, plus tunneling peaks and QE broadening	Quasi-elastic scattering, backscattering	✅	✅	❌	❌/✅ (Quasielastic broadening + tunnel peaks)	(✅ analytic approach)	✅
10	Phonon_simple *McStas team / Kim Lefmann*	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	❌	❌	❌	✅ (phonon, at this point FCC lattice only)	❌	❌
11	Isotropic_Sqw *McStas team / Emmanuel Farhi*	Structure and dynamics in isotropic materials (liquids, powders etc.)	Inelastic scattering, diffraction, isotropic materials, imaging	✅	✅	✅ (Debye-Scherrer cones)	✅ isotropic inelastic scattering	✅	✅
12	Res_sample *McStas team*	Resolution-oriented sample component	Generic	"✅"	❌	❌	"✅" flat, isotropic inelastic scattering	❌	❌
13	TOFRes_sample *McStas team / Kim Lefmann*	Idem Res_sample, with TOF support	Generic	"✅"	❌	❌	"✅" flat, isotropic inelastic scattering	❌	❌
14	Spot_sample *Garrett Granroth, SNS/ORNL*	Resolution-oriented sample component Dirac delta-functions in (Q and energy)	Inelastic scattering	❌	❌	"✅"	"✅"	❌	❌
15	Union components, Mads Bertelsen, ESS	A set of components that allows to build a complex sample/sample environment from basic geometries and physics/material properties	Generic	✅	✅	✅ Single crystalline or Powder crystalline	(✅ - single acoustic phonon being included 2018)	✅	(✅ - if built from cylinders, spheres, boxes, ...)
16	Single_crystal_inelastic Duc Le, ISIS STFC	4D-equivalent of Isotropic_Sqw / Single_crystal	Elastic and inelastic experiments with crystals	✅	✅	✅	✅	✅	?¿?
17	Magnon_bcc *McStas team / Kim Lefmann*	FM / AFM magnon in BCC lattice	Inelastic scattering magnon	❌	❌	❌	✅ (magnon, at this point BCC lattice only)	❌	❌
18	NCrystal_sample Xiao Xiao Cai, DTU Nutech/ESS	Single crystal and powder diffraction, with isotropic inelastic scattering	Powder and Single_crystal diffraction, imaging	✅	✅	✅	✅ (in an isotropic form)	✅	

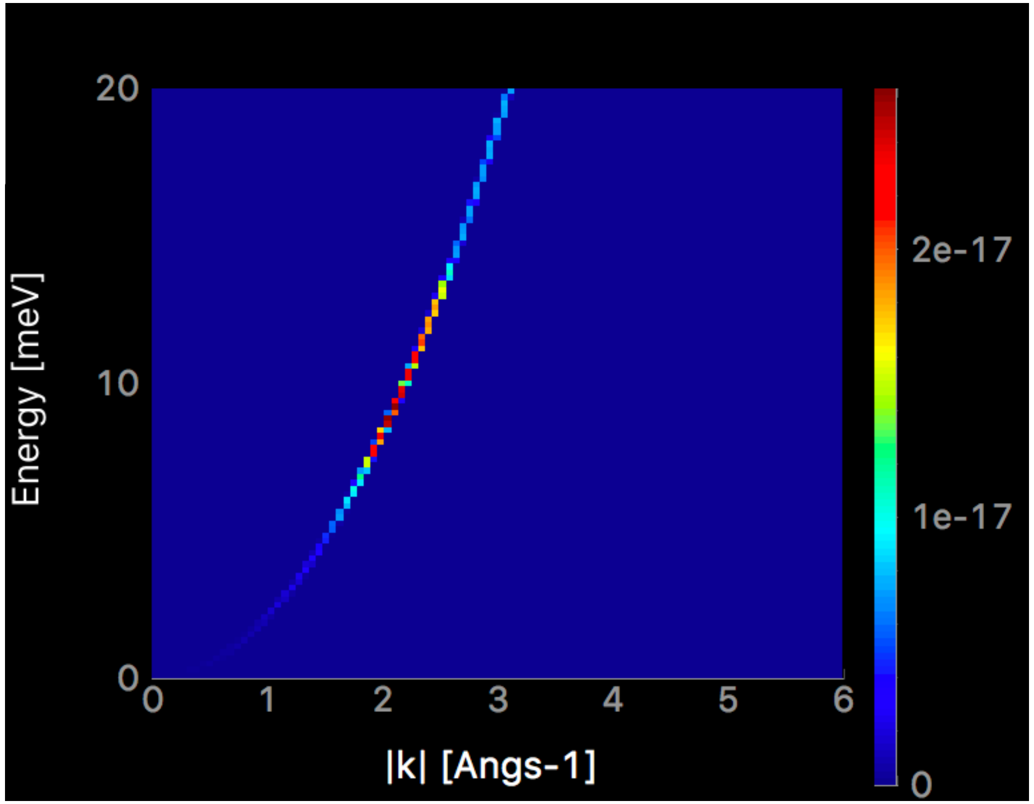
Example component: Phonon_simple

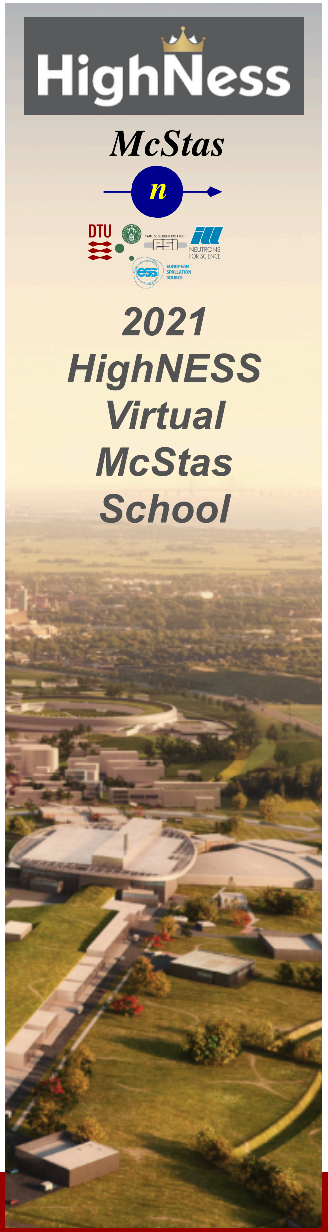
- One isotropic acoustic phonon branch in all Brillouin zones on FCC Bravais single crystal

  Dispersion $d_1(\mathbf{q}) = c_1/a\sqrt{z - s_q}$

- Dispersion relation, theory and mcstas



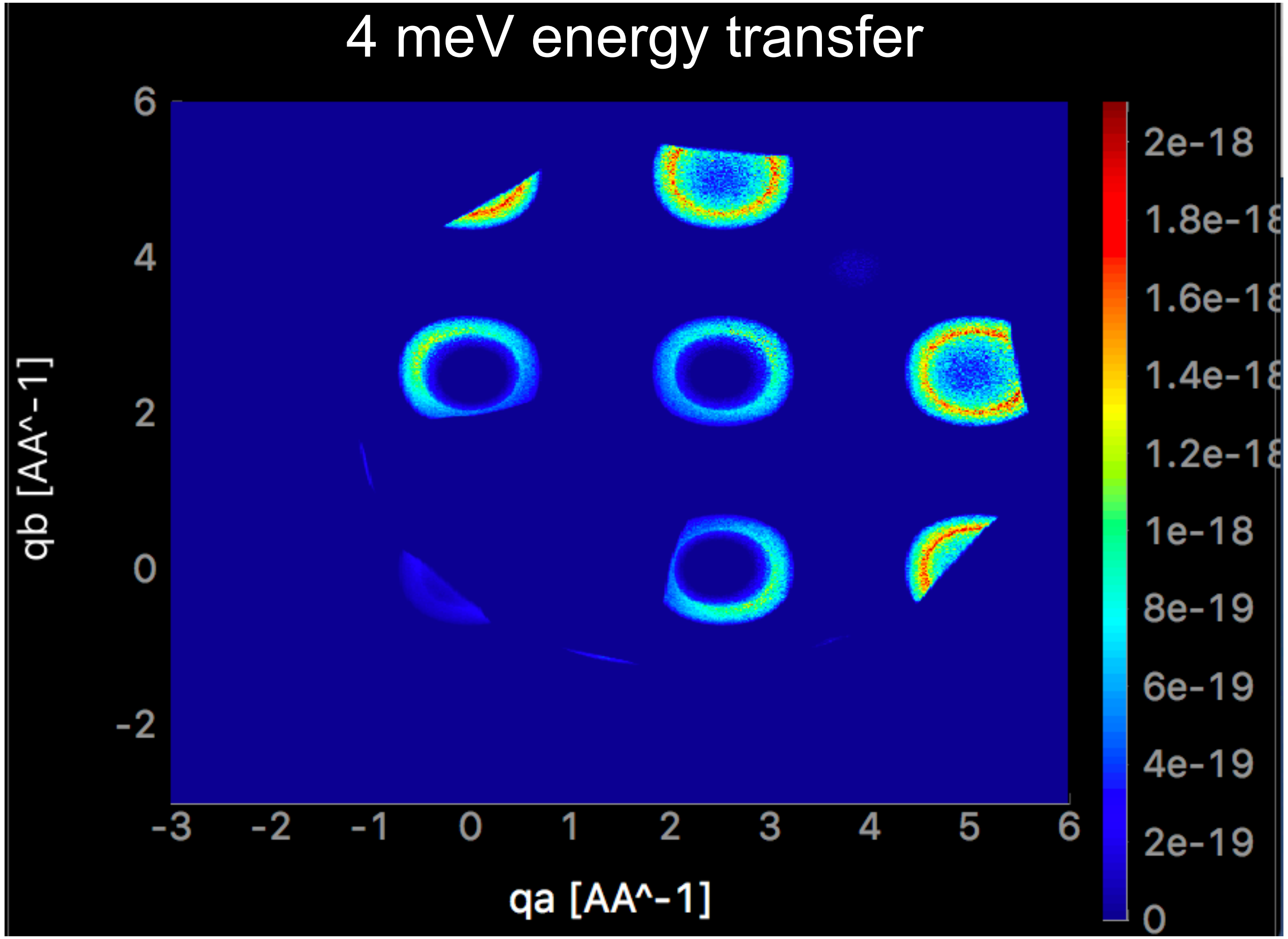


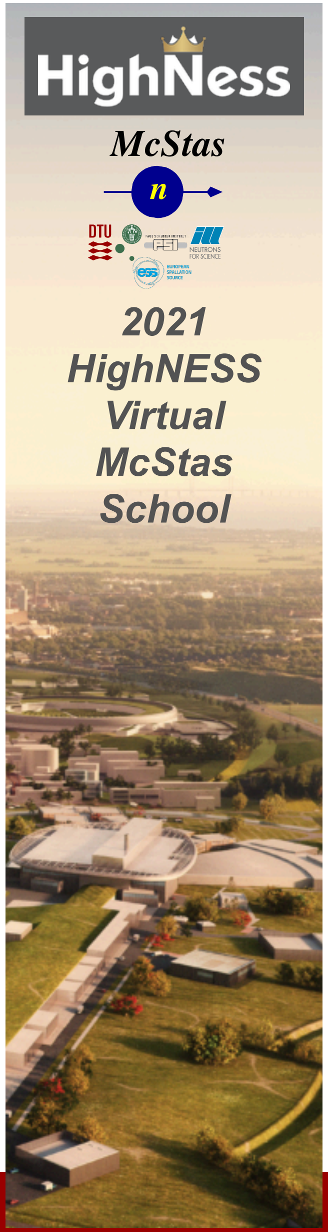


Example component: Phonon_simple

- Example of the output
- Elastic scattering only
- Combine with Single_crystal for elastic-inelastic scattering

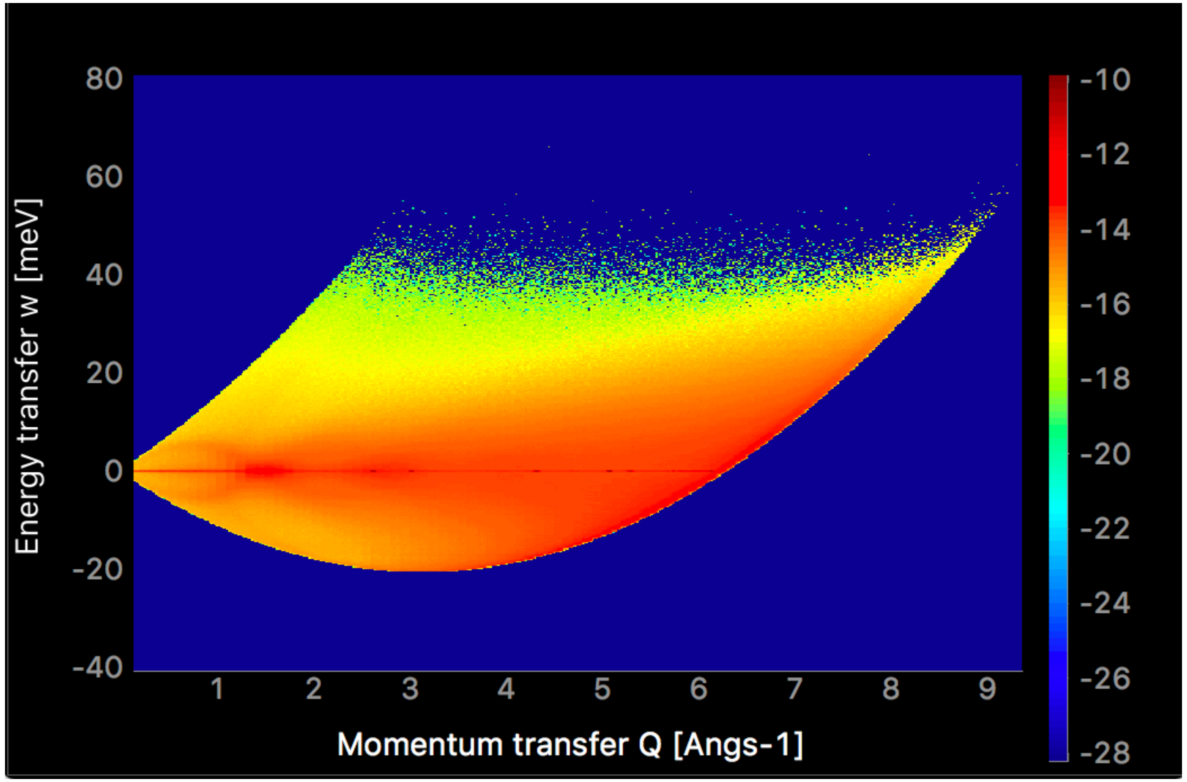
- Magnon_fcc is conceptually very similar

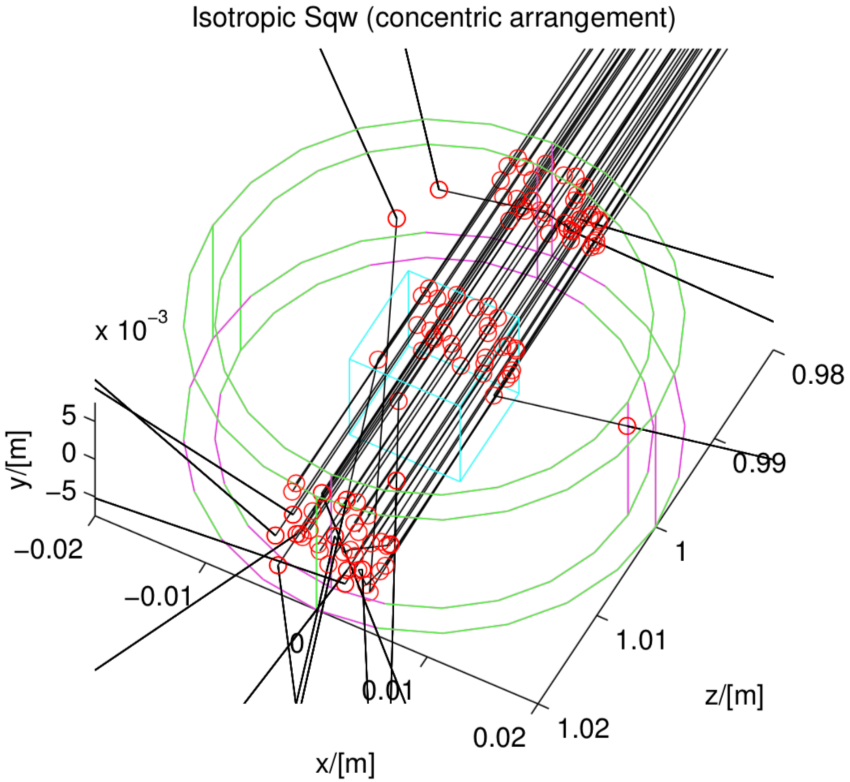


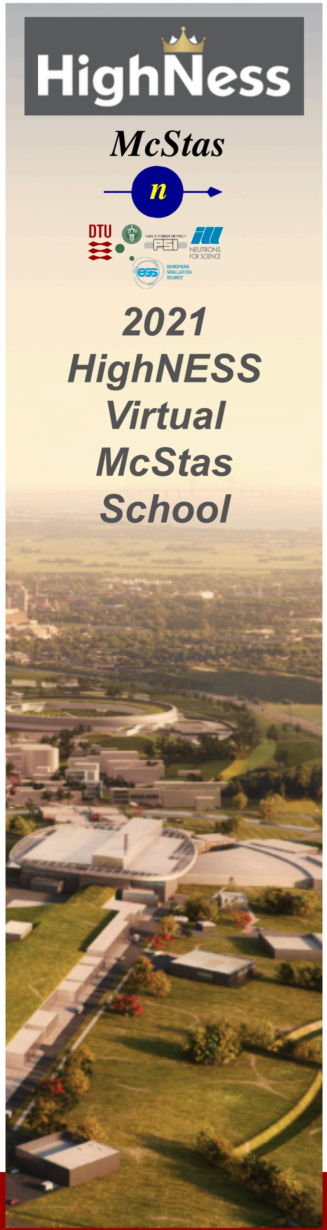


Example component: Isotropic_sqw

- Isotropic processes (powder, liquid, …)
- Use data files to describe S(|q|,w) directly, coherent and incoherent - isotropic scattering
- Supports concentric geometries







Example component

- Single_crystal_inelastic
- Contribution from Duc Le, ISIS
- “Marriage” between Single_crystal and 4D equivalent of Isotropic_Sqw

- BIG tables, lots of memory, close to impossible to use for anything but “locally” in reciprocal space, i.e. in TAS settings

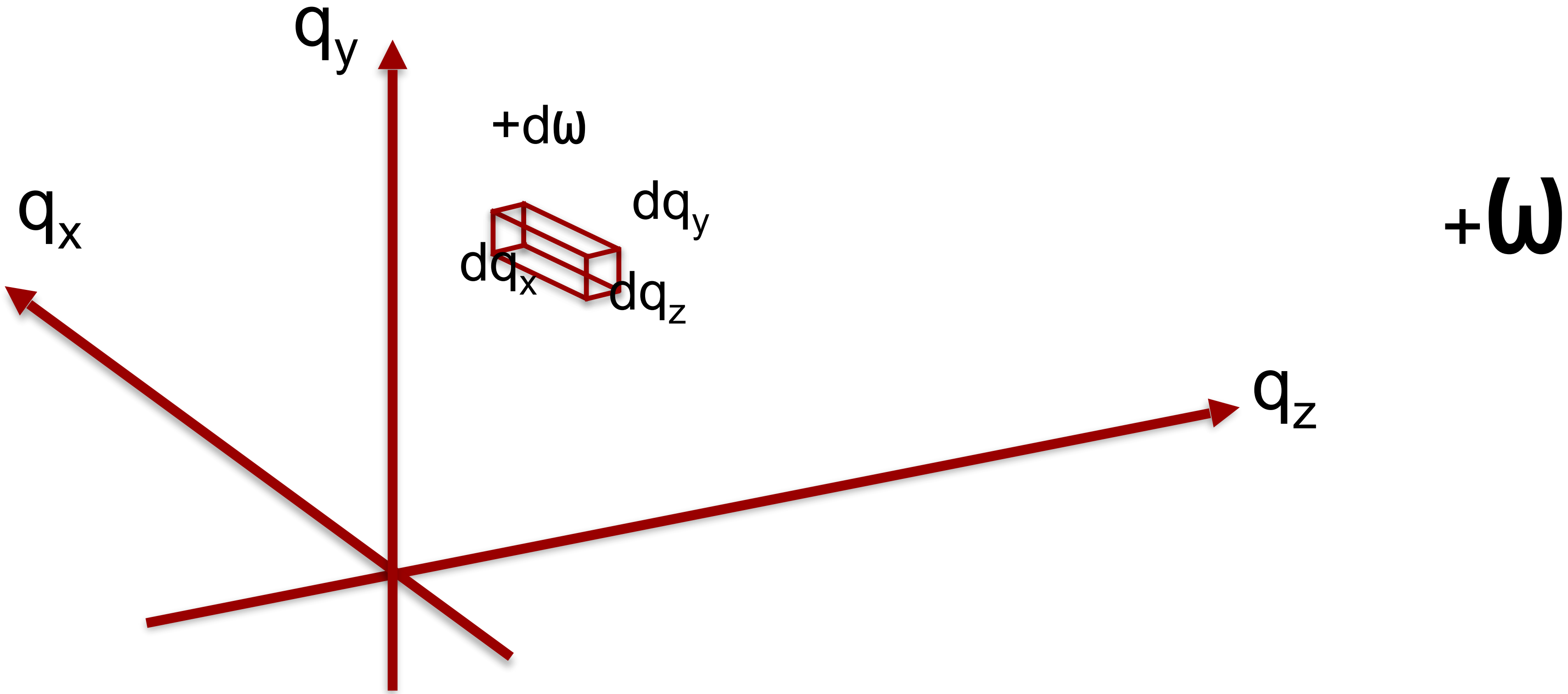
DTU

EUROPEAN SPALLATION SOURCE

HighNess

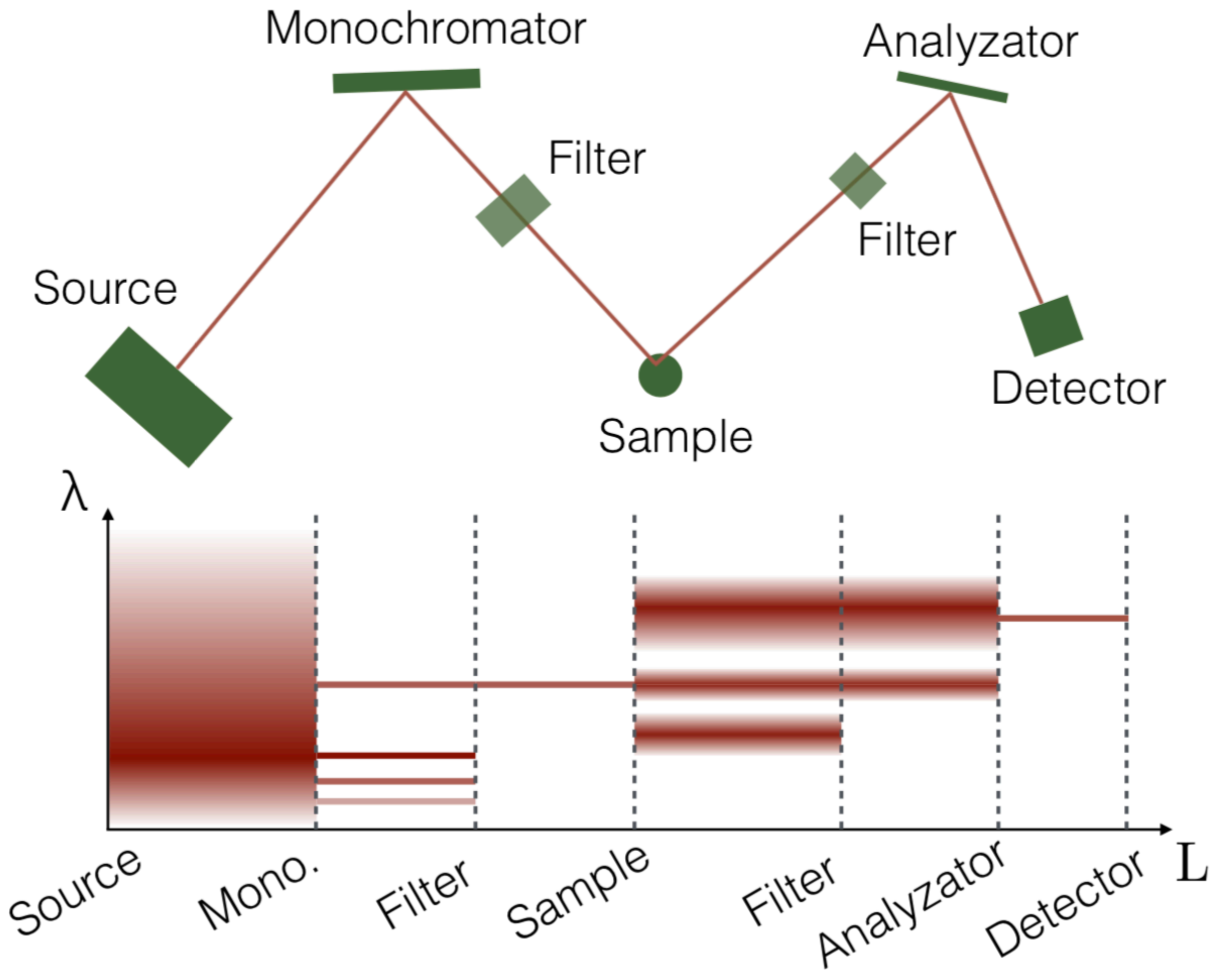
Inelastic scattering in McStas

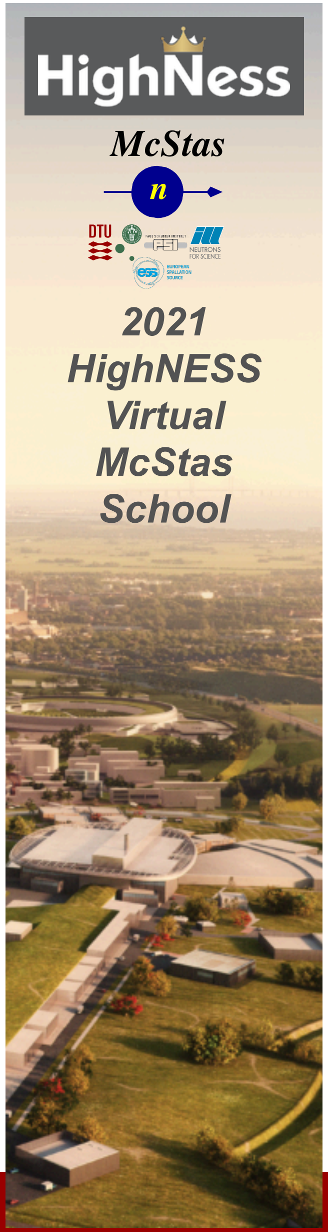
- Monte carlo sampling issues
- Need to sum over large amount of possible final states to find cross section
- Need large amount of rays to sample all the options



TAS

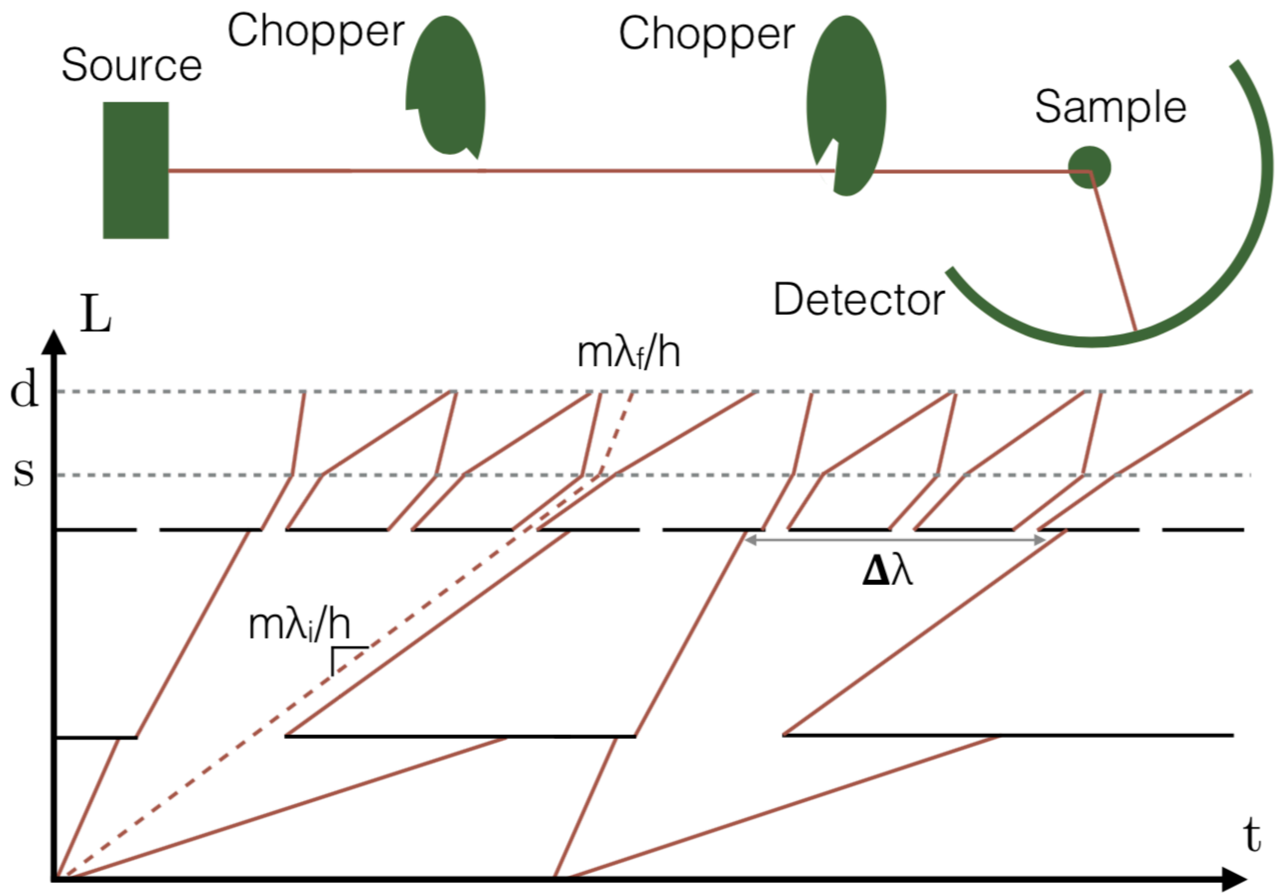
- Only a small fraction of neutrons arrive, most are simulated in vain

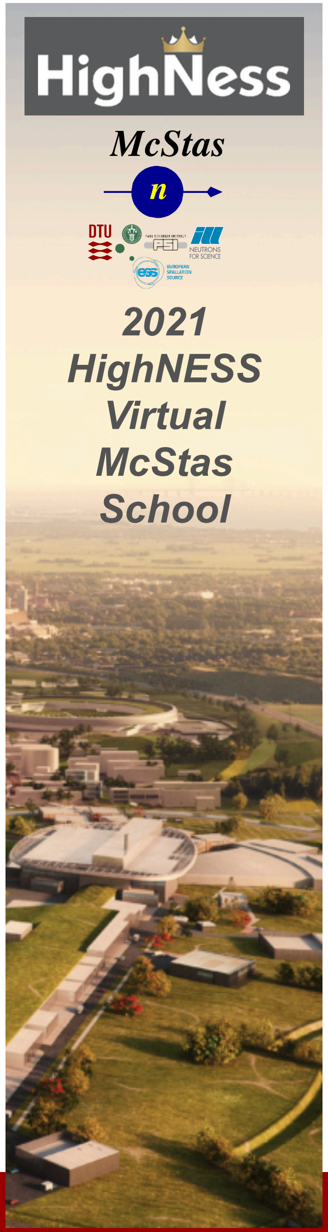




Chopper spectrometers

- Only a small fraction of neutrons arrive, most are simulated in vain





Conclusions

- SANS
  - Lots of choice, many models (challenge can be to decide what to choose)

- Reflectometry:
  - Only little choice, Multilayer_sample or “a mirror”

- Inelastic scattering
  - Inelastic scattering supported in McStas, not all cases fully covered
  - Longer computational times required
  - Advantages from simulation especially important for spectroscopy (resolution function)