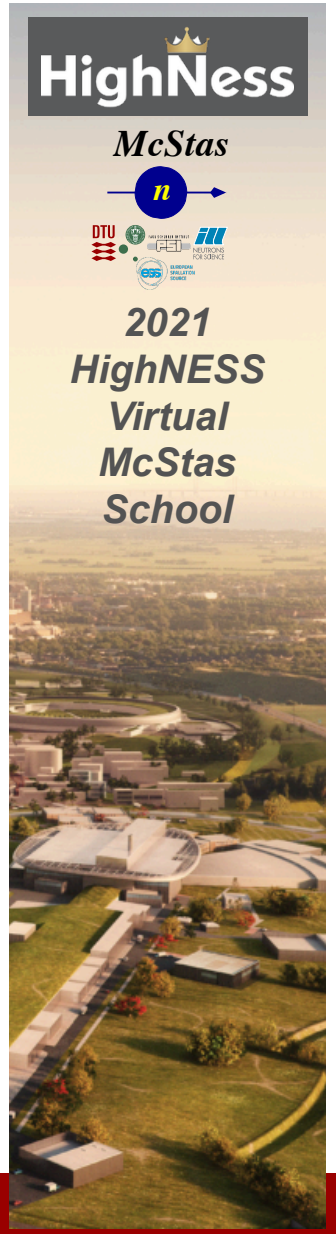
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Peter Willendrup

Further samples…

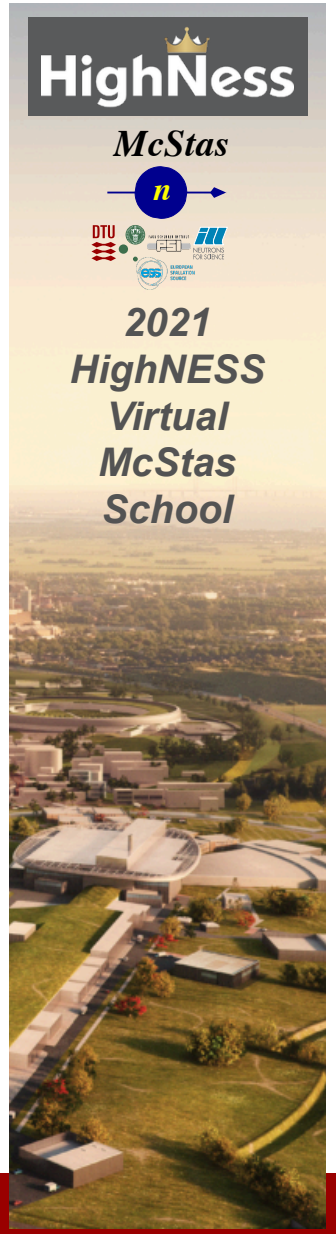
SANS, reflectometry, imaging, inelastic scattering



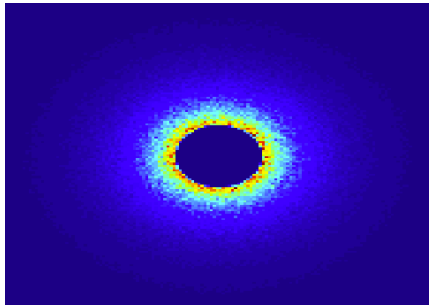
Further samples in McStas

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

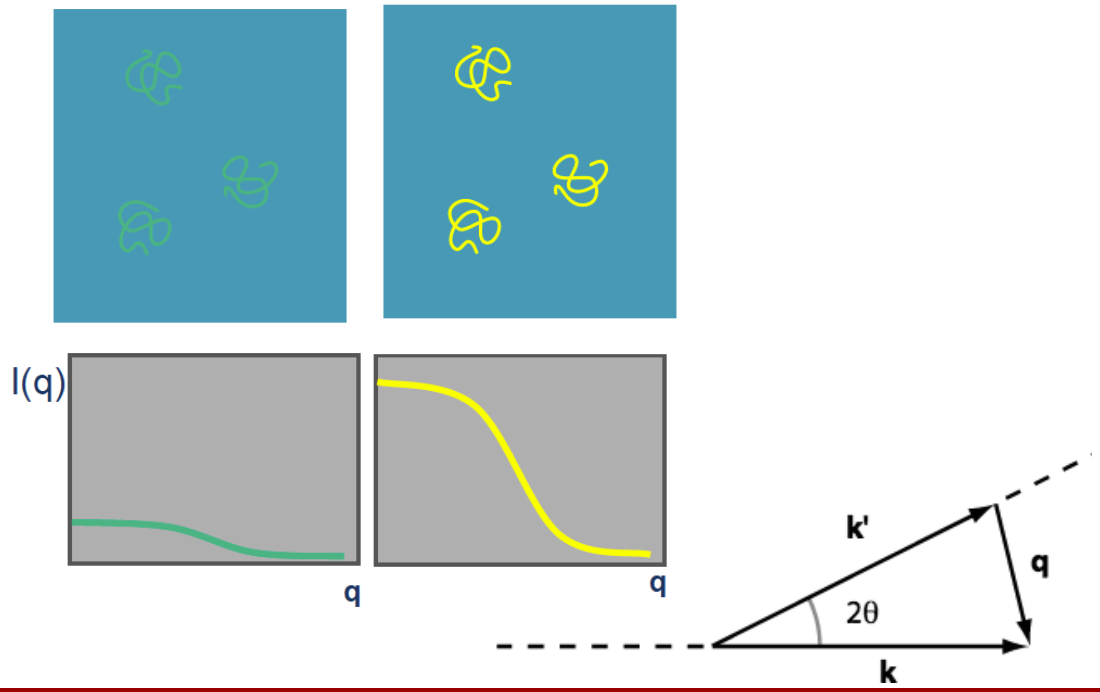
Small angle scattering SANS



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



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

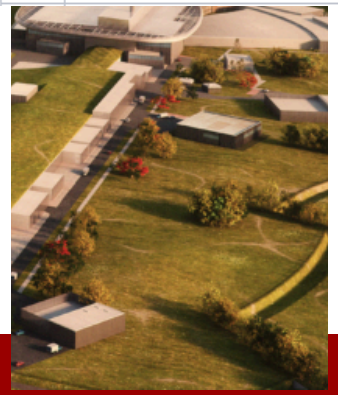


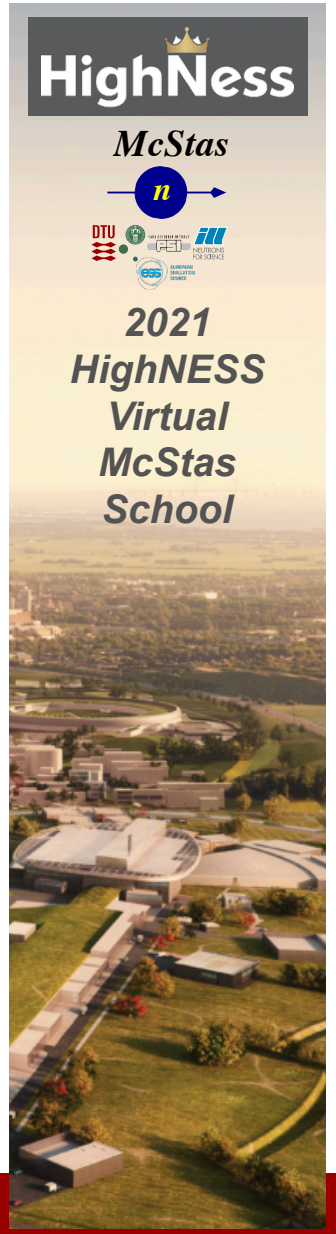
Small Angle Neutron Scattering

- 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	❌





Example: SANS spheres

Input parameters

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

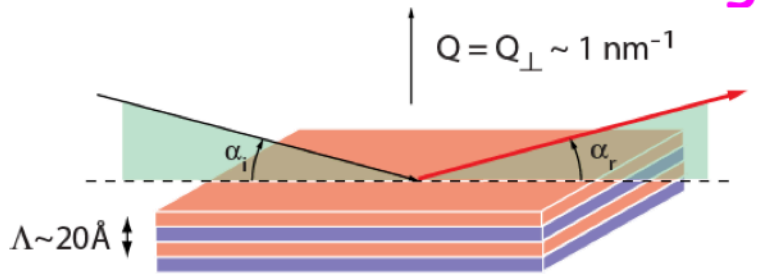
Name	Unit	Description	Default
R	AA	Radius of scattering hard spheres	100
Phi	1	Particle volume fraction	1e-3
Delta_rho	fm/AA^3	Excess scattering length density	0.6
sigma_abs	m^-1	Absorption cross section density at 2200 m/s	0.05
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert . dimension 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

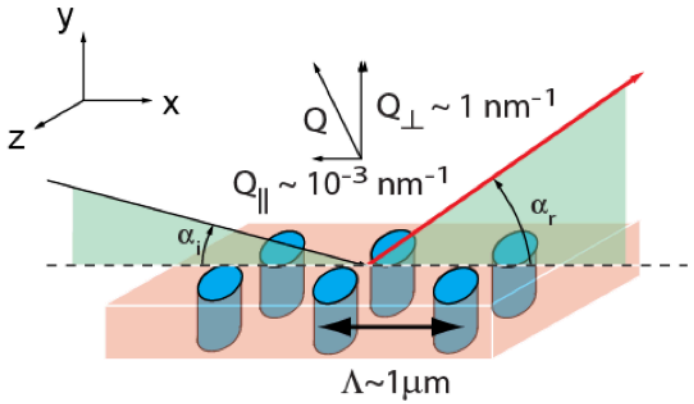
Reflectometry

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

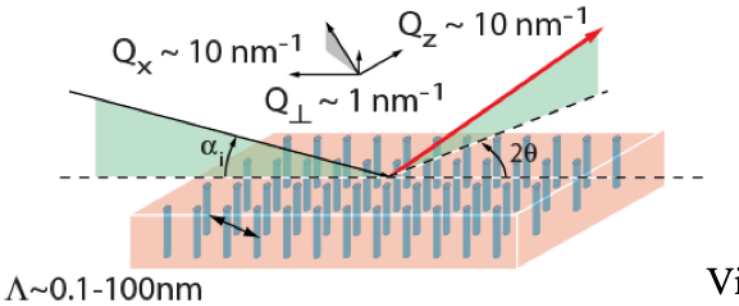
Various forms of small angle neutron reflection



Specular reflectometry
Depth profiles
(nuclear and/or magnetic)



Off-specular (diffuse) scattering
In-plane correlated roughness
Magnetic stripes
Phase separation (polymers)

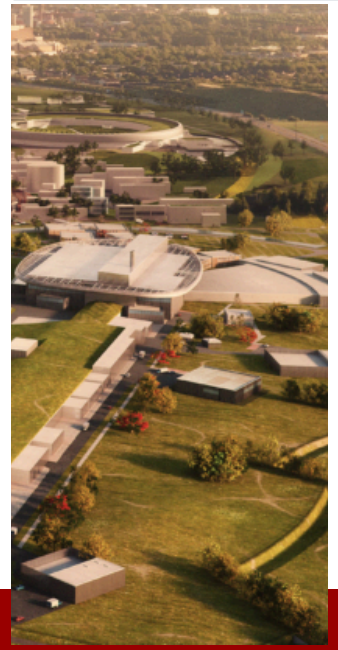


Glancing incidence diffraction
Ordering in liquid crystals
Atomic structures near surfaces
Interactions among nanodots

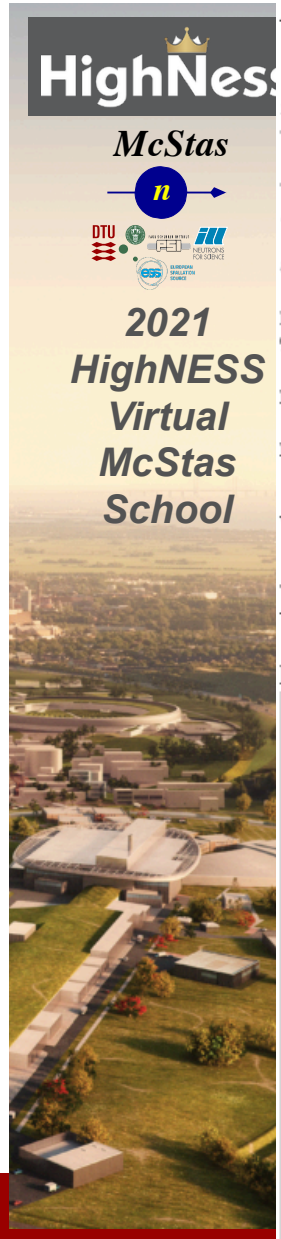
Viewgraph from M. R. Fitzsimmons

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.**

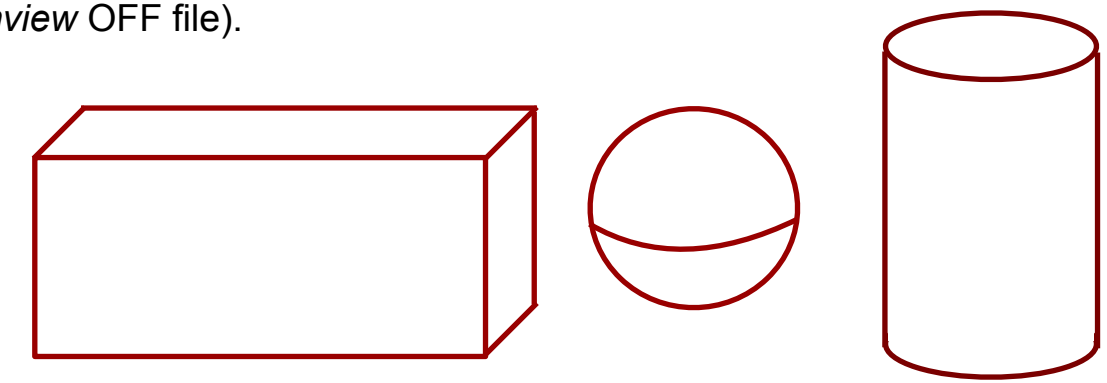
Input parameters

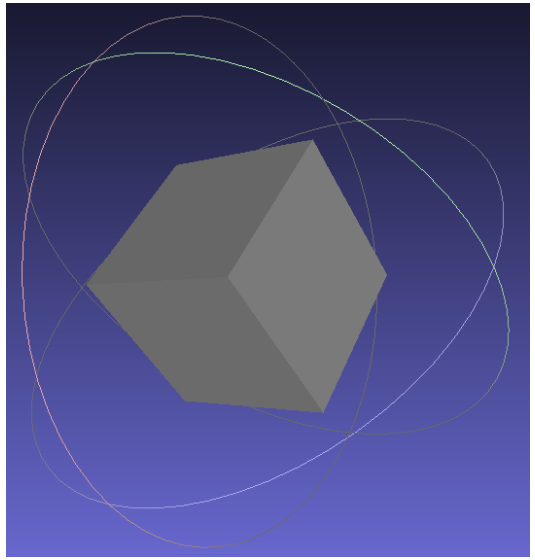
Parameters in **boldface** are required; the others are optional.

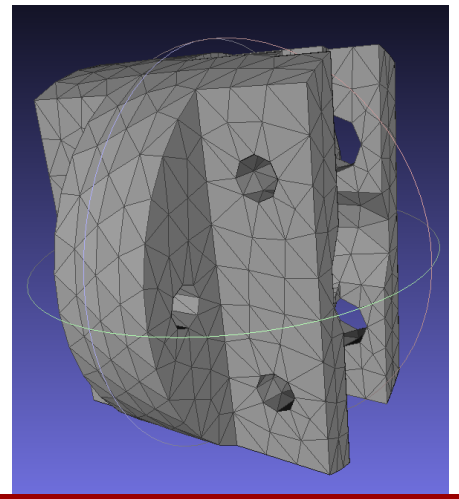
Name	Unit	Description	Default
sldPar	1	(Angstoms ^-2) Scattering length Density's of layers	{0.0
dPar	1	(Angstroms) Thicknesses of film layers	{20.0}
sigmaPar	1	(Angstroms) r.m.s roughnesses of the interfaces	{5.0
xwidth	m	Width of substrate	0.2
zlength	m	Length of substrate	0.2
nlayer	1	Number of film 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

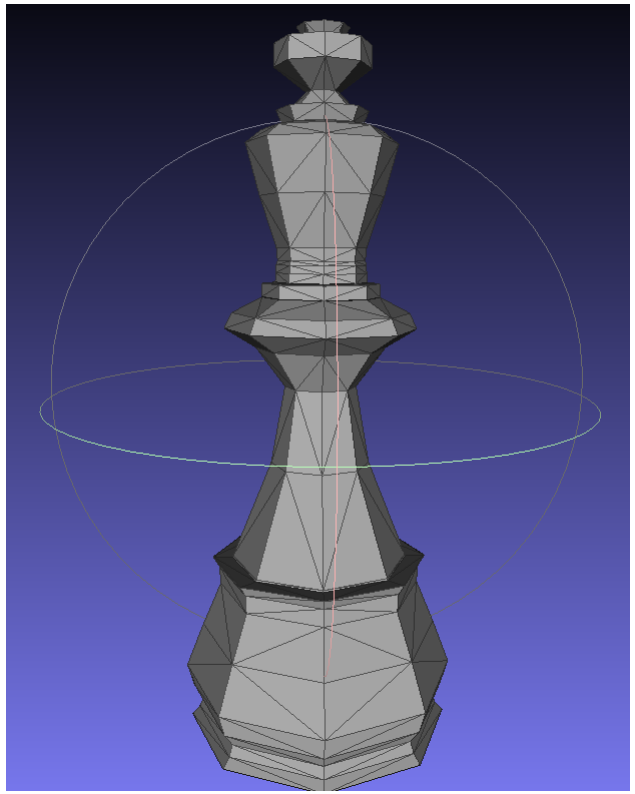
Absorption Imaging - simple shapes or OFF's of single-phase material blocks

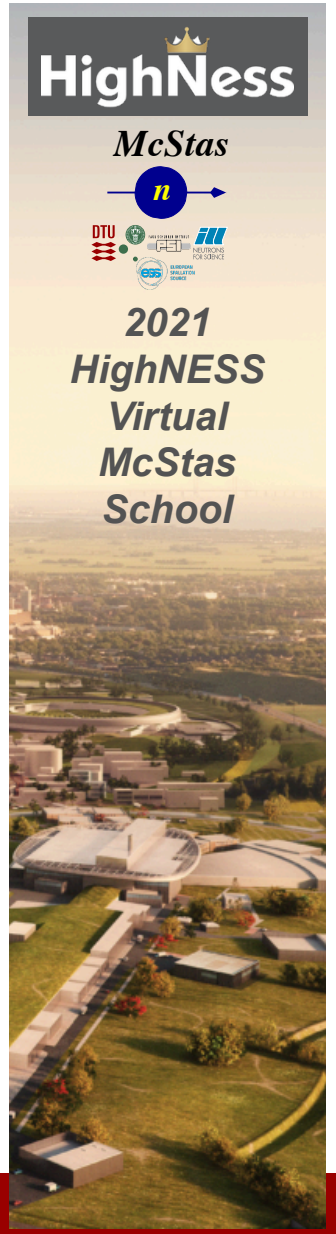
An additional complex geometry enables to use any point set to describe the material volume (*geomview* OFF file).





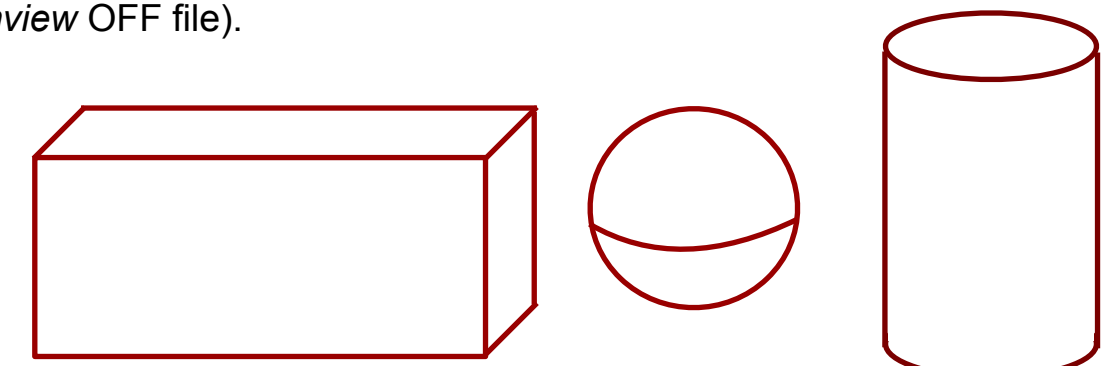


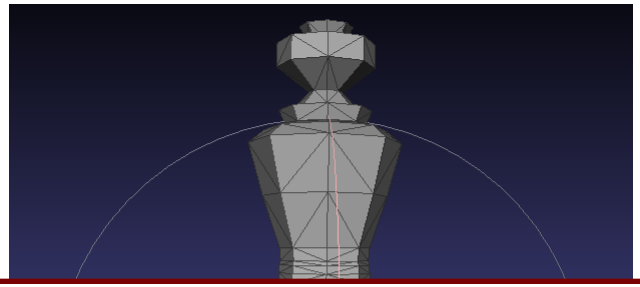


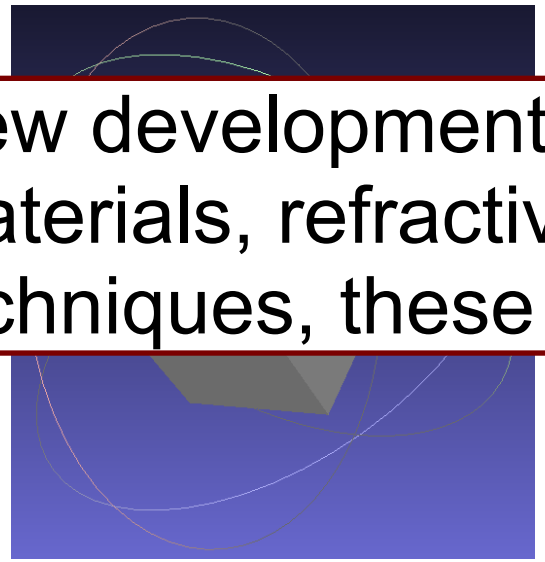


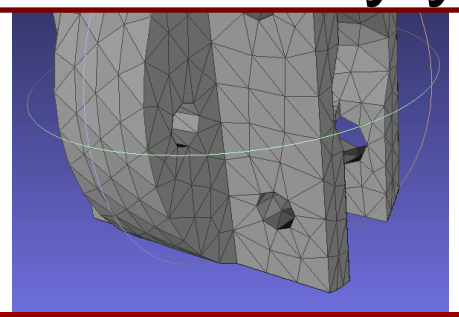
Absorption Imaging - simple shapes or OFF's of single-phase material blocks

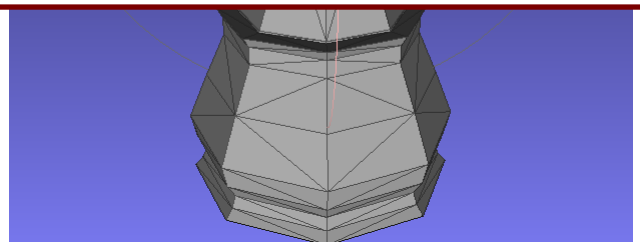
An additional complex geometry enables to use any point set to describe the material volume (*geomview* OFF file).



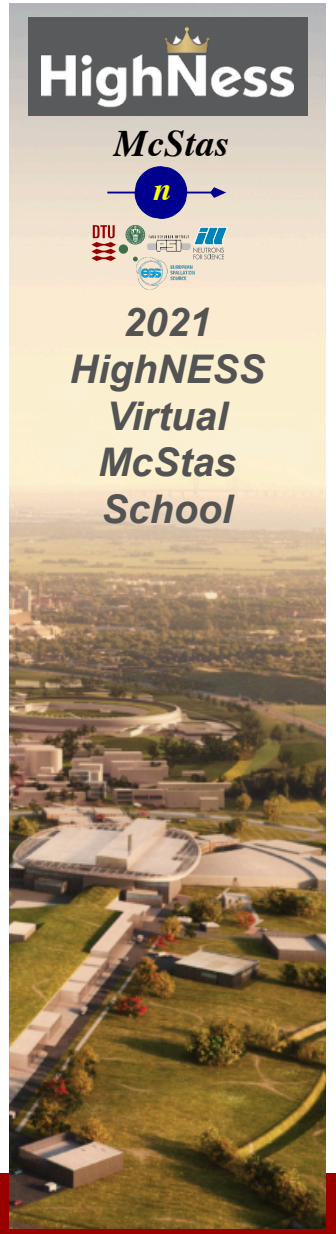


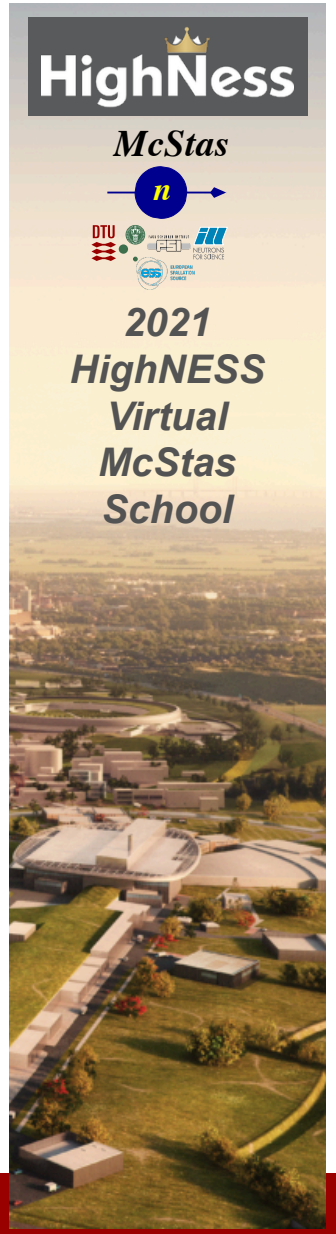






New developments are in the pipe e.g. for multi-phase materials, refractive effects, phase-contrast imaging techniques, these are not ready yet.

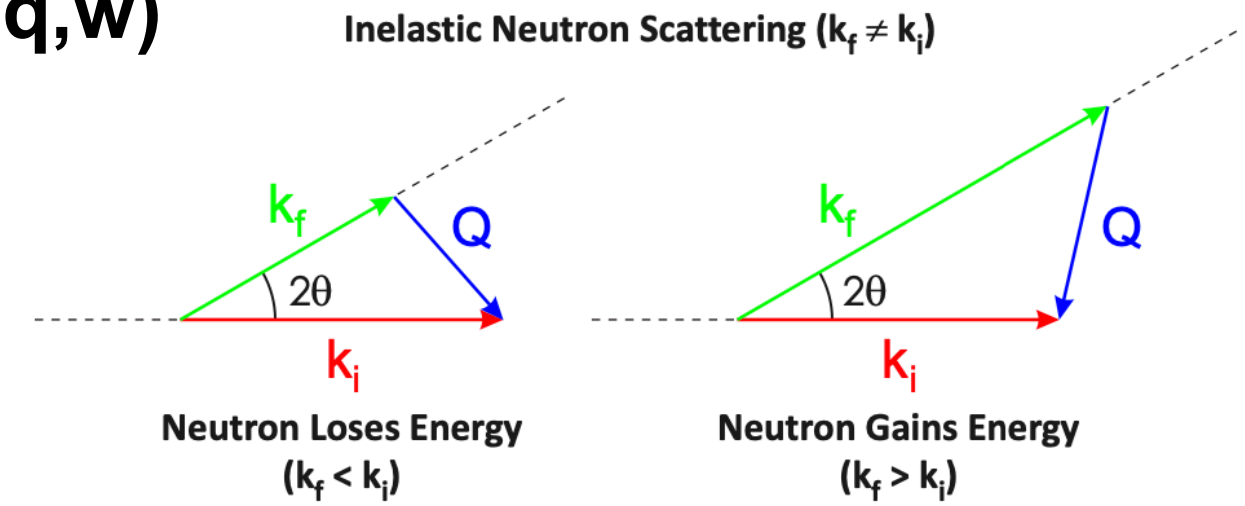




Inelastic scattering S(q,w)

- 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

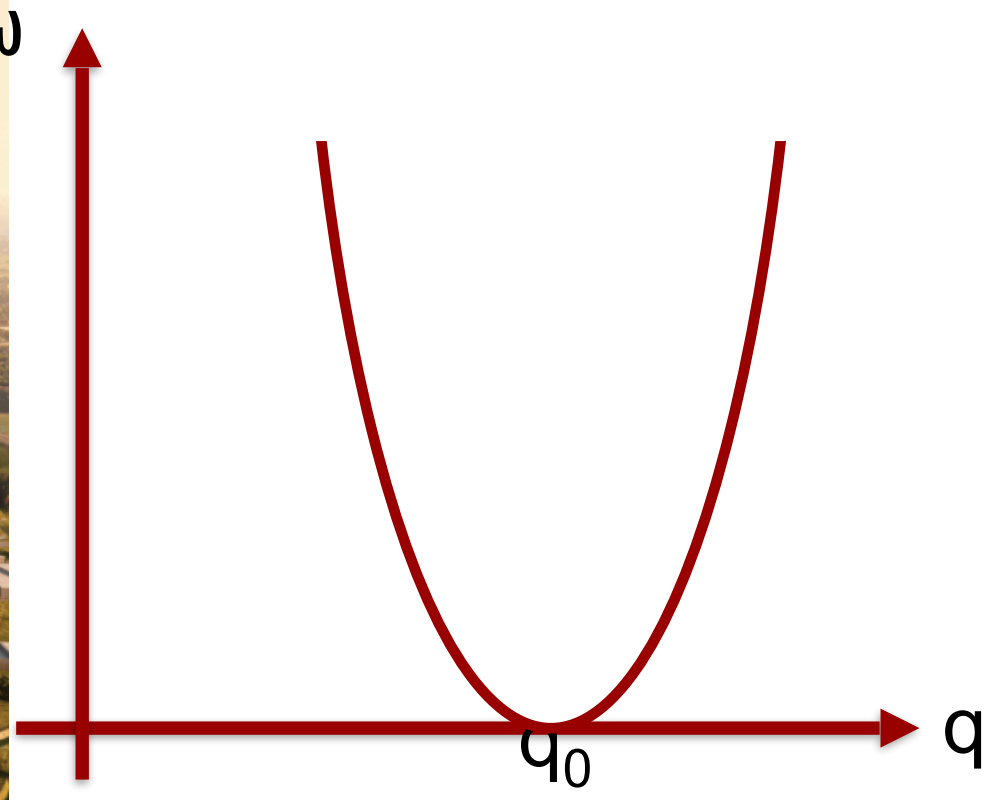
2	Tunelling_sample *McStas team / Kim Lefmann*	Idem 1, plus tunneling peaks and QE broadening	Quasi-elastic scattering, backscattering	✅	✅	❌	❌/✅ (Quasielastic broadening + tunnel peaks)	(✅ analytic approach)	✅
10	Phonon_simple *McStas team / Kim Lefmann*	Single-branch acoustic phonon in FCC lattice	Inelastic 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)	✅	

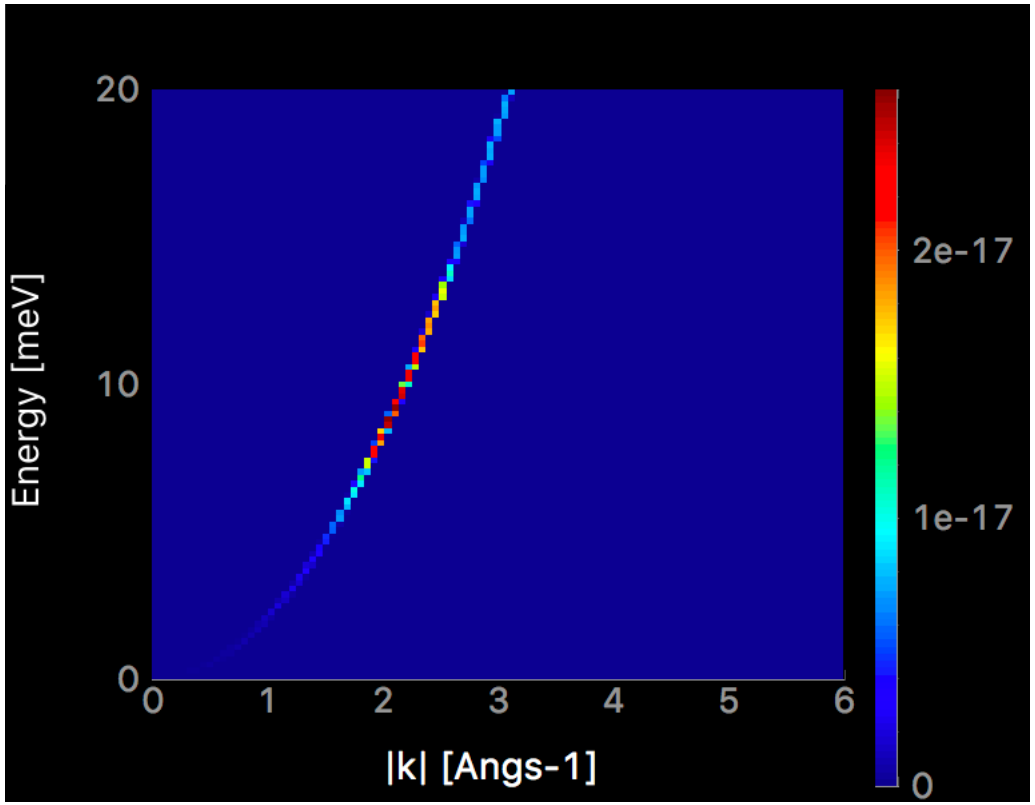
Example component: Phonon_simple

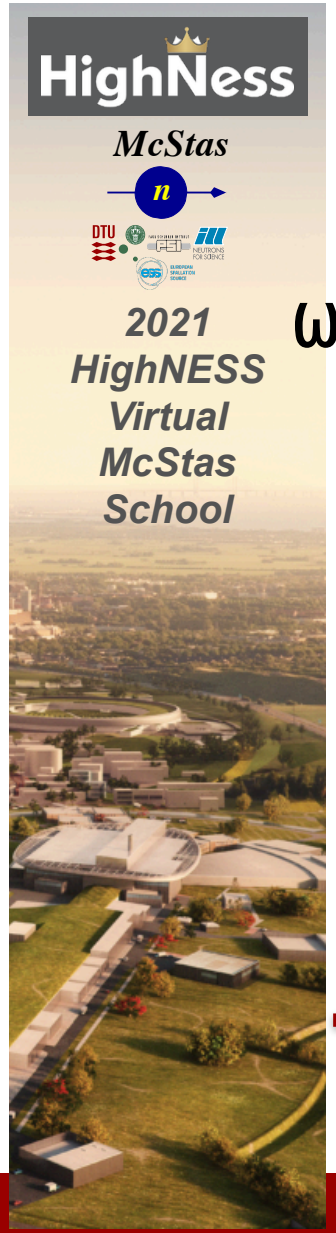
- One isotropic acoustic phonon branch in all Brillouin zones on FCC Bravais single crystal

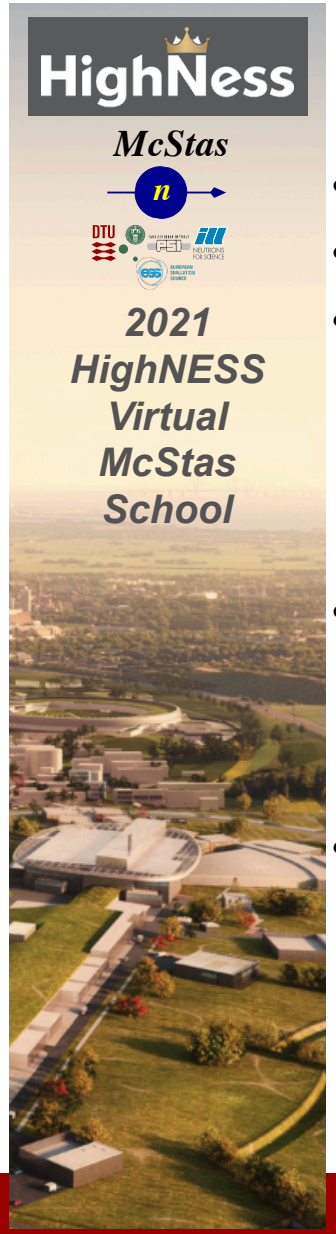
  Dispersion $d_1(\mathbf{q}) = c_1/a\sqrt{z - s_q}$

- Dispersion relation, theory and mcstas







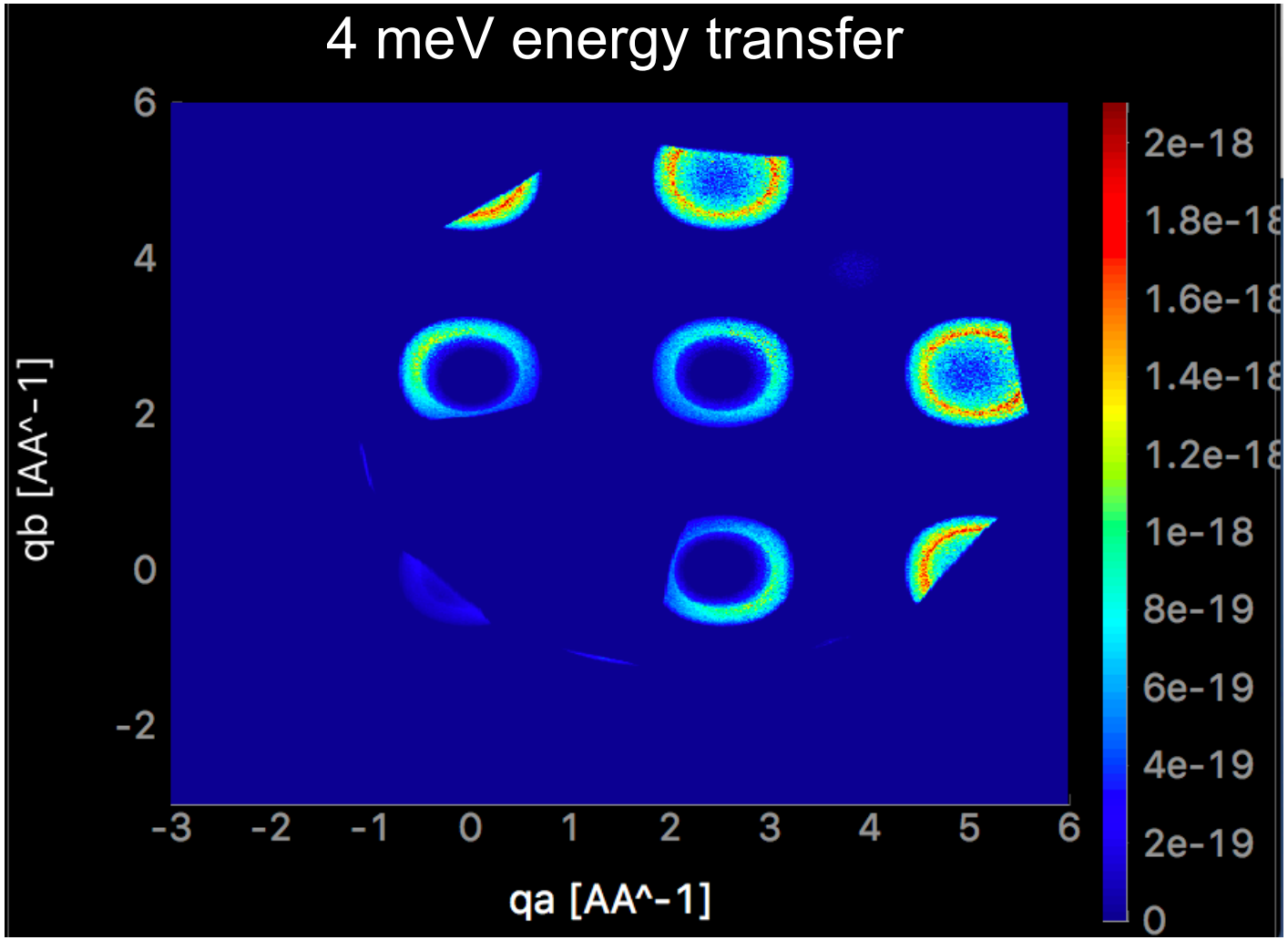


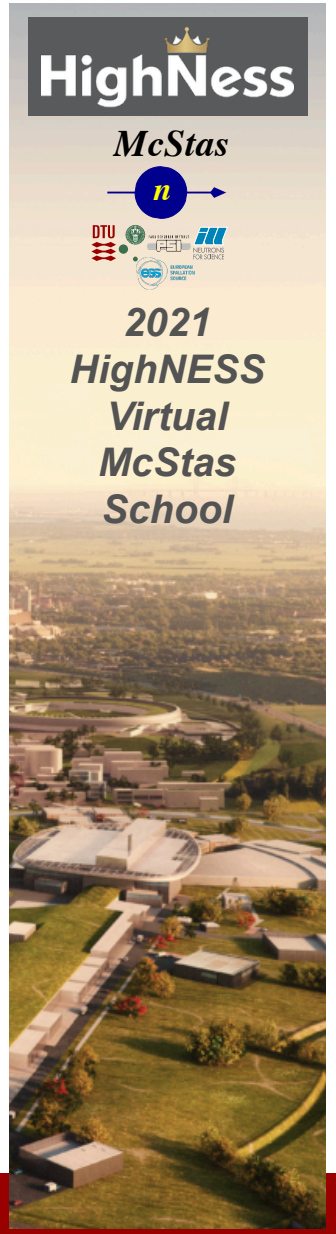
Example component: Phonon_simple

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

- Magnon_fcc is conceptually very similar

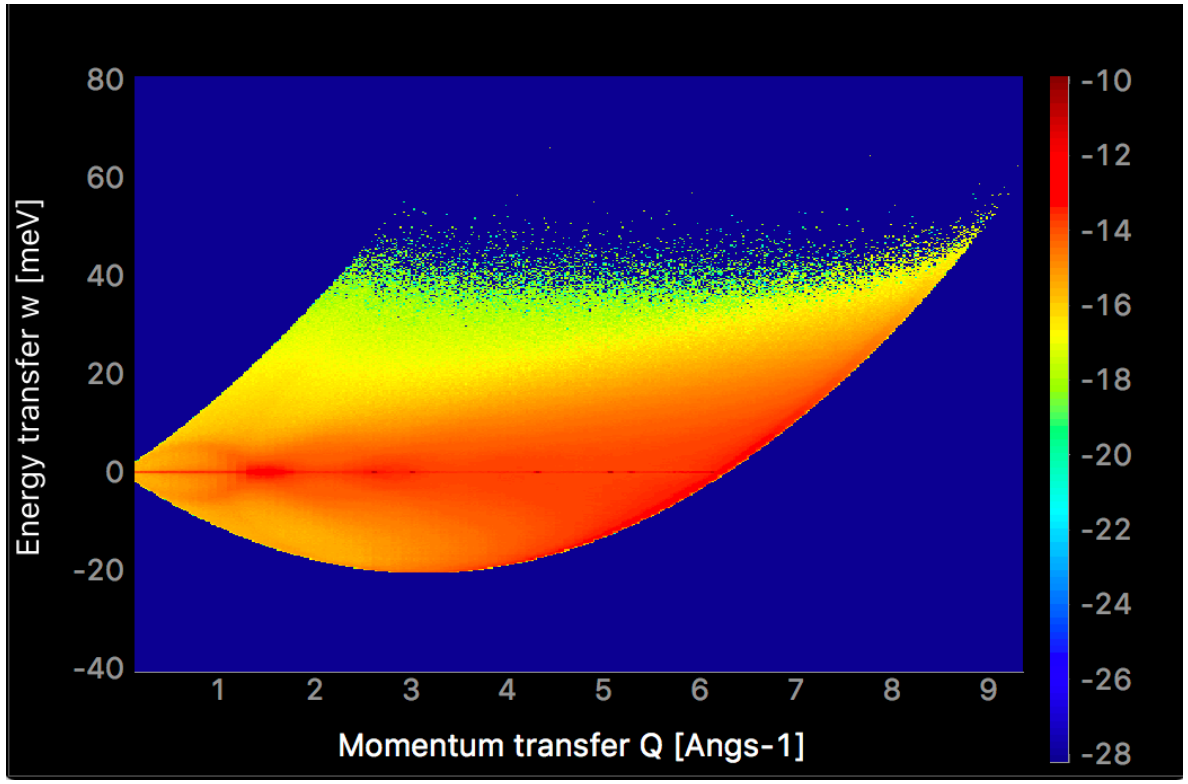
- Describes coherent “closed-form” inelastic scattering, generalisations foreseen, different lattice-dep. Other dispersion shapes?

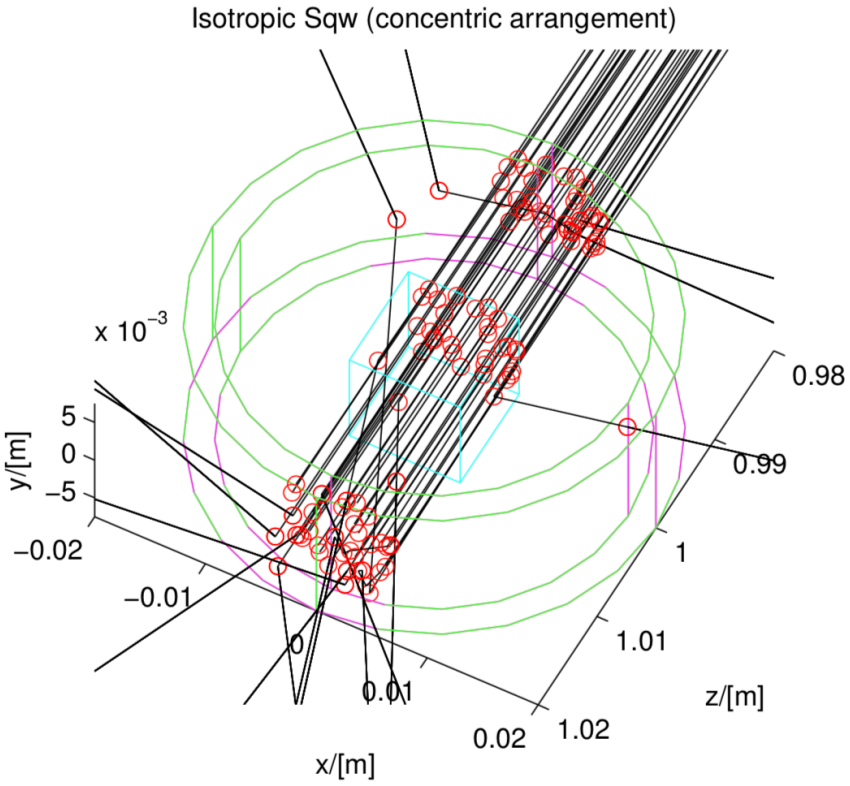


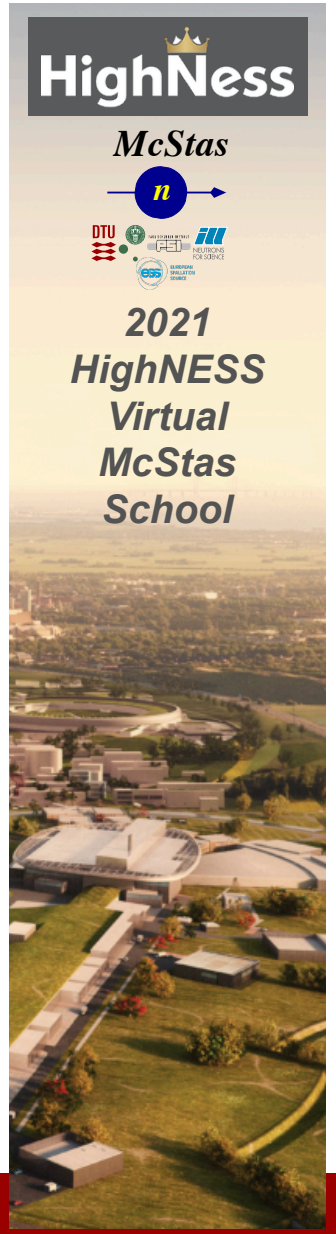


Example component: Isotropic_sqw

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





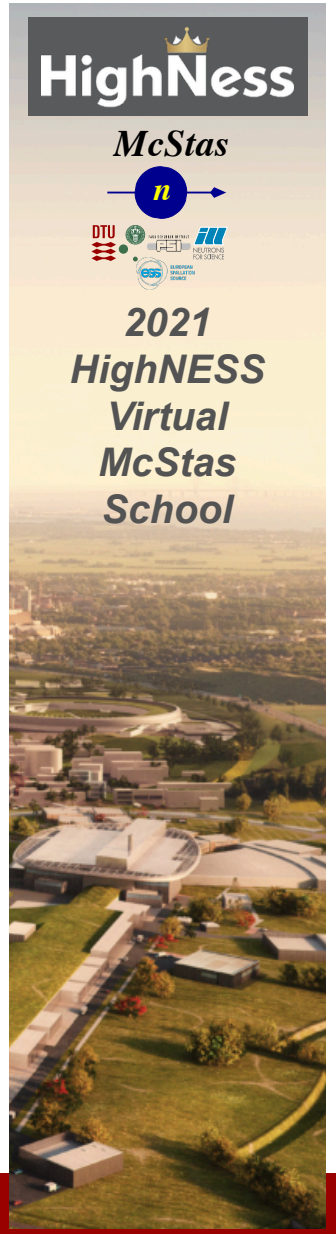


Example component

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

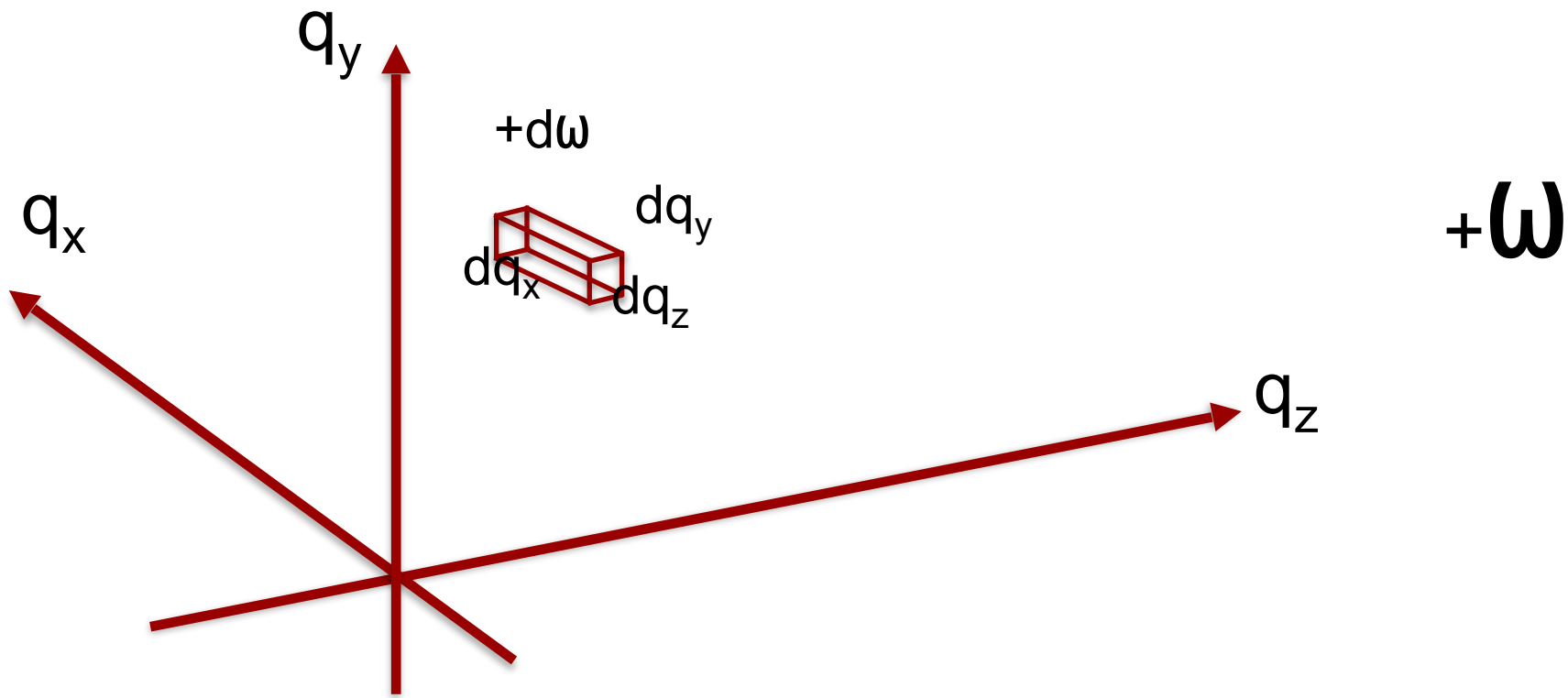
- BIG tables, lots of memory, close to impossible to use for anything but “locally” in reciprocal space, i.e. in TAS settings

- We are looking for good alternatives



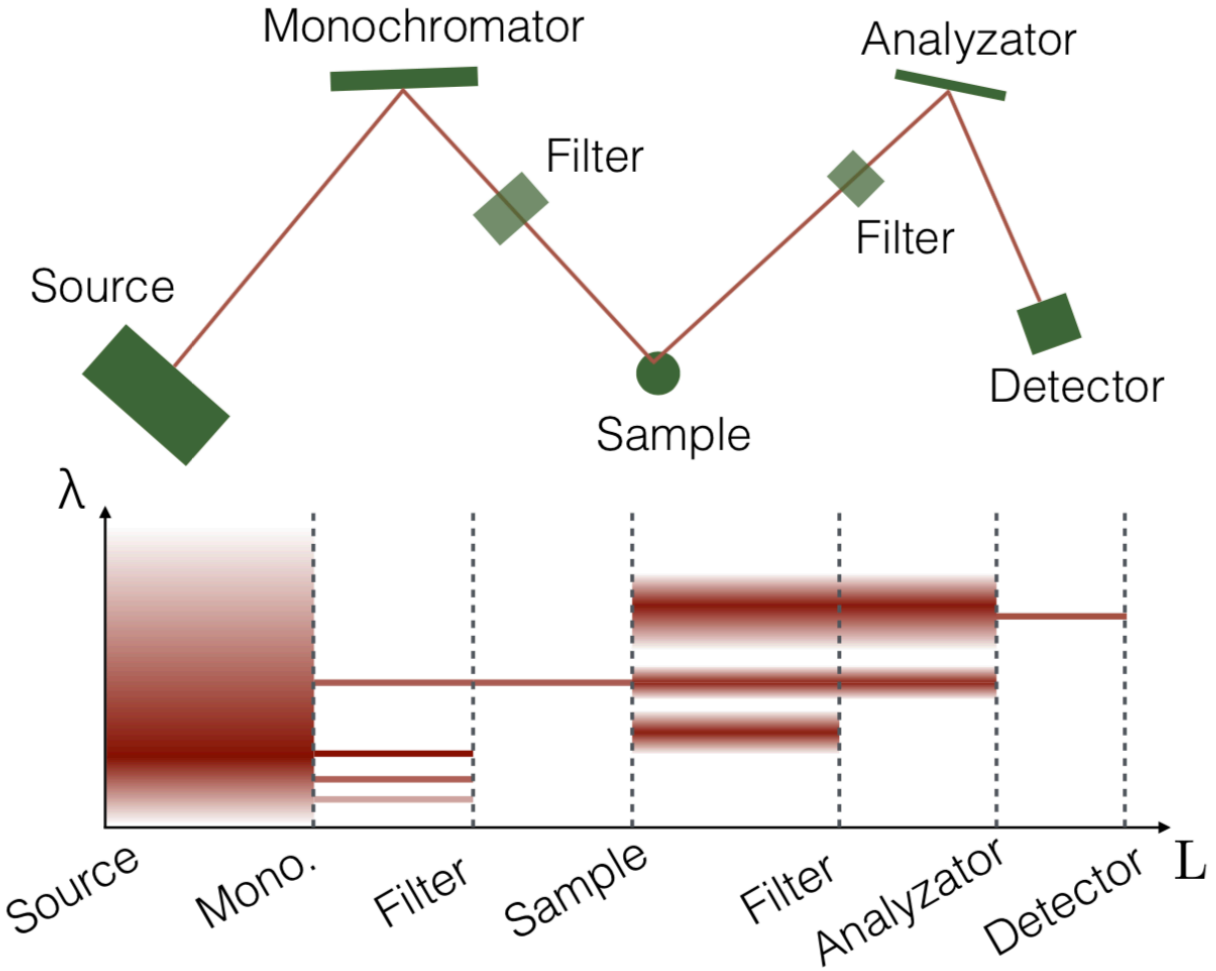
Inelastic scattering in McStas

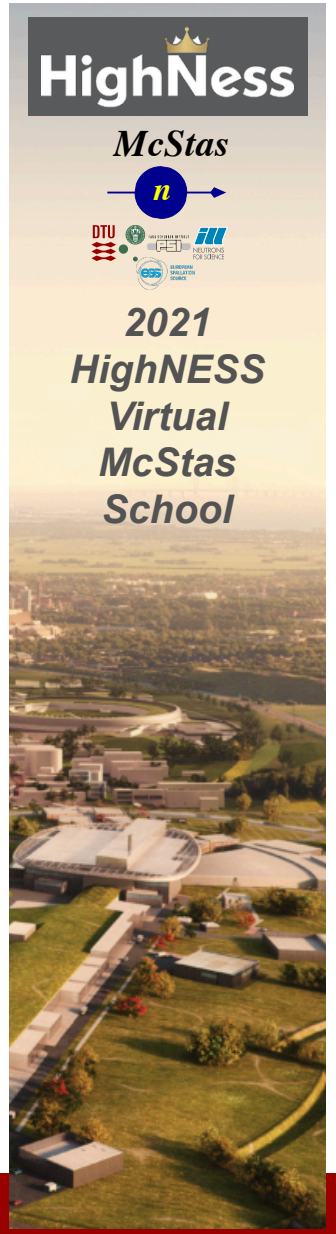
- Monte carlo sampling issues
- Need to sum over large amount of possible final states to find cross section
- Need large amount of rays to sample all the options



TAS

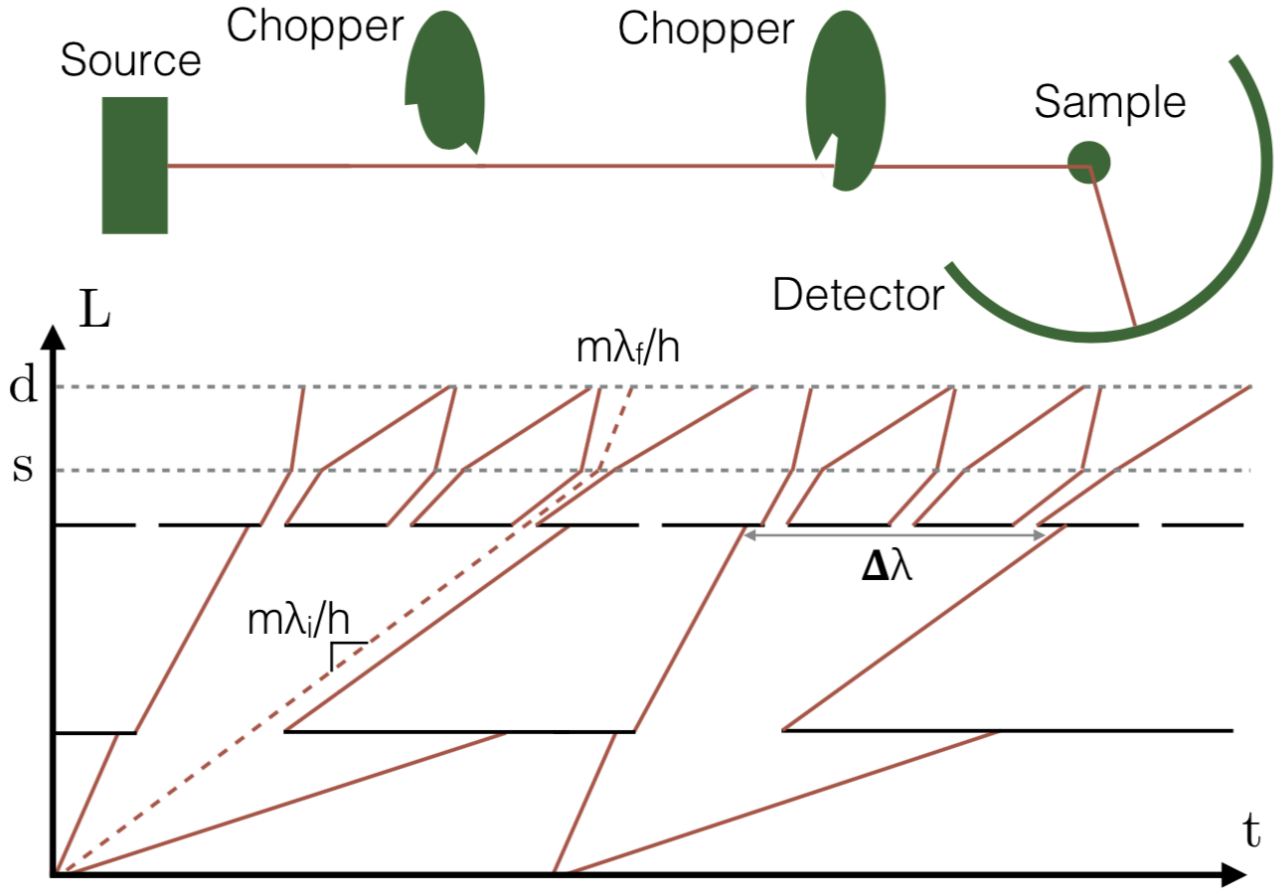
- Only a small fraction of neutrons arrive, most are simulated in vain

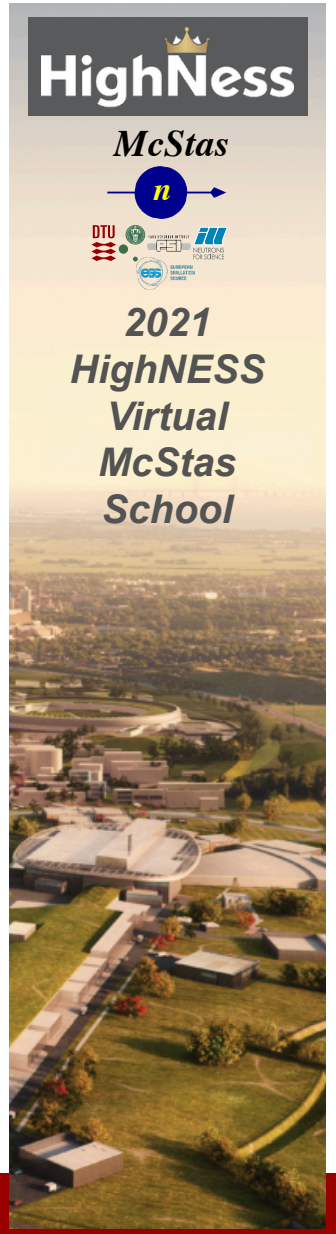


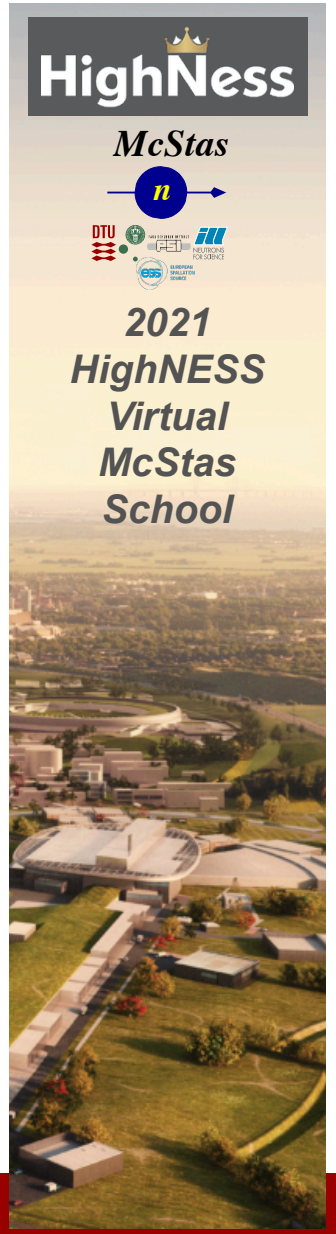


Chopper spectrometers

- 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”
- Imaging:
  - Single-phase “blocks” of material, new developments are in the pipe
- 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)