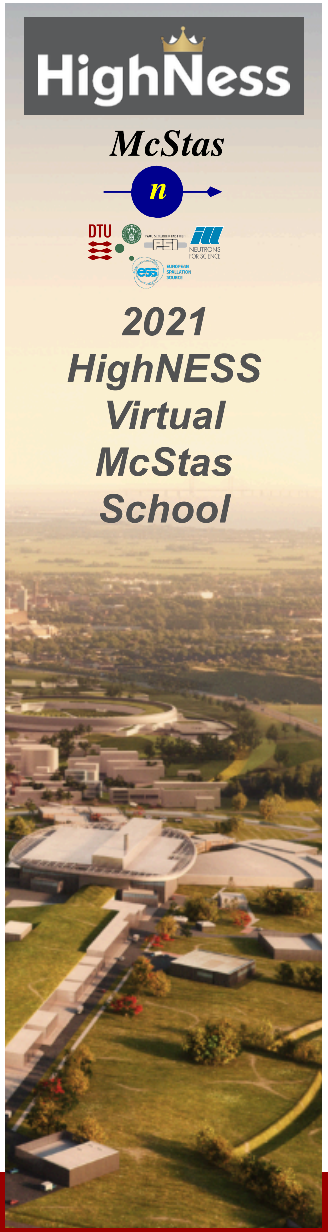
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Peter Willendrup

Further samples...



Further samples in McStas

- A look at the "Sample functionality matrix"

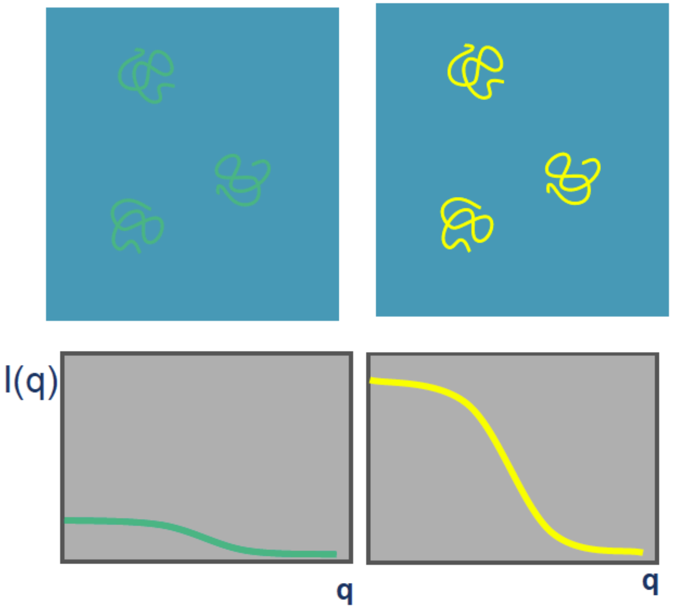
- Models for SANS

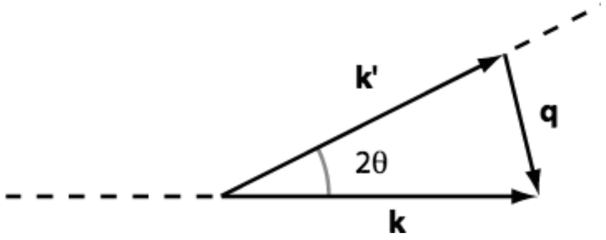
- Inelastic scattering, examples:
  - Phonon_simple
  - Isotropic_sqw

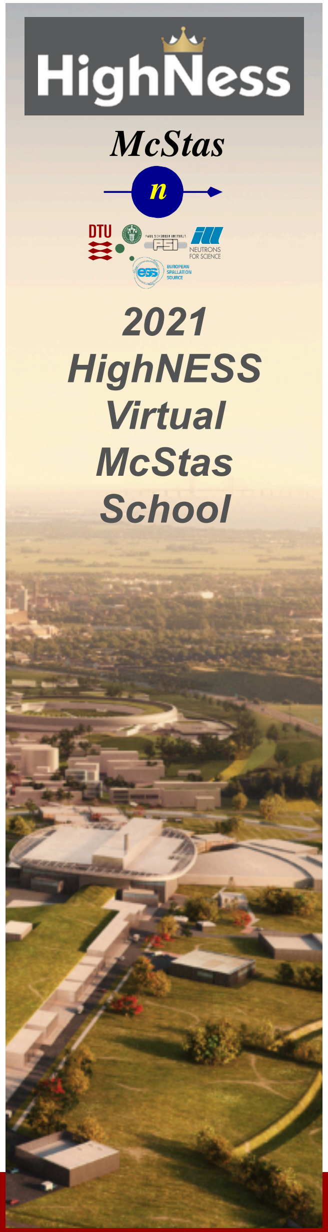
- McStas performance, TAS / Chopper

Small angle scattering SANS

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



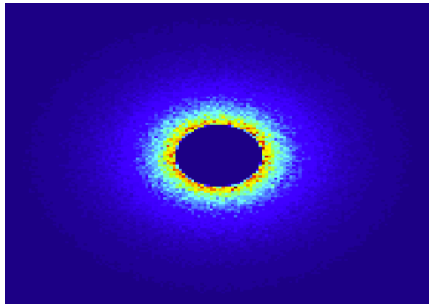




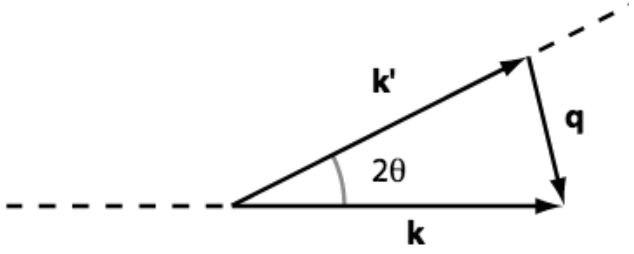
SANS

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.



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



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McStas

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SANS other samples

McStas has a suite of SANS-models:

Try ellipsoidal and cylindrical particles

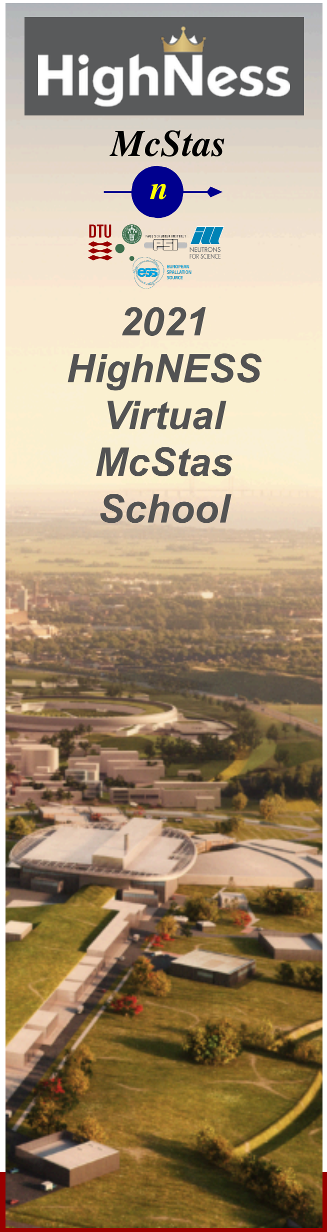
-or-

Elliptic cylinders

Go for Nanodiscs and Liposomes

- 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



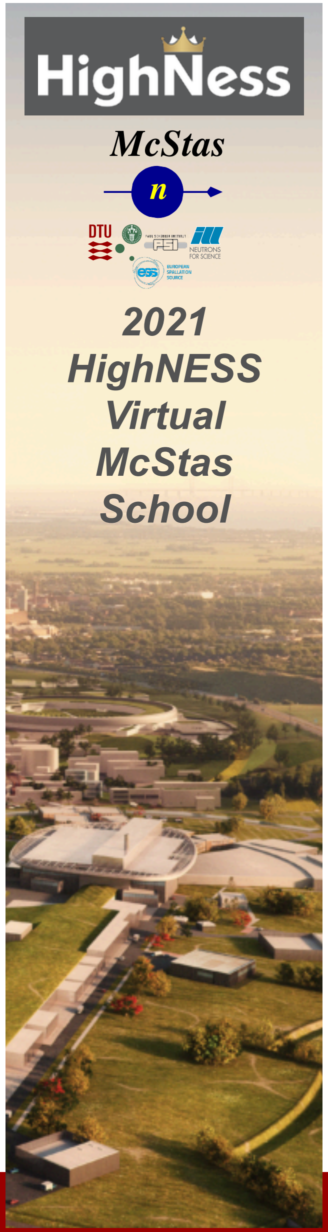
SANS spheres

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

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



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)

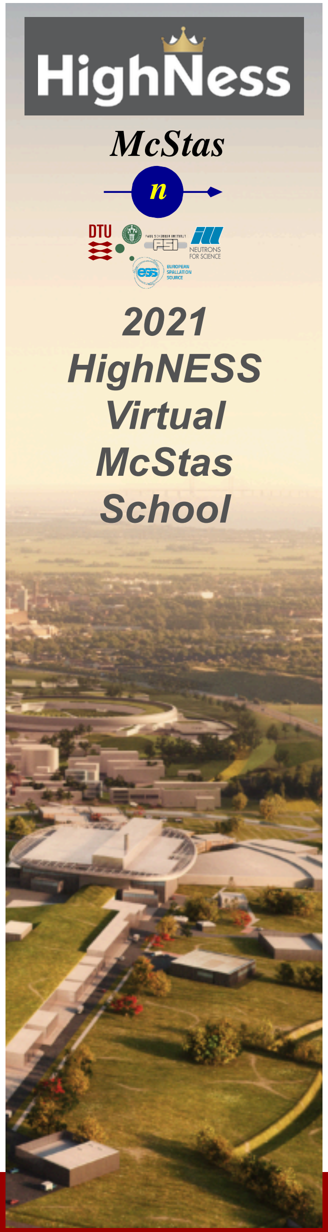
Inelastic scattering S(q,w)

- partial differential cross section
- Scattering function

- Phonons, Spin waves, …

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

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



Popular component: Phonon_simple

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

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

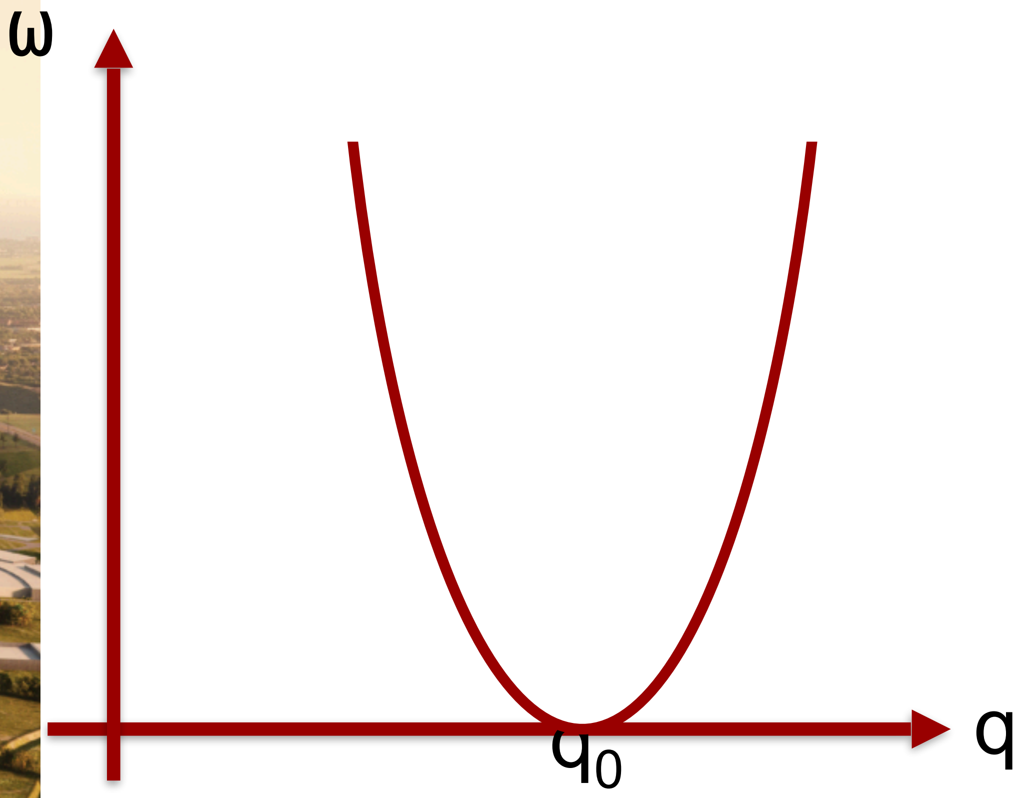
Dispersion $d_1(\mathbf{q}) = c_1/a\sqrt{z - s_q}$

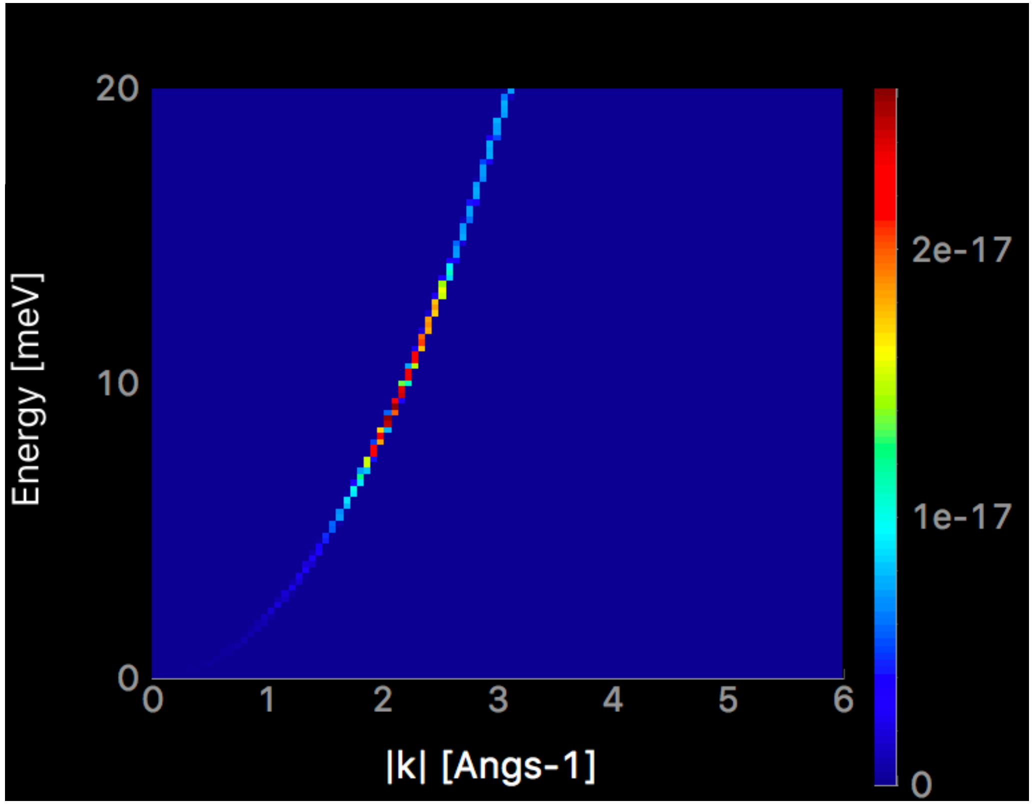
For FCC Bravis $z = 12 \quad s_q = \sum_\mathrm{nn} \cos(\mathbf{q}\cdot\mathbf{r}_\mathrm{nn})$

- 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

Popular component: Phonon_simple

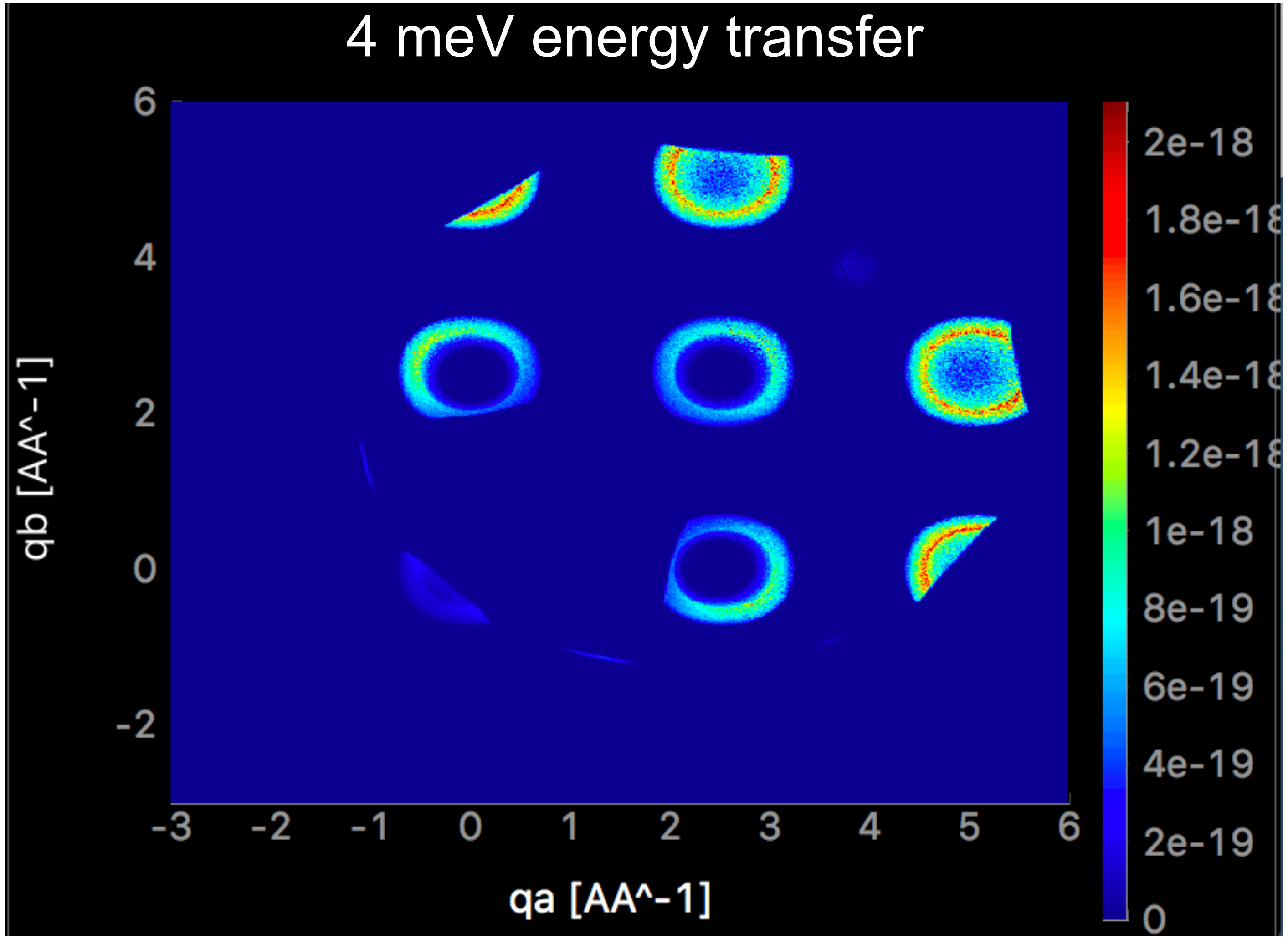
- Dispersion relation, theory and mcstas





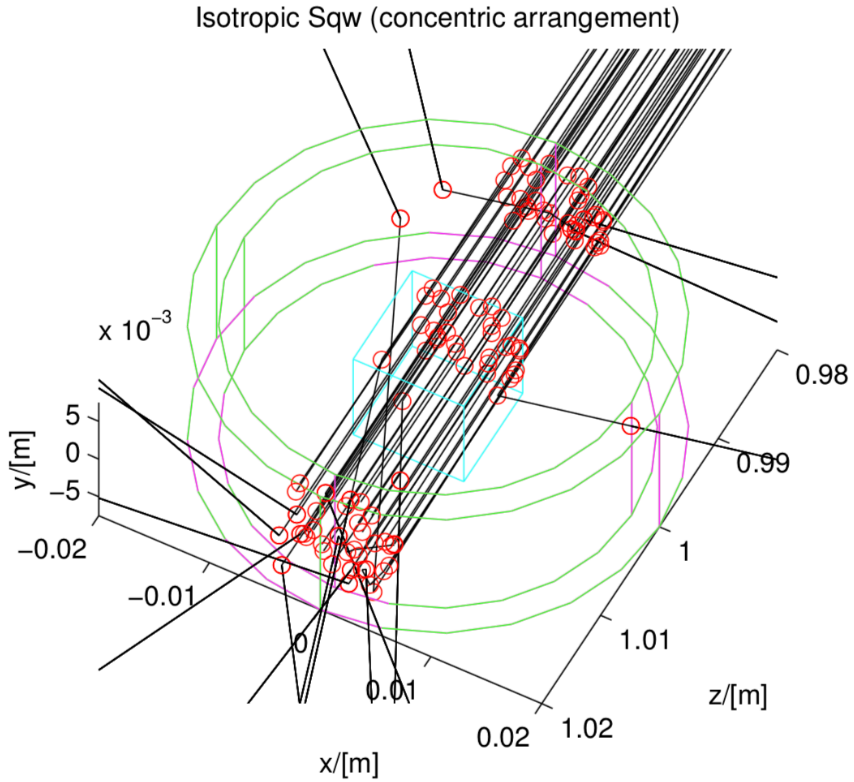
Popular component: Phonon_simple

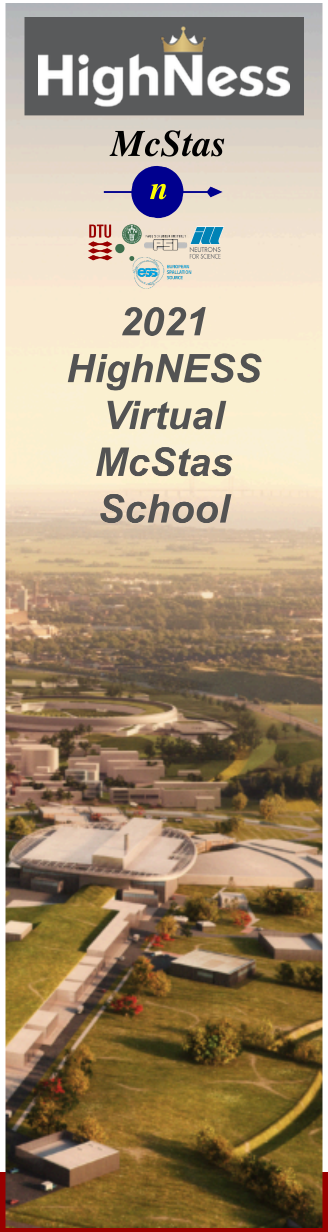
- Example of the output



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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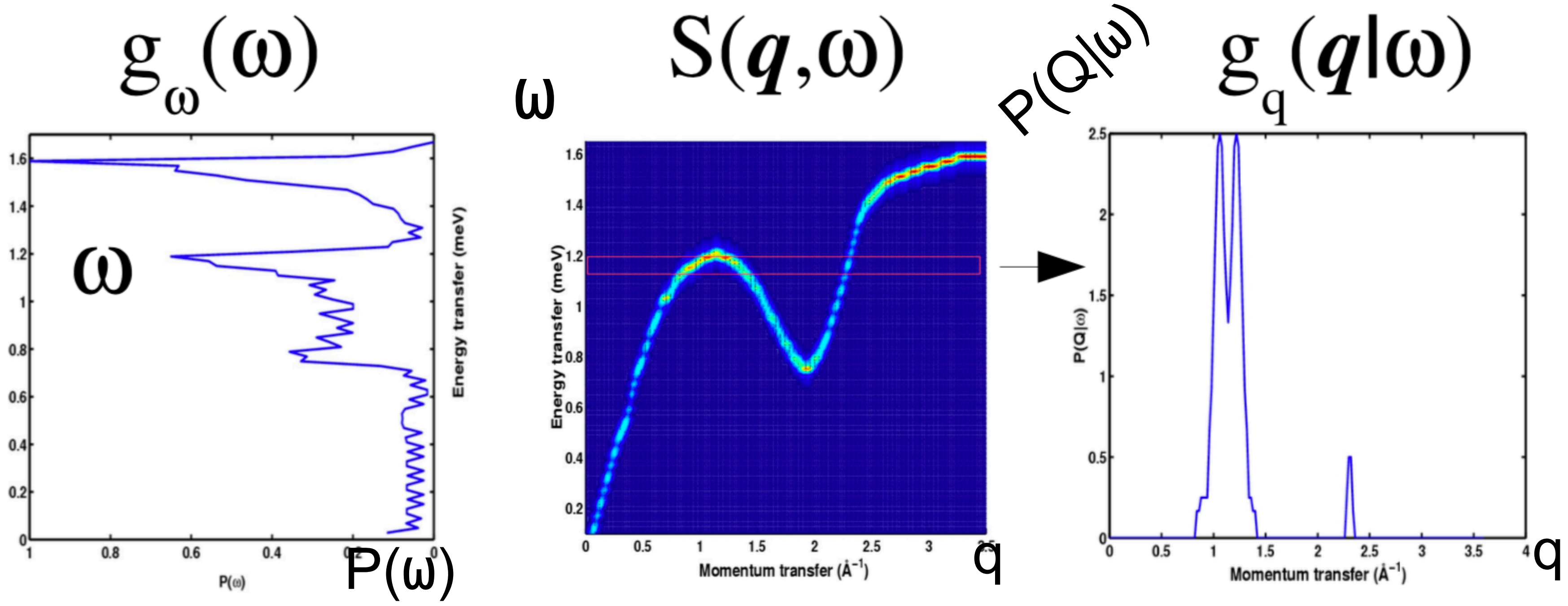
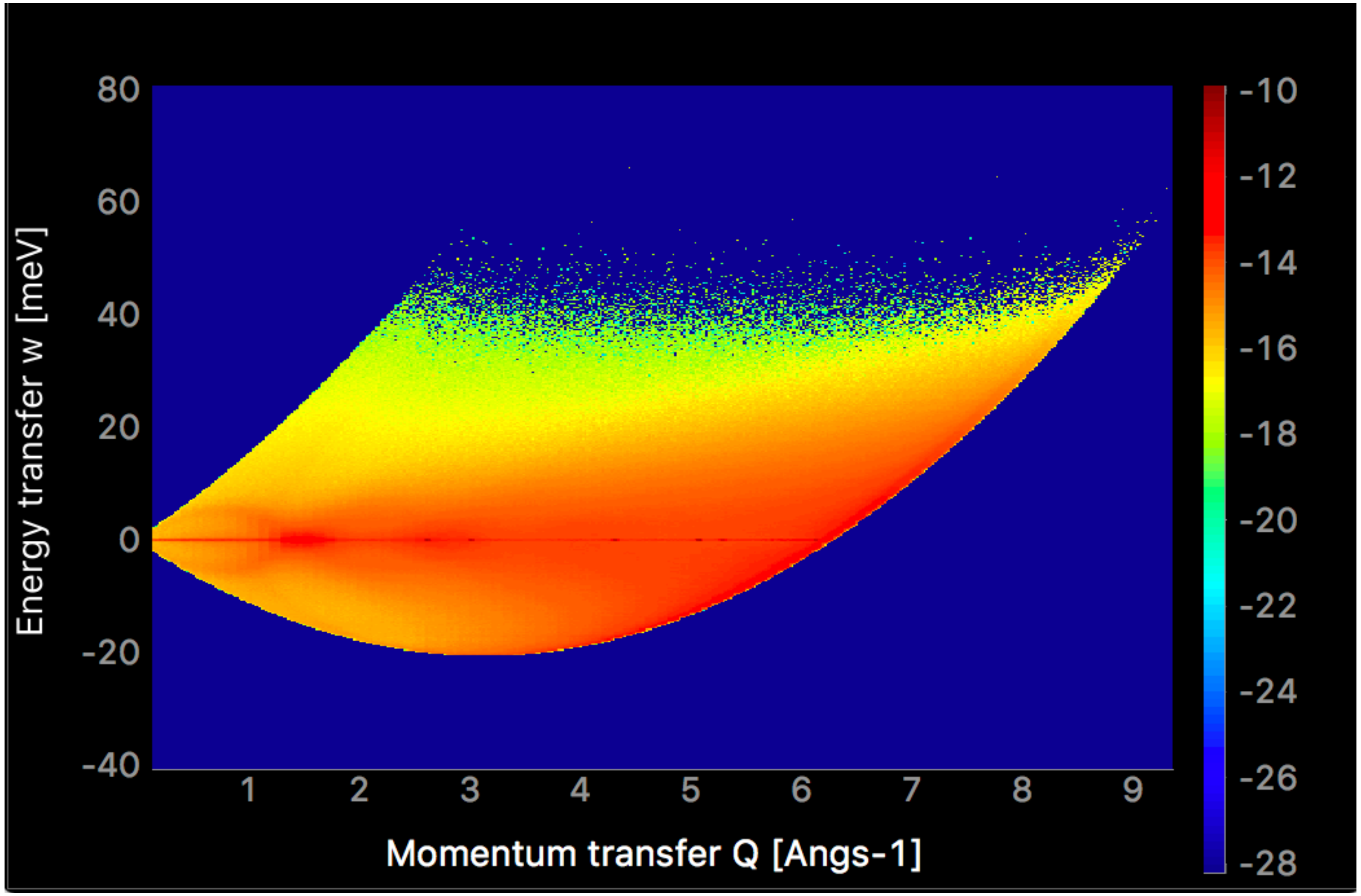


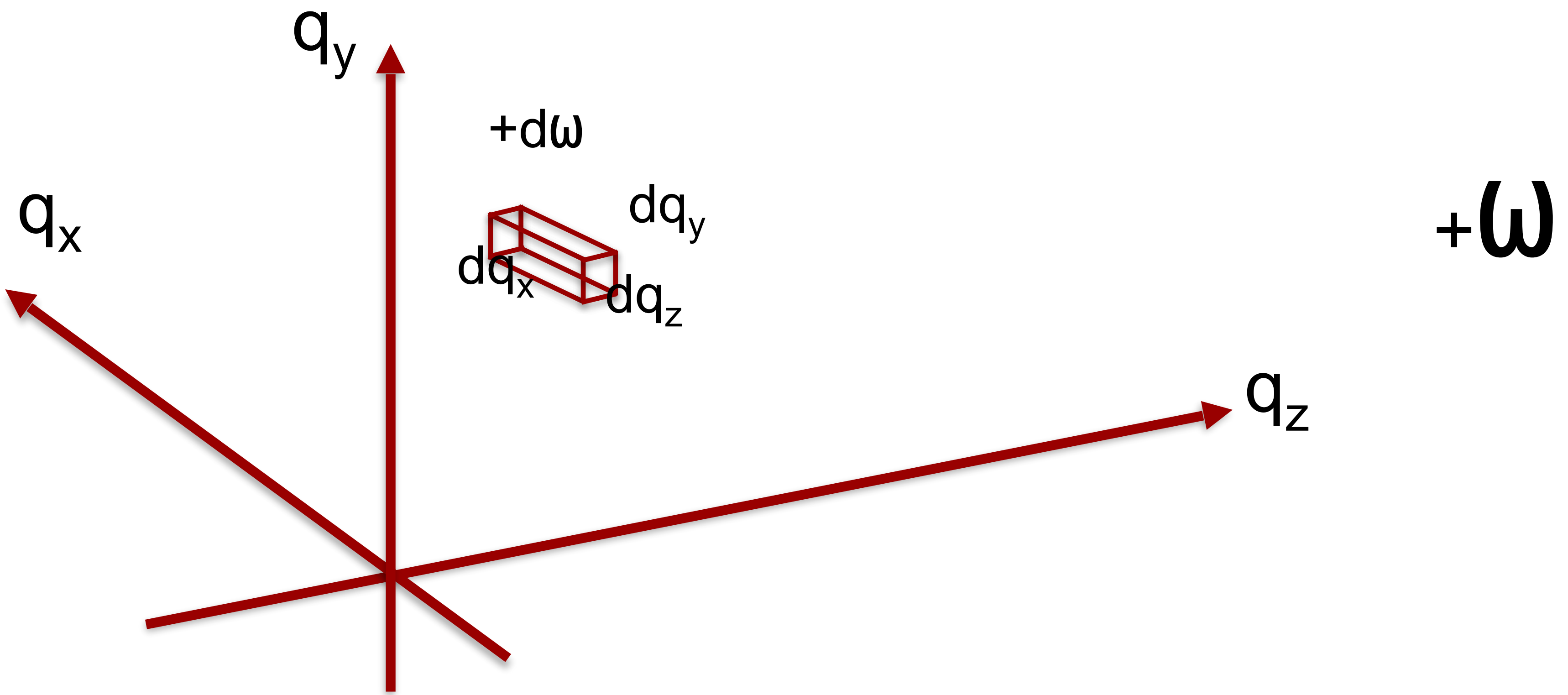
Popular component: Isotropic_sqw

- Rb liquid in time of flight
- Coherent and incoherent



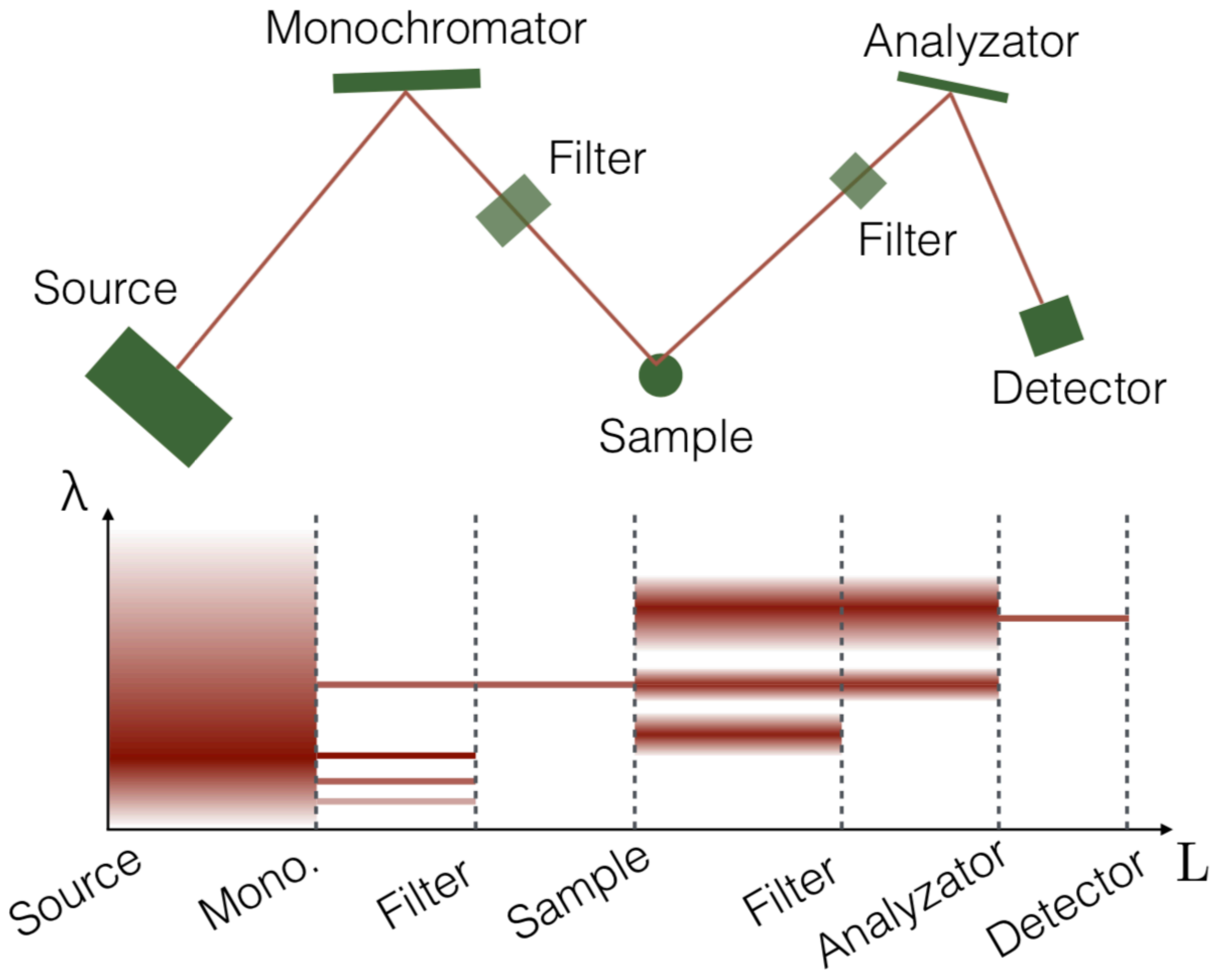
Inelastic scattering in McStas

- 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



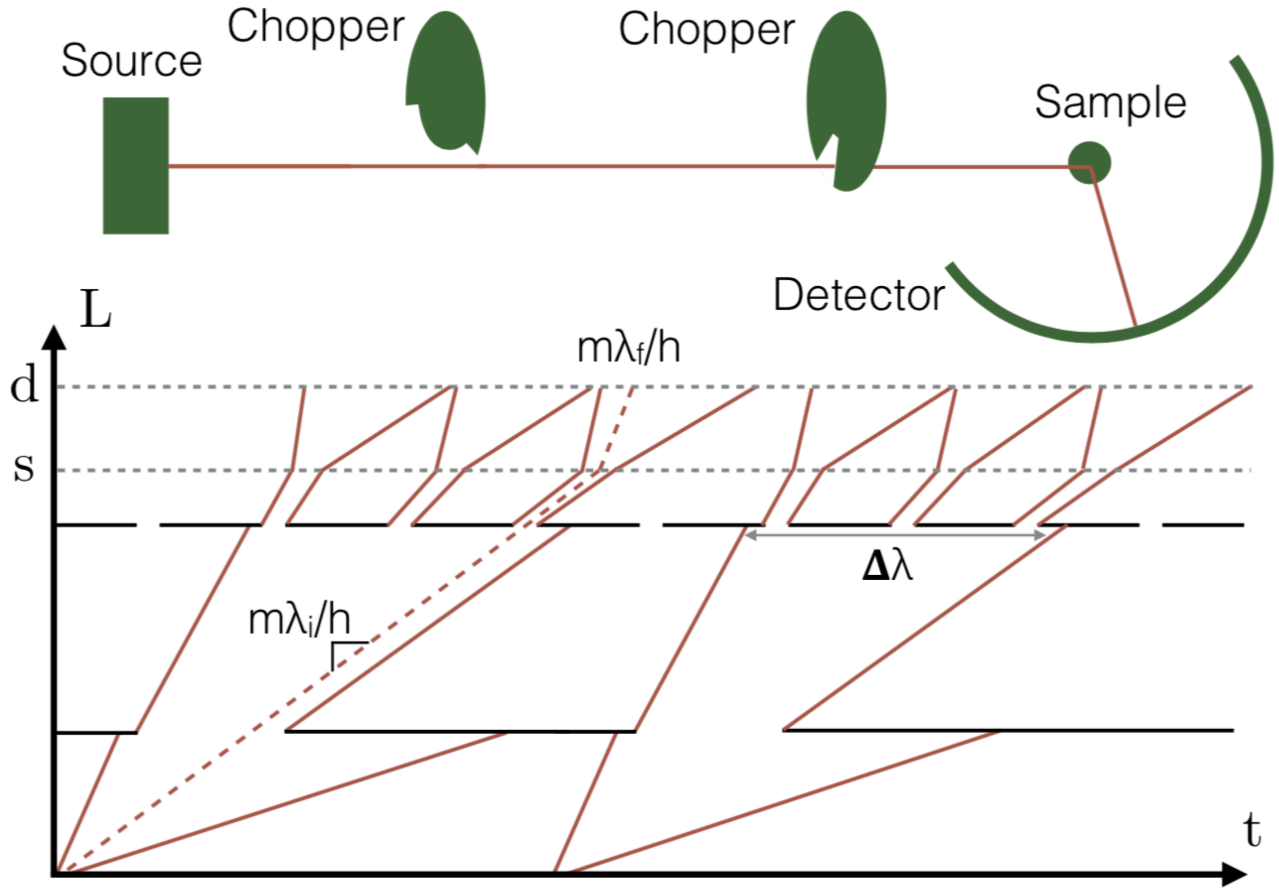
TAS

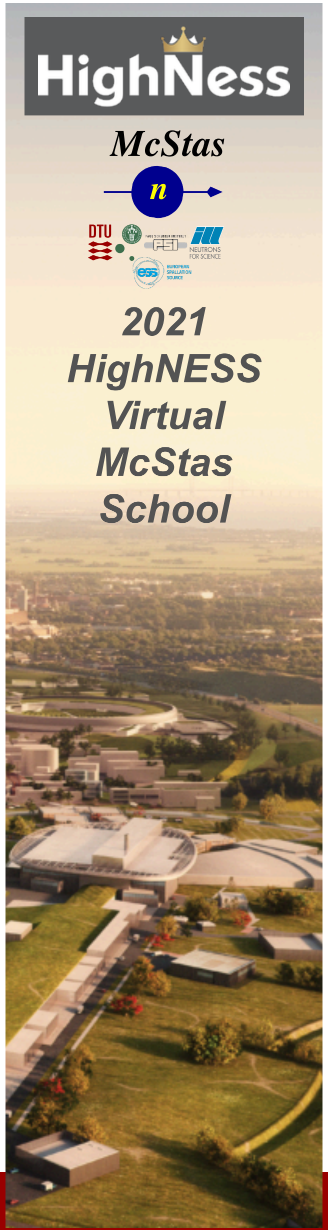
- Only a small fraction of neutrons arrive, most are simulated in vain



Chopper spectrometers

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





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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)