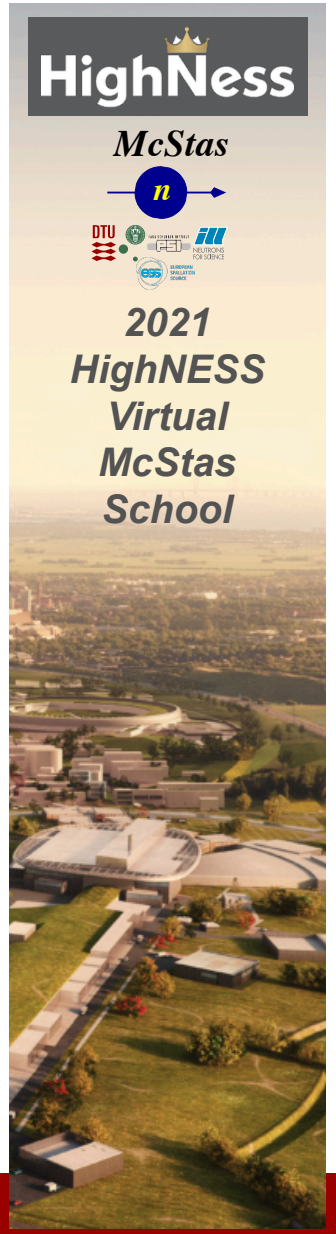
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Peter Willendrup

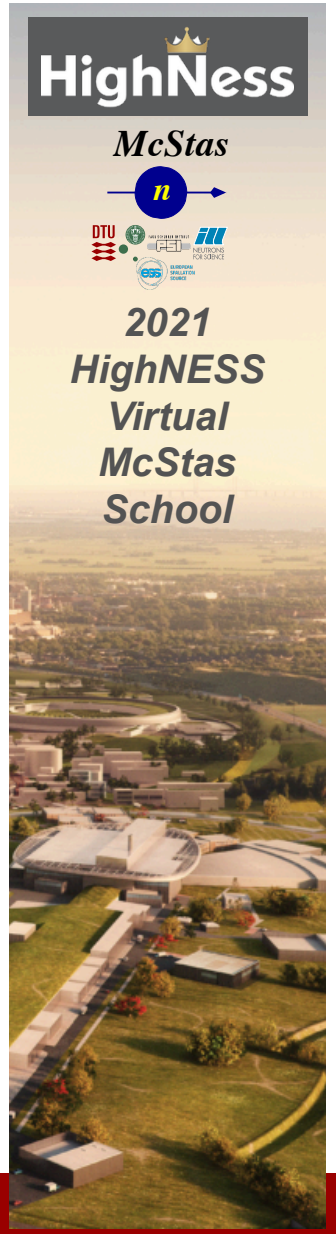
Further samples…

Slides adapted from Mads Bertelsen, ESS DMSC



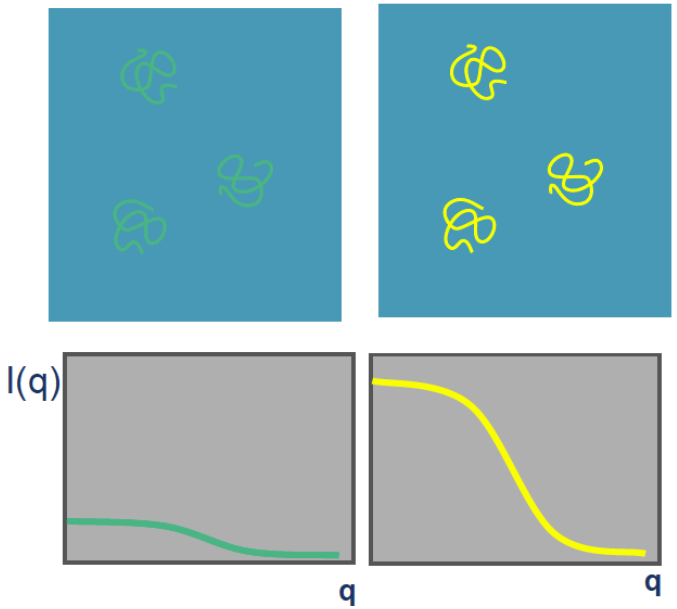
Further samples in McStas

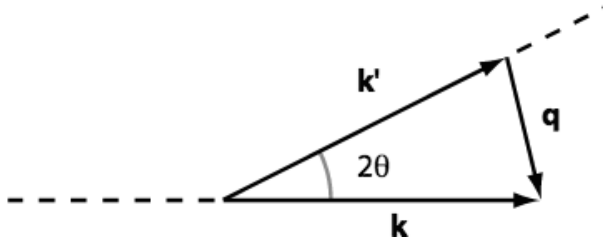
- Models for SANS and reflectometry
- Inelastic scattering, examples:
  - Phonon_simple
  - Isotropic_sqw
- McStas performance, TAS / Chopper

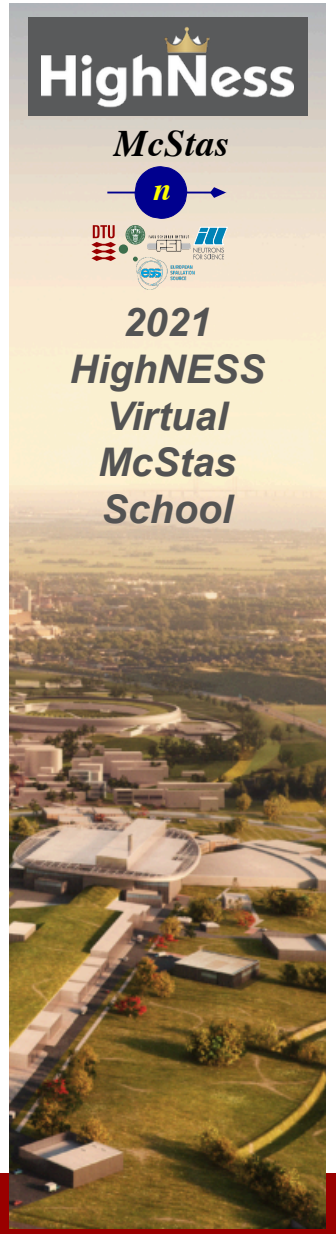


Small angle scattering SANS

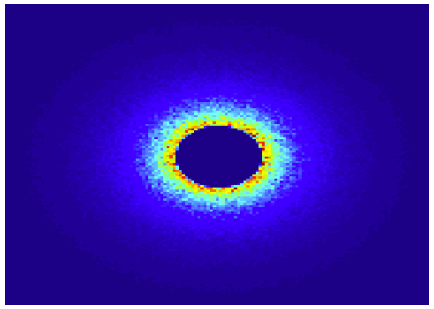
- SANS method can be used for many types of material
- Often: Molecule + Liquid (buffer solution)
- Isotropic scattering







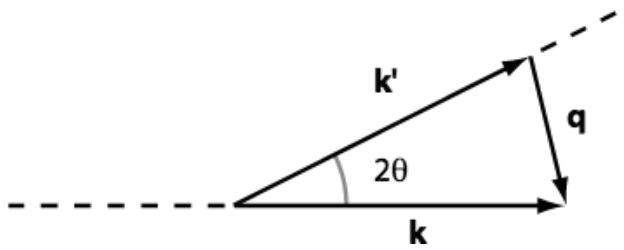
SANS



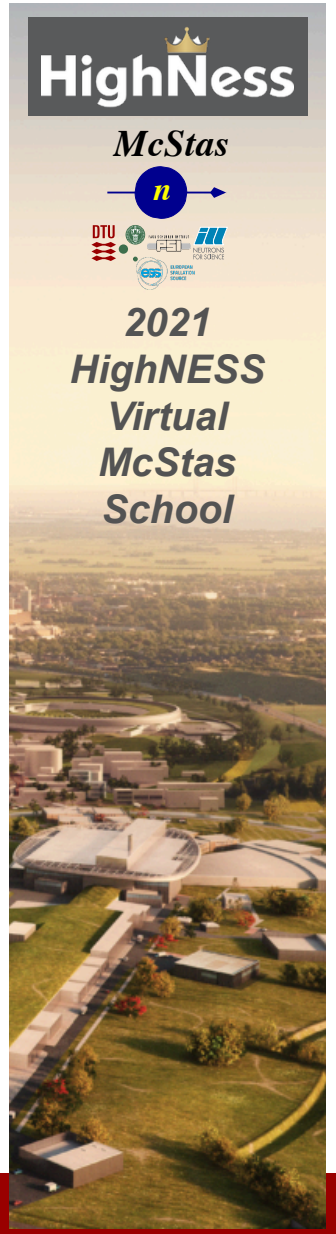
$$q = \frac{4\pi}{\lambda}\sin(\theta)$$

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.



McStas has a suite of SANS-models:

Try ellipsoidal and

cylindrical particles

-or-

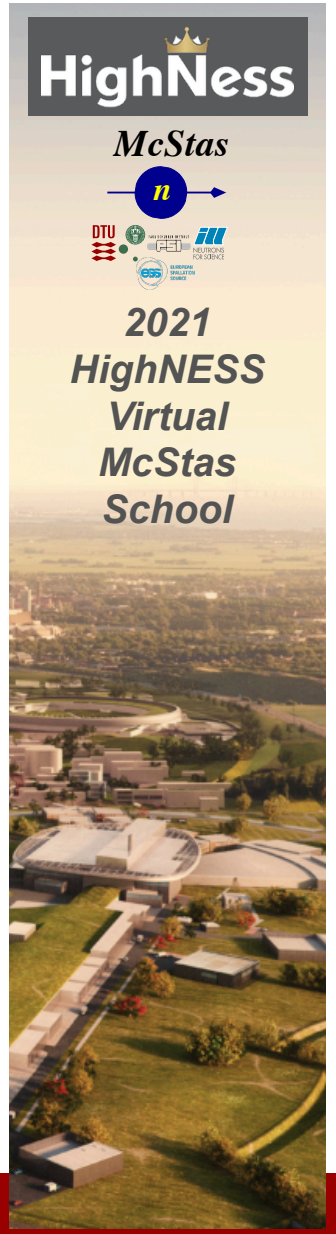
Elliptic cylinders

Go for Nanodiscs and Liposomes

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

Also – SASmodels from SASview



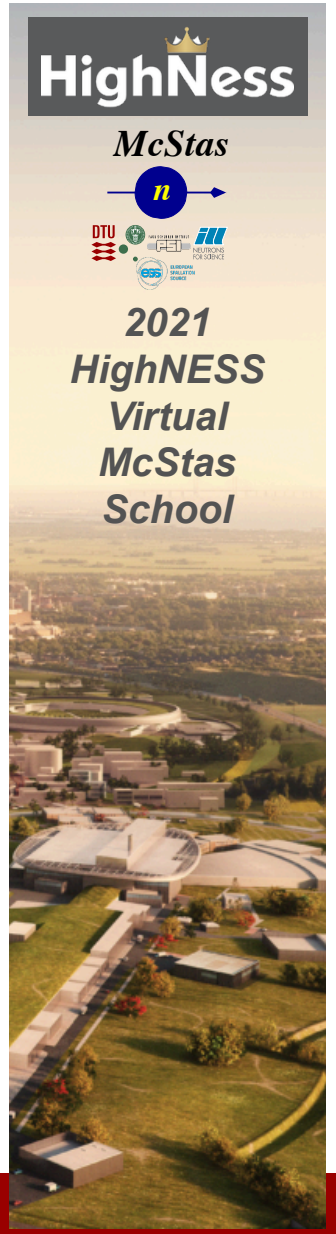
SANS spheres

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

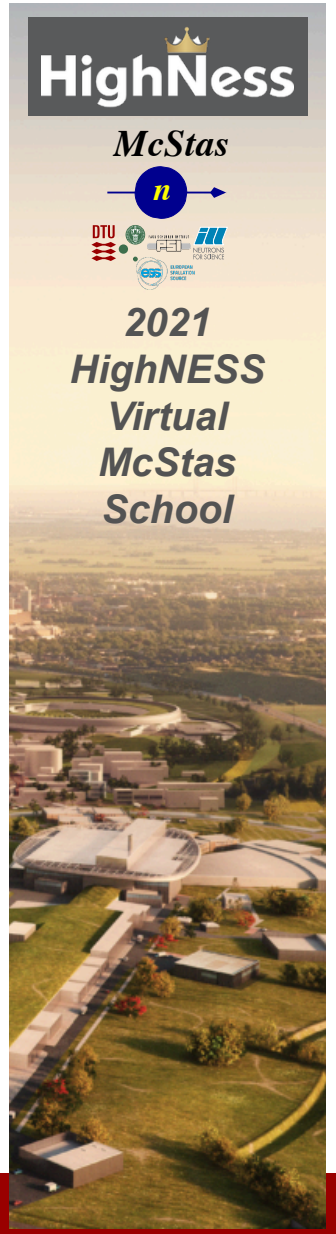


SasView_models

Input parameters

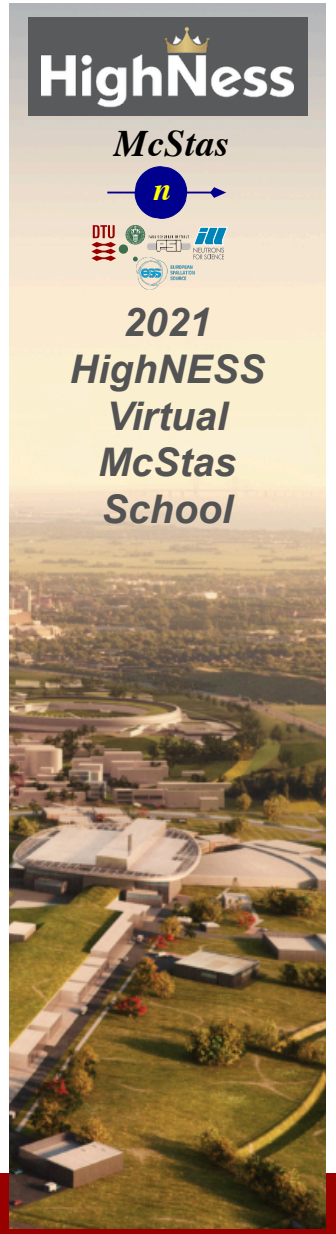
Parameters in **boldface** are required; the others are optional.

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)



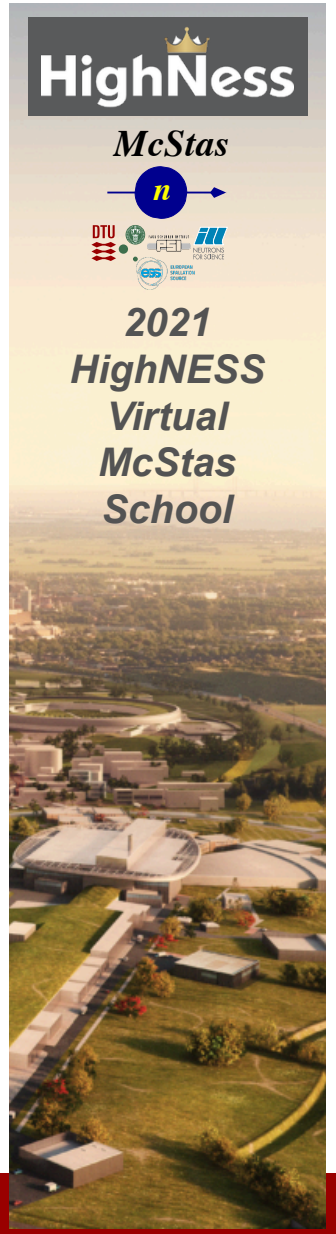
Inelastic scattering S(q,w)

- partial differential cross section
- Scattering function

- Phonons, Spin waves, …

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

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



Popular component: Phonon_simple

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

$$\frac{d^2\sigma'}{d\Omega dE_\mathrm{f}} = b^2\frac{k_\mathrm{f}}{k_\mathrm{i}}\frac{(2\pi)^3}{V_0}\frac{1}{2M}\exp(-2W)$$
$$\times \sum_{\tau,q,p}\frac{(\boldsymbol{\kappa}\cdot\mathbf{e}_{q,p})^2}{\omega_{q,p}}\left\langle n_{q,p}+\frac{1}{2}\mp\frac{1}{2}\right\rangle\delta(\omega\pm\omega_{q,p})\delta(\kappa\pm\mathbf{q}-\tau)$$

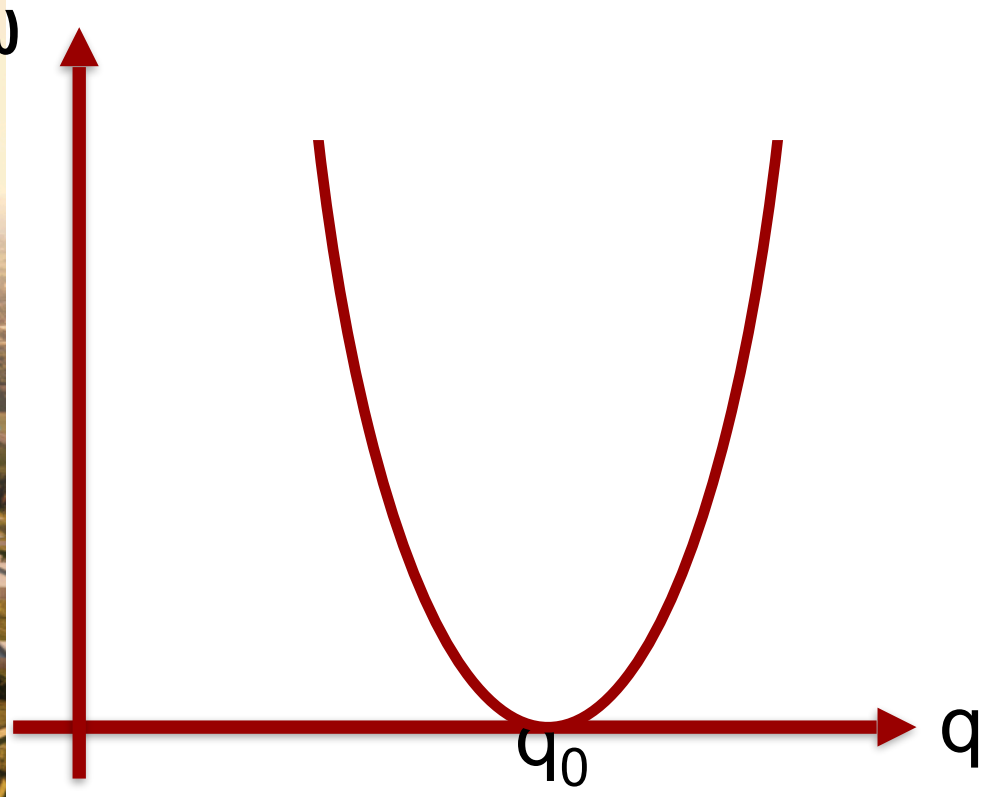
Dispersion $d_1(\mathbf{q}) = c_1/a\sqrt{z-s_q}$

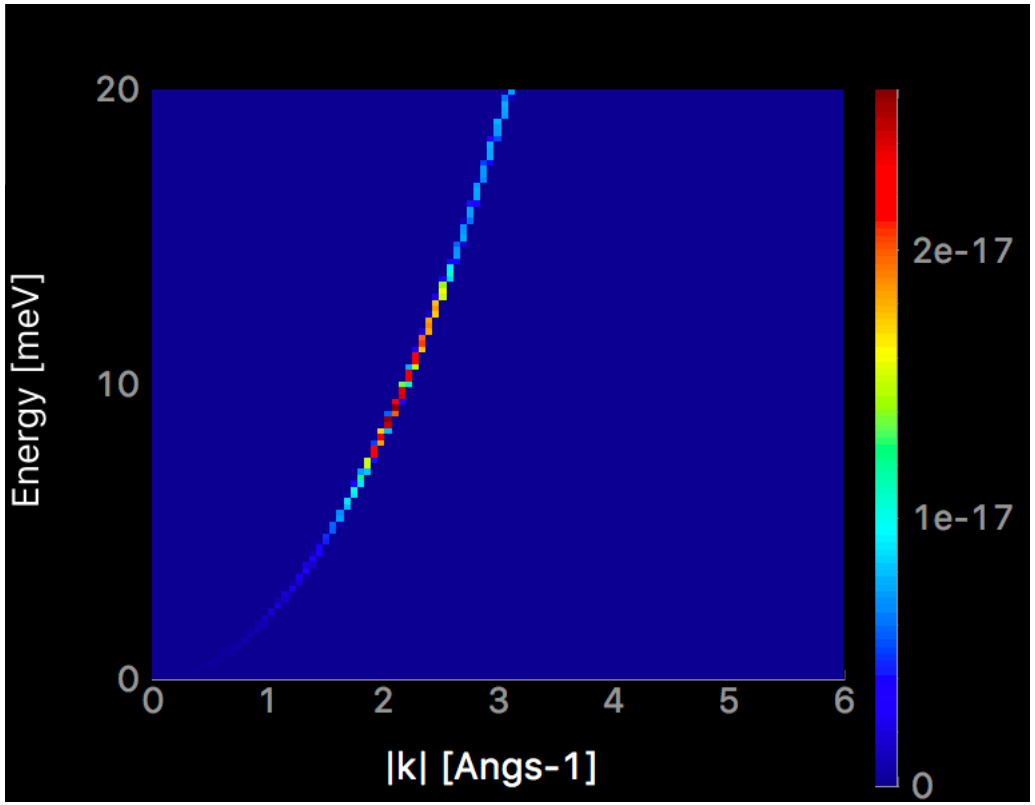
For FCC Bravis $z = 12 \quad s_q = \sum_{\mathrm{nn}}\cos(\mathbf{q}\cdot\mathbf{r}_{\mathrm{nn}})$

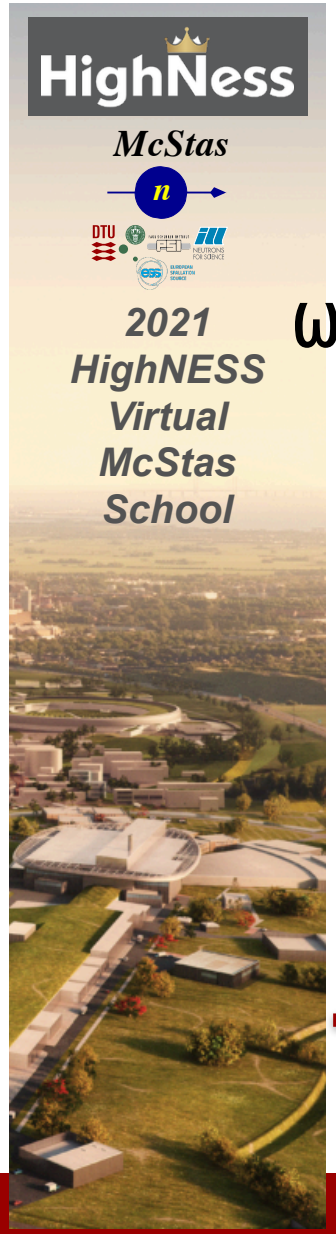
- M - Atomic mass
- b – scattering length
- *n* – bose factor
- a – fcc lattice spacing
- c - speed of sound
- $\boldsymbol{\kappa}$ – measured q vector
- **q** – Phonon scattering vector

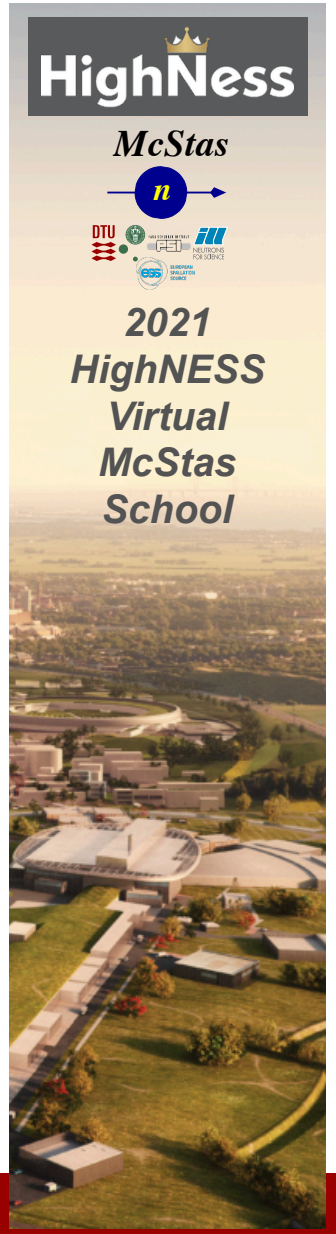
Popu _simple

- Dispers



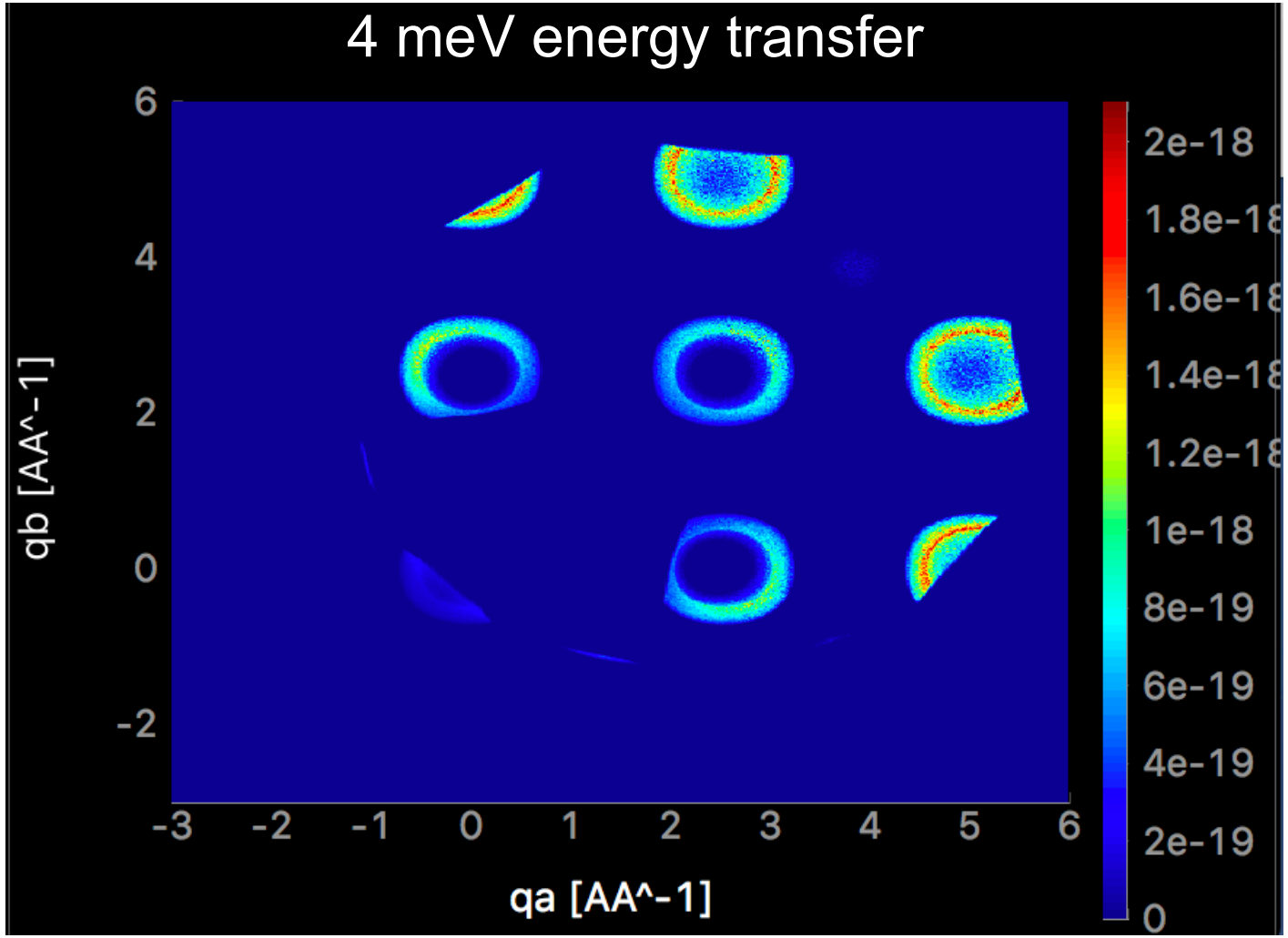


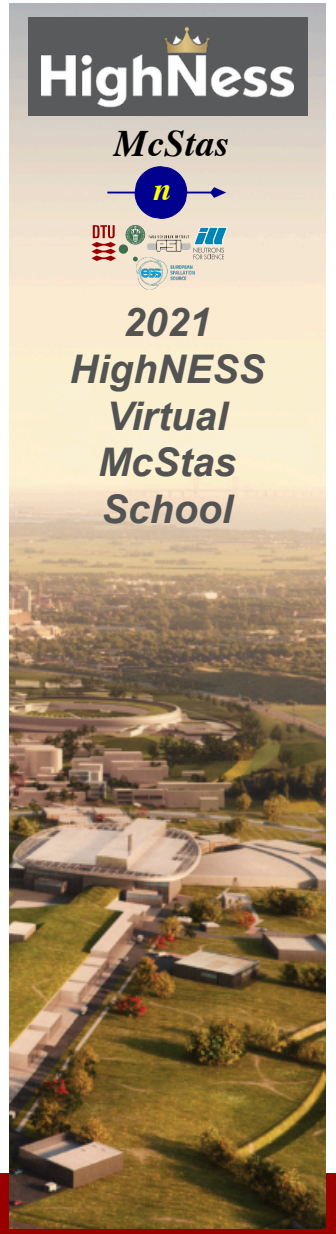




Popular component: Phonon_simple

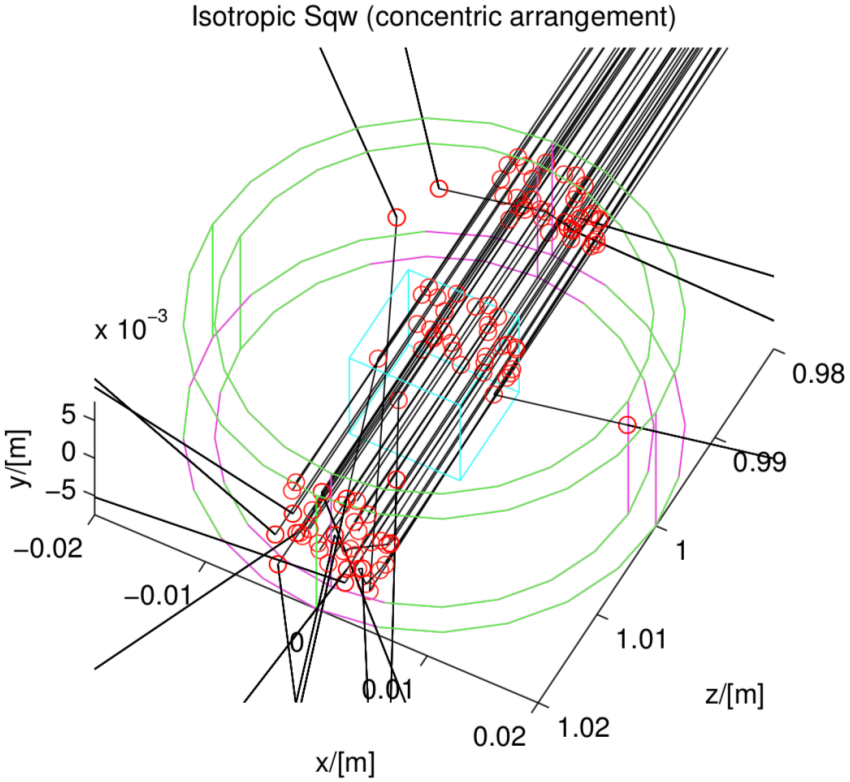
- Example of the output

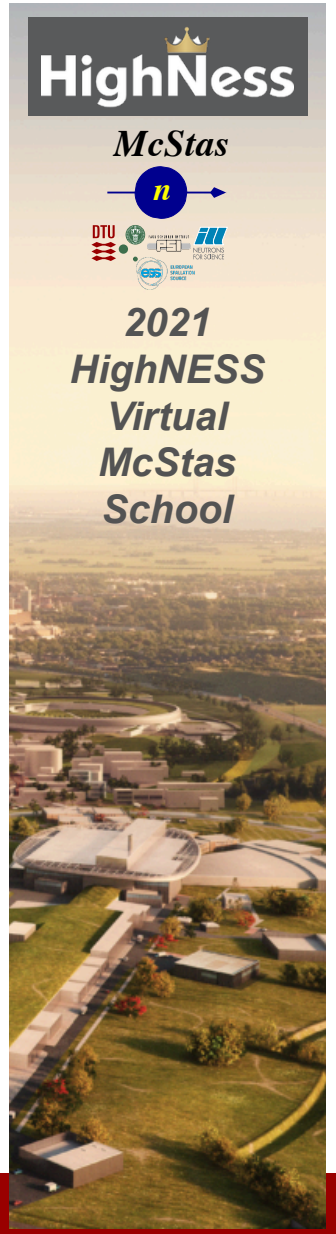




Popular component: Isotropic_sqw

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





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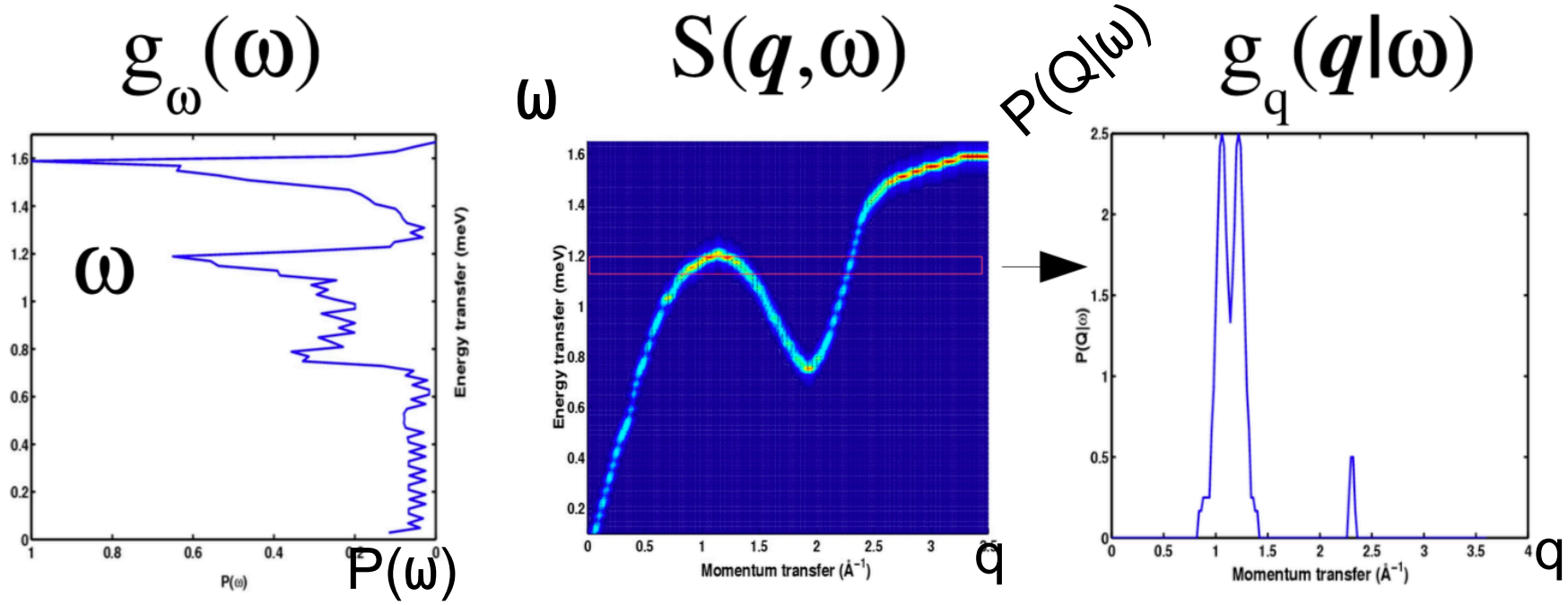
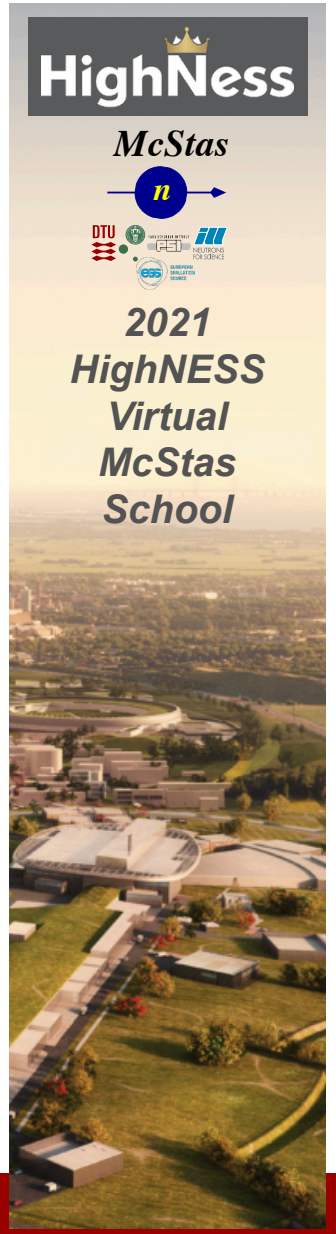
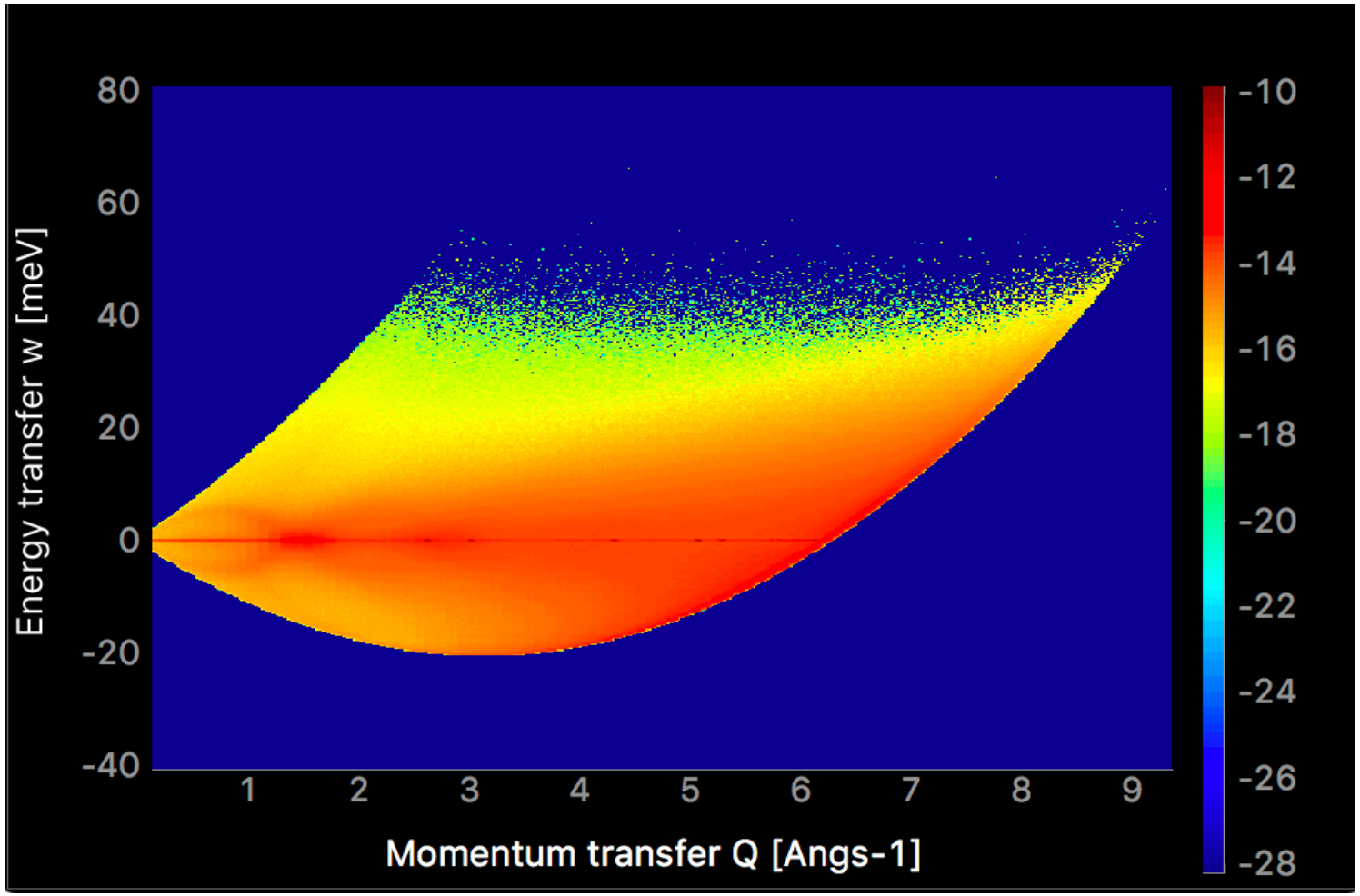
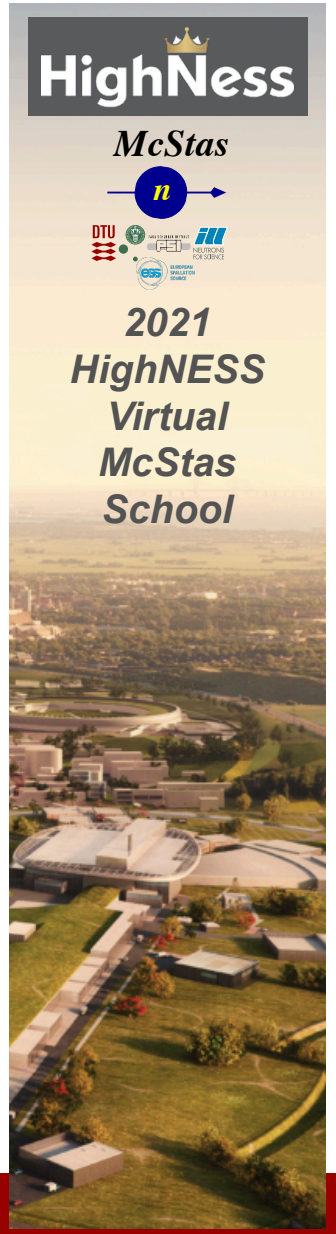




Popular component: Isotropic_sqw

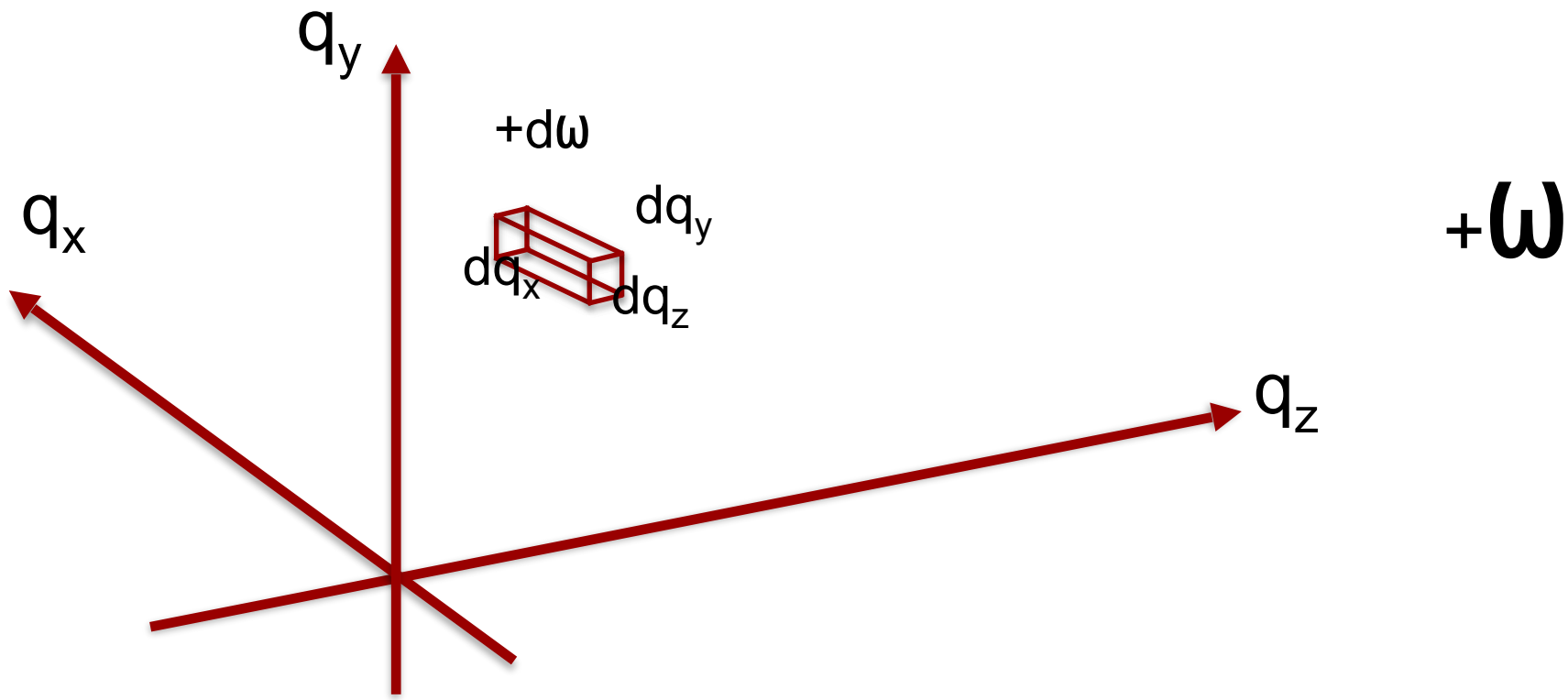
- Rb liquid in time of flight
- Coherent and incoherent

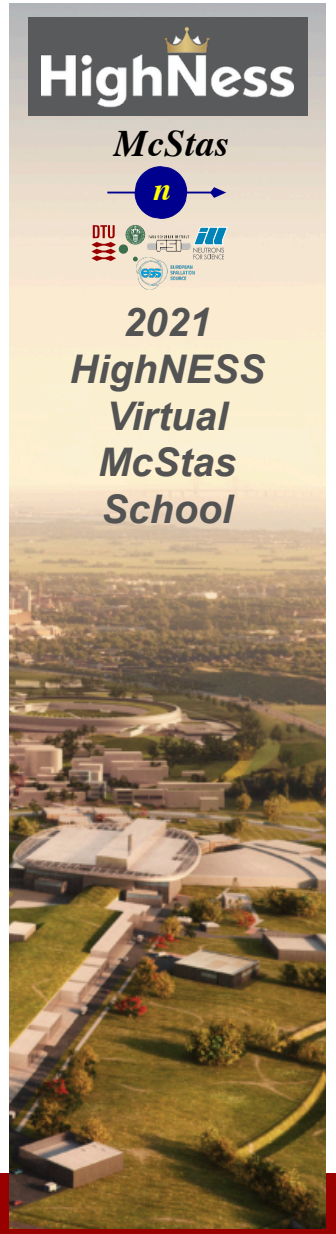




Inelastic scattering in McStas

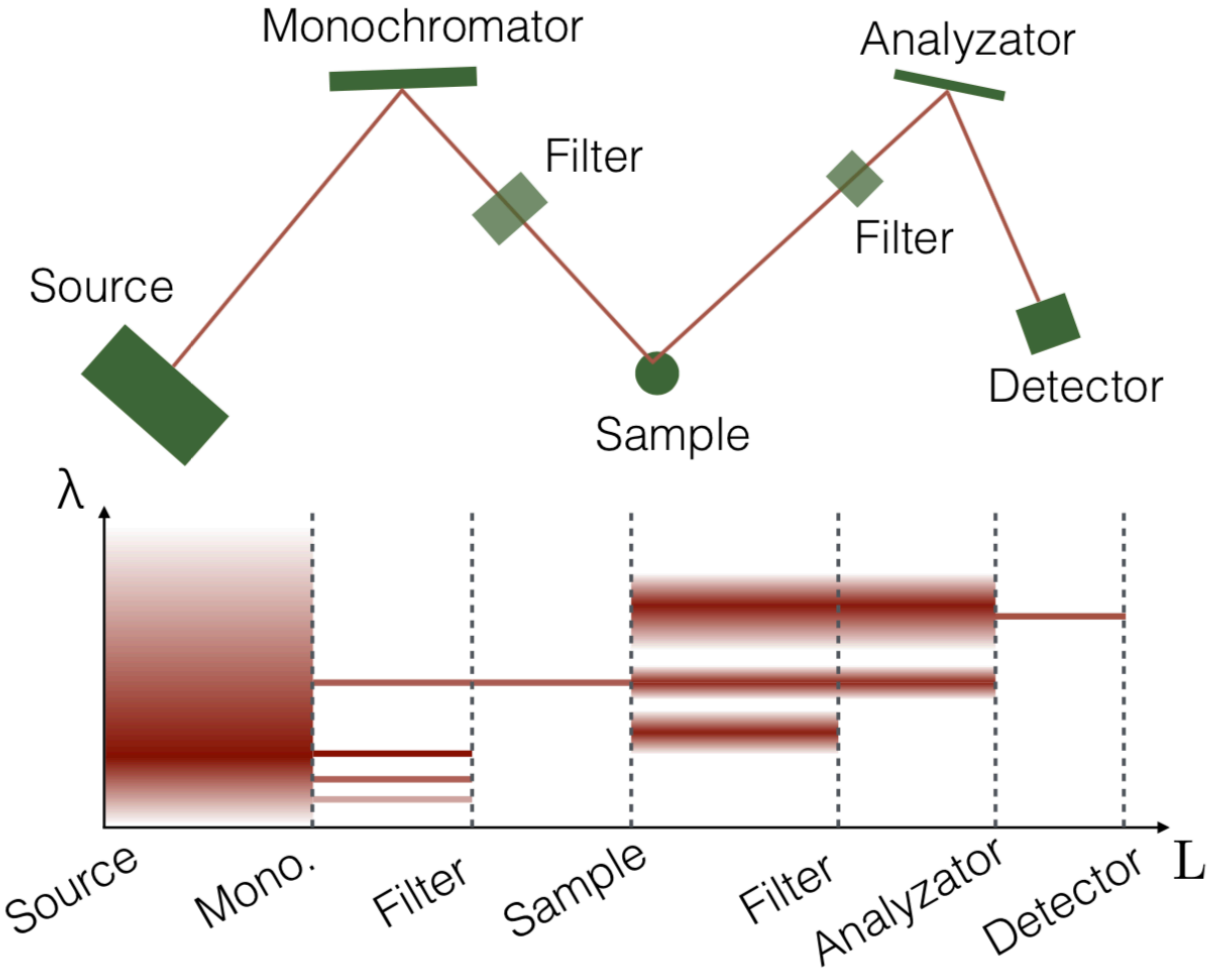
- Monte carlo sampling issues
- Need to sum over large amount of possible final states to find cross section
- Need large amount of rays to sample all the options

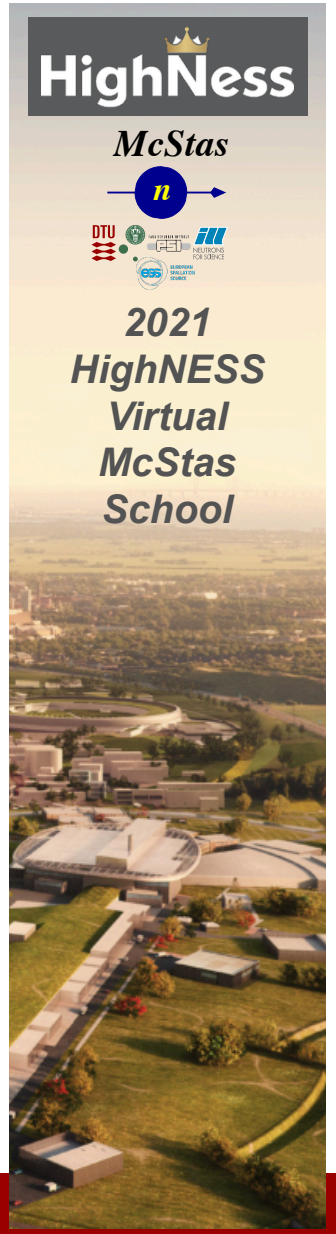




TAS

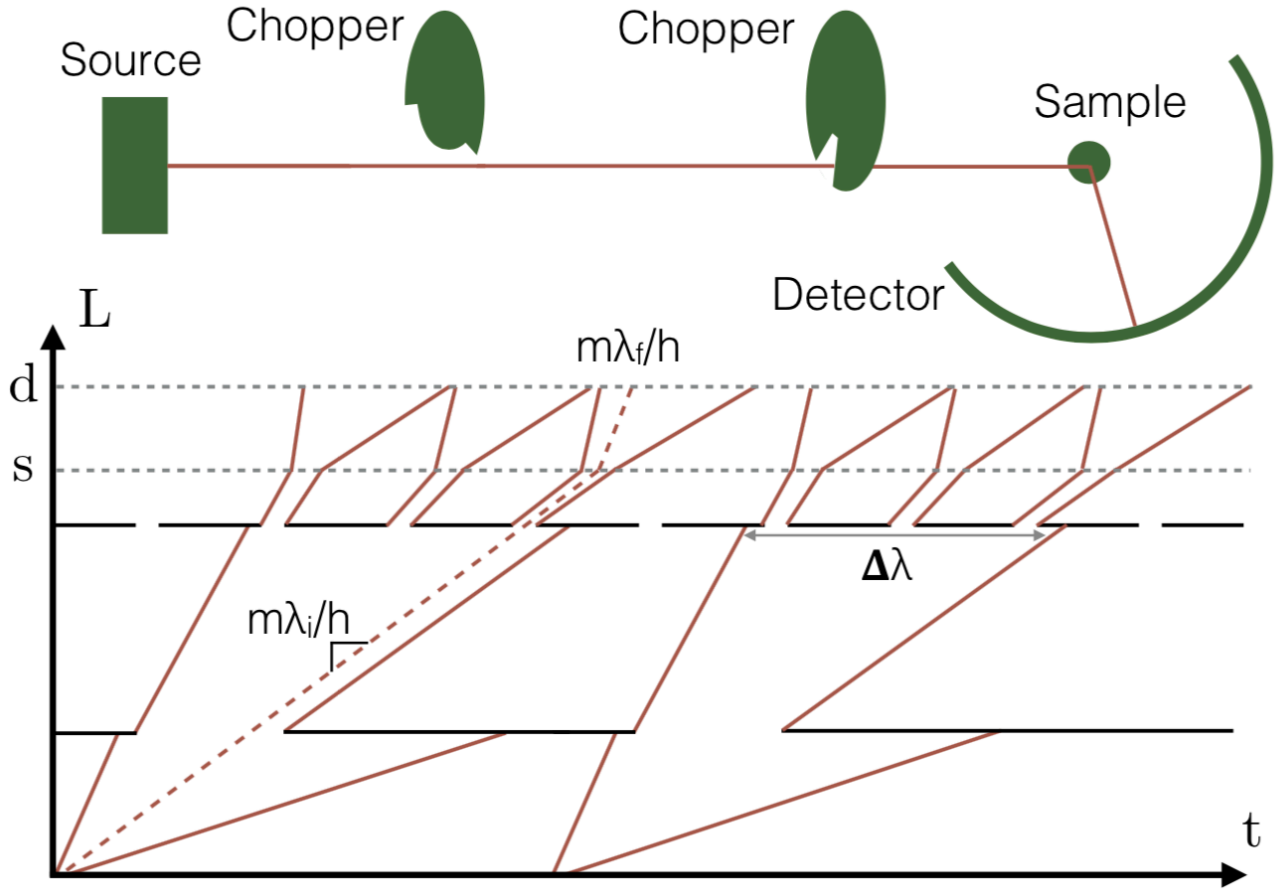
- Only a small fraction of neutrons arrive, r

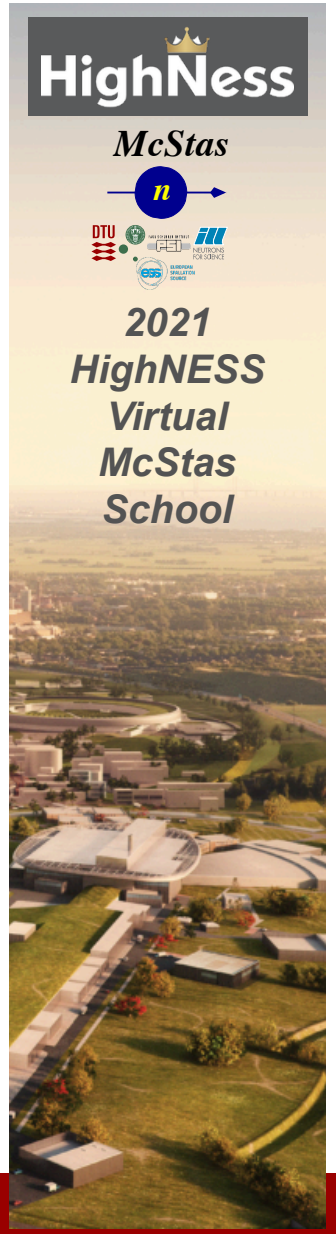




Chopper spectrometers

- Only a small fraction of neutrons arrive





Conclusion

- Inelastic scattering supported in McStas, but could use more sample components
- Longer computational times required
- Advantages from simulation especially important for spectroscopy (resolution function)