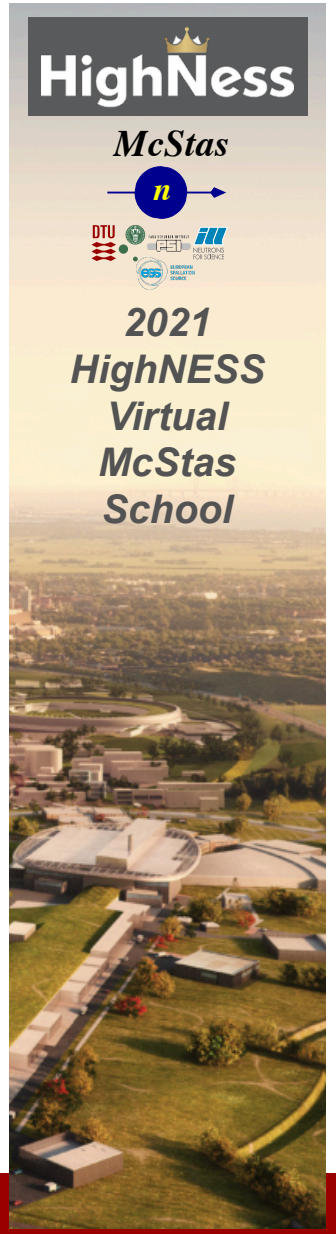
HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Peter Willendrup

Inelastic samples

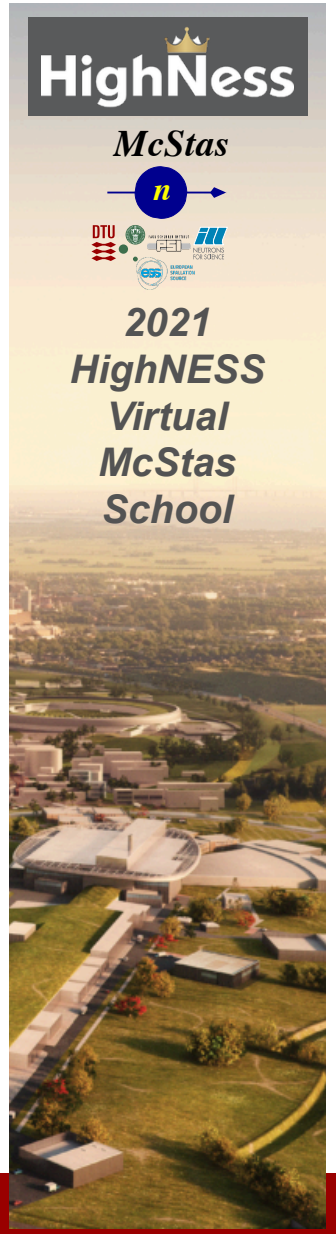
Slides adapted from Mads Bertelsen, ESS DMSC



Inelastic scattering in McStas

- Introduction to inelastic scattering
- Included components
  - Phonon_simple
  - Isotropic_sqw
- Sampling performnace with data approach

- McStas performance, TAS / Chopper
- Exercise



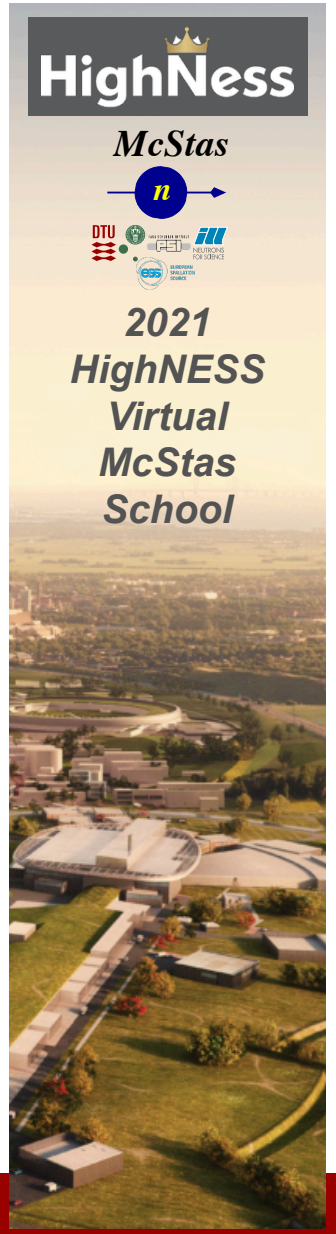
Inelastic scattering S(q,w)

- 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

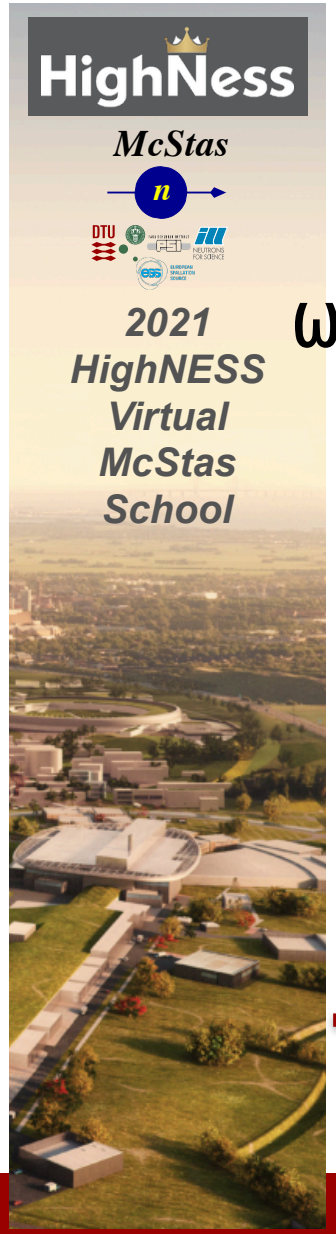
- One isotropic acoustic phonon branch in all Briullion zones on FCC bravis single crystal

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

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

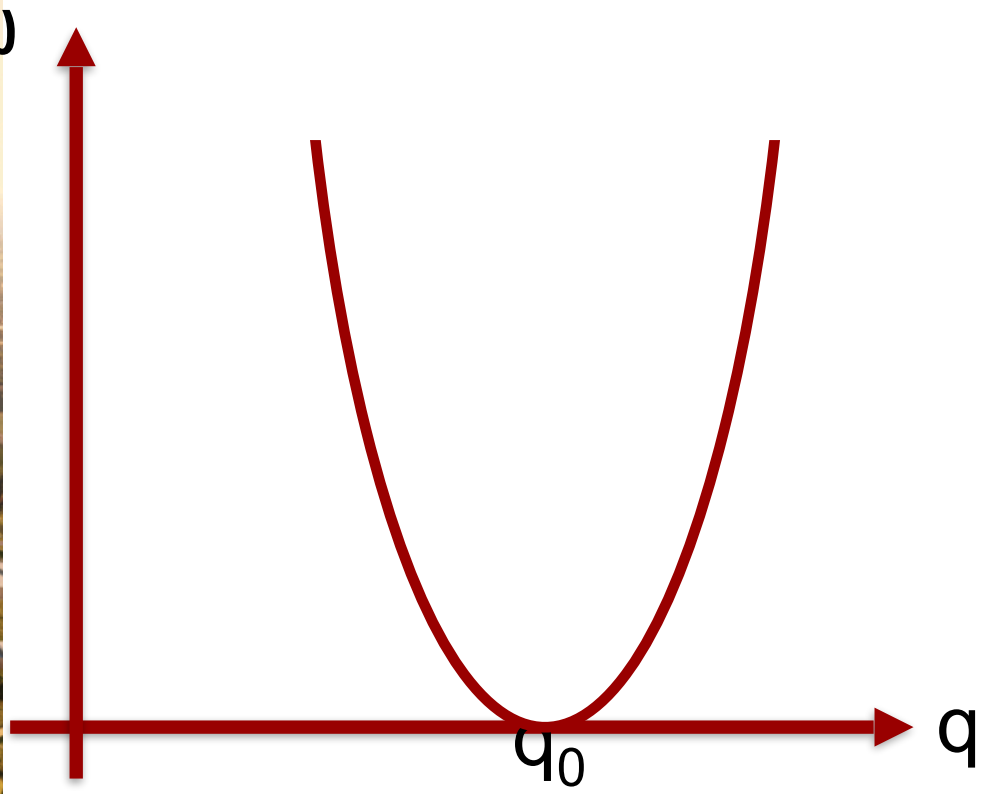
For FCC Bravis $z = 12 \quad s_q = \sum_{\rm nn}\cos(\mathbf{q}\cdot\mathbf{r}_{\rm nn})$

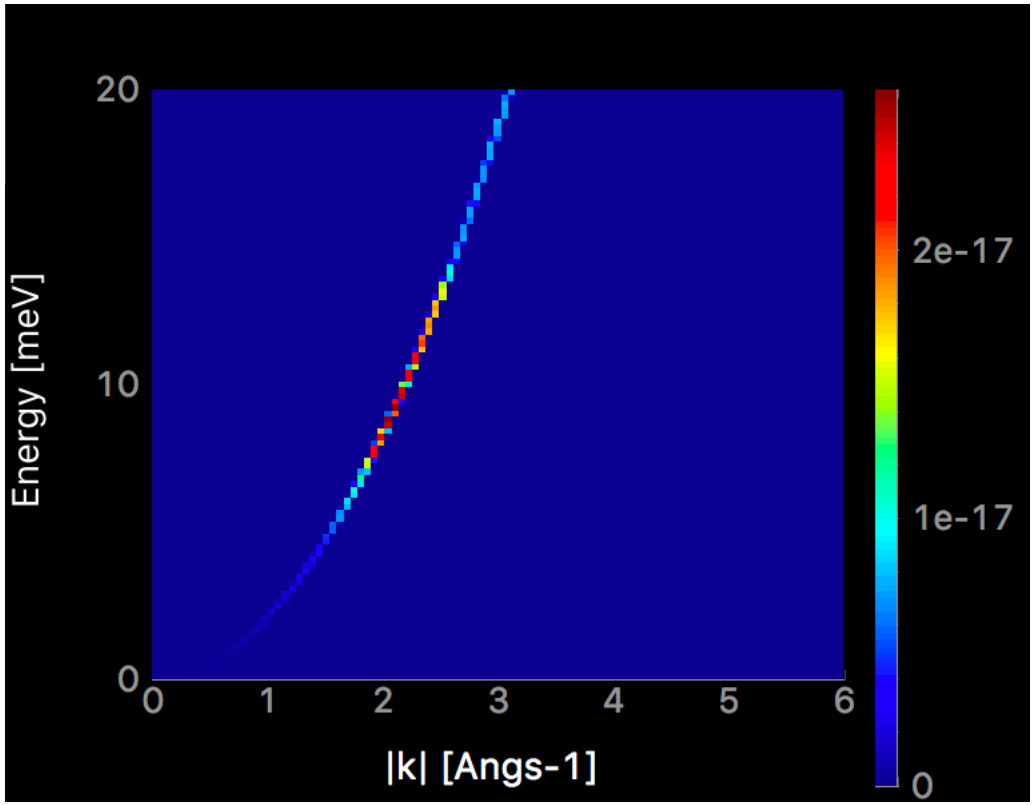
- M - Atomic mass
- b – scattering length
- *n* – bose factor
- a – fcc lattice spacing
- c - speed of sound
- $\boldsymbol{\kappa}$ – measured q vector
- **q** – Phonon scattering vector

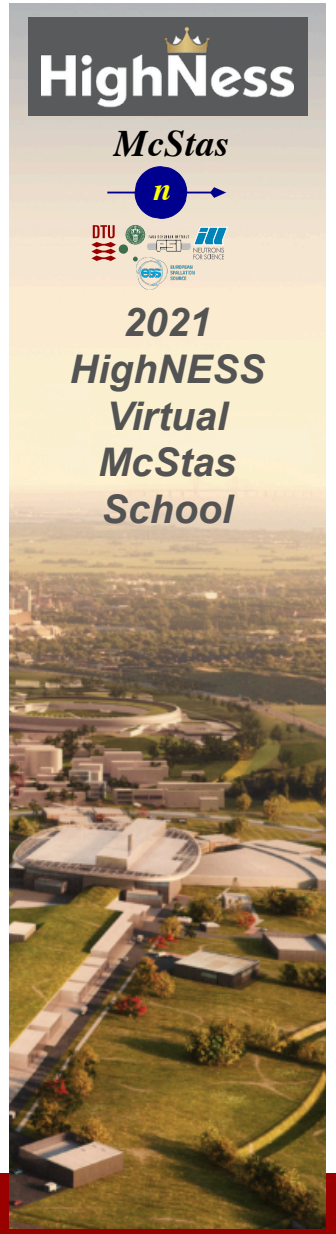


Popu _simple

- Dispers

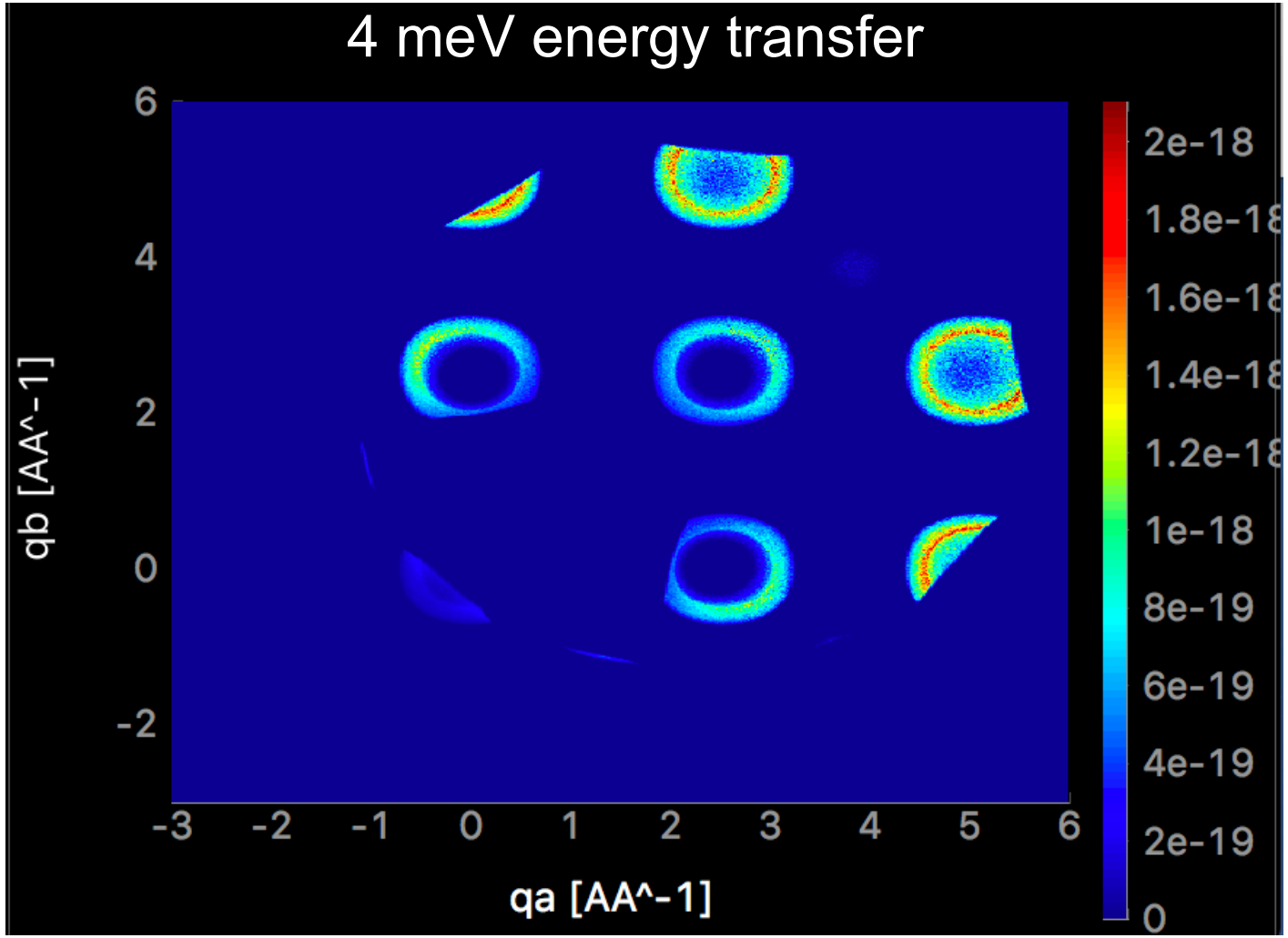


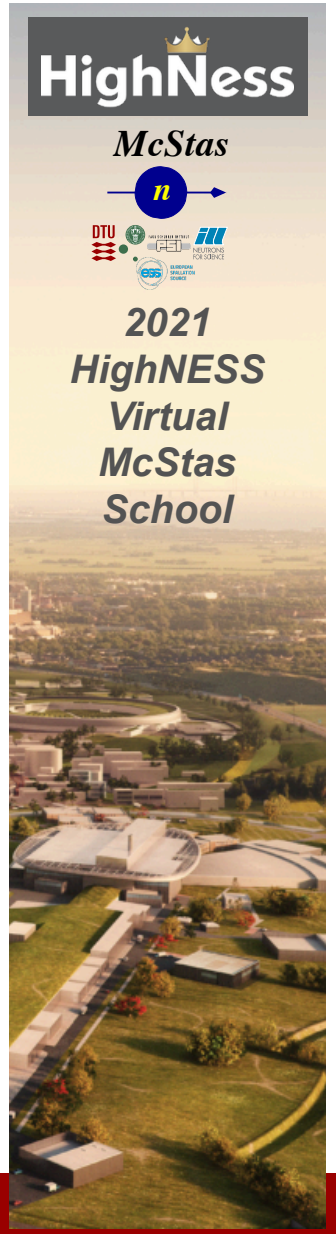




Popular component: Phonon_simple

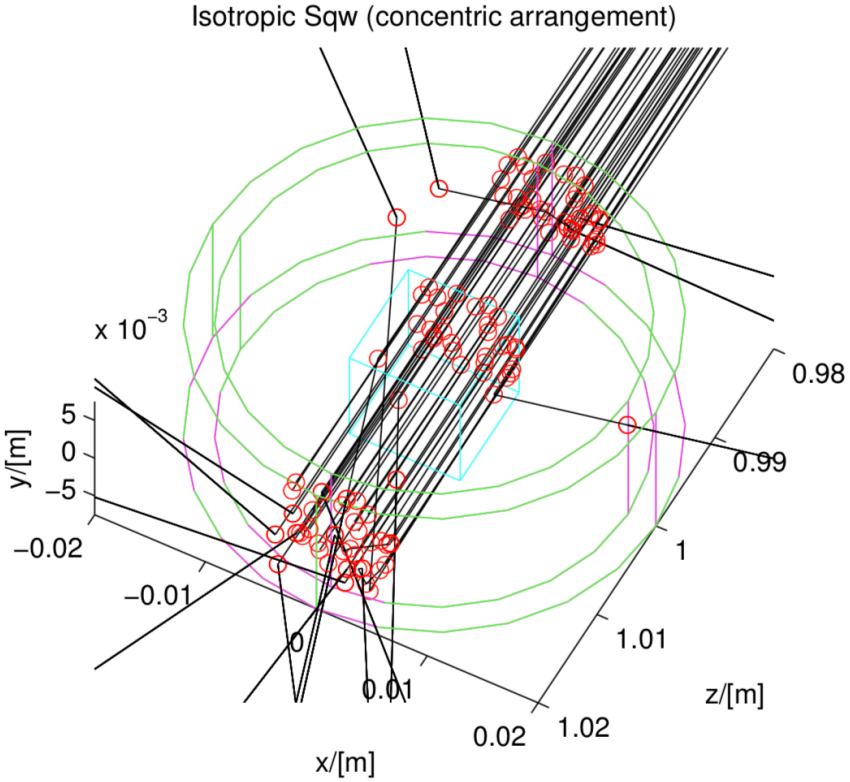
- Example of the output





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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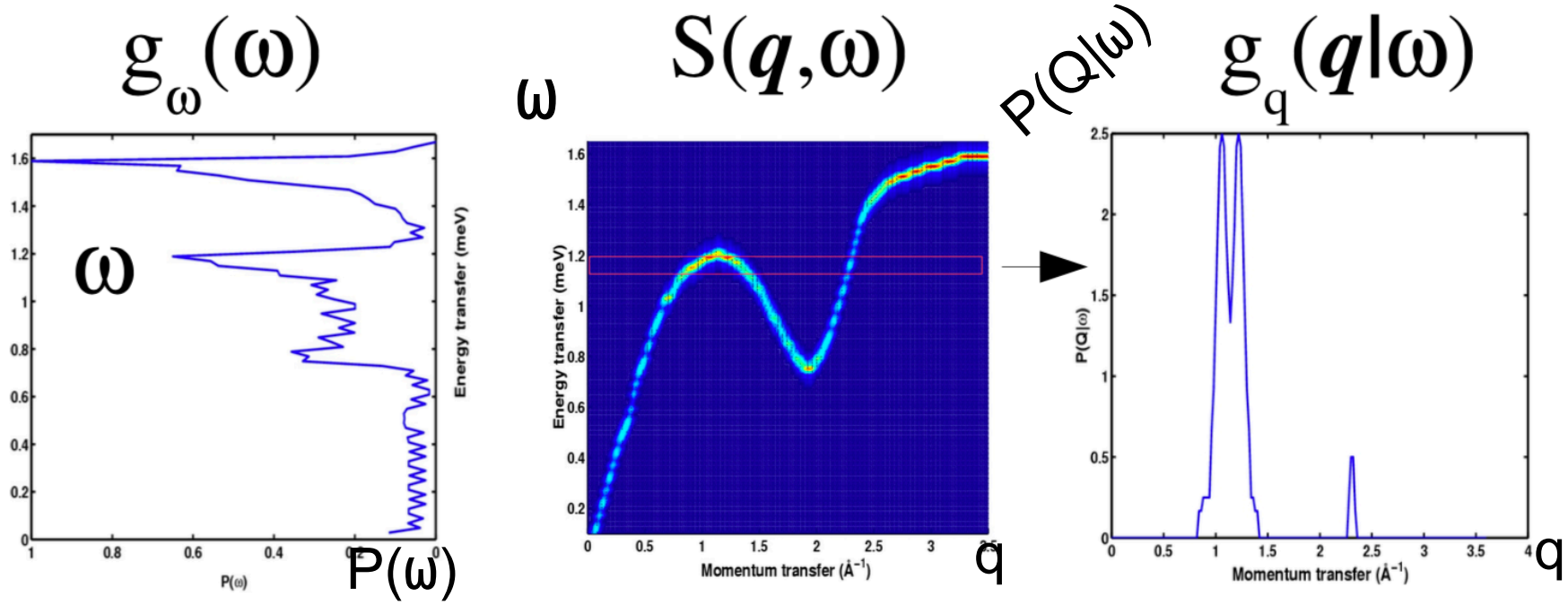
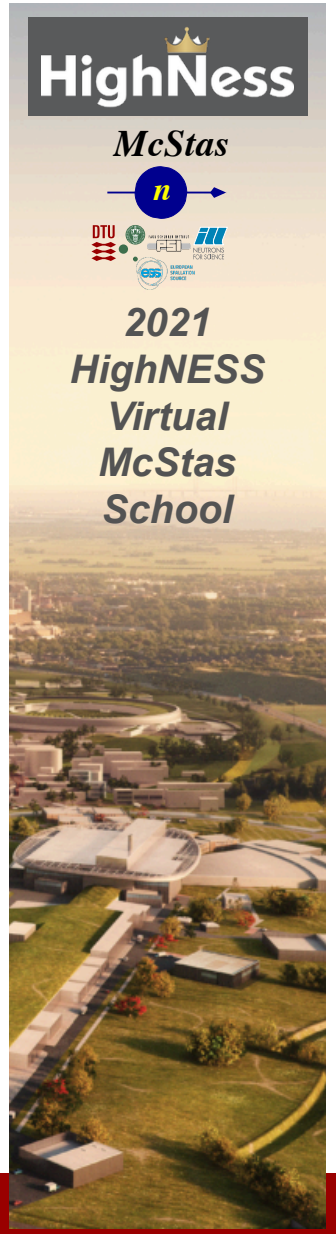
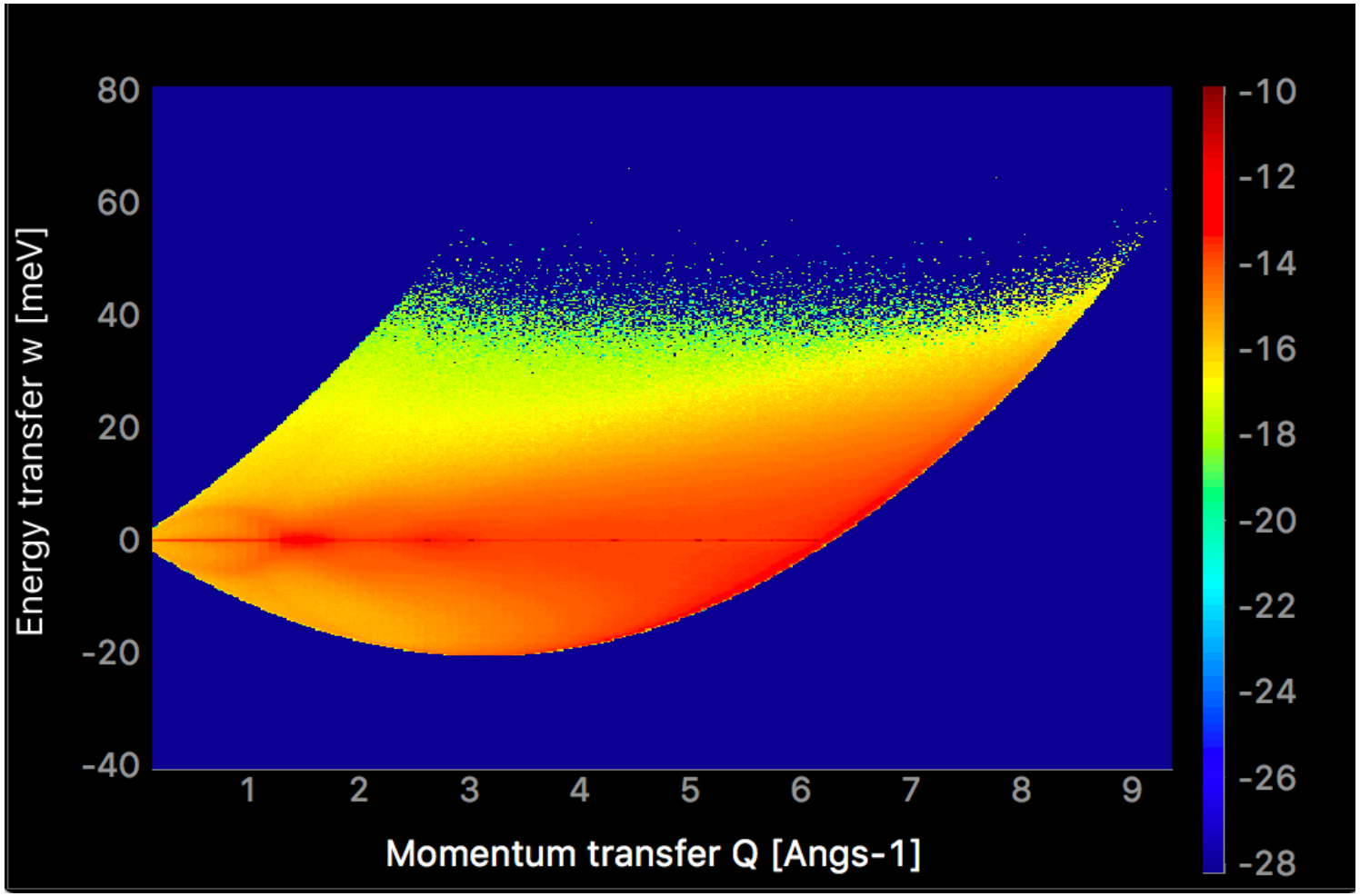
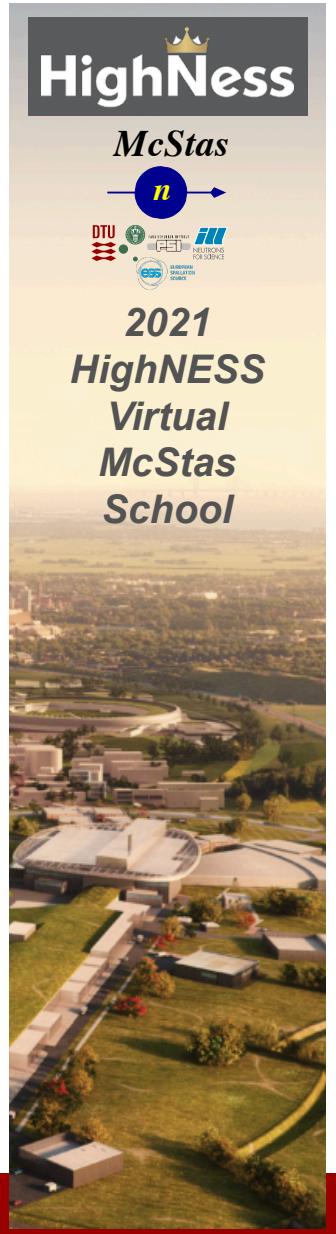




Popular component: Isotropic_sqw

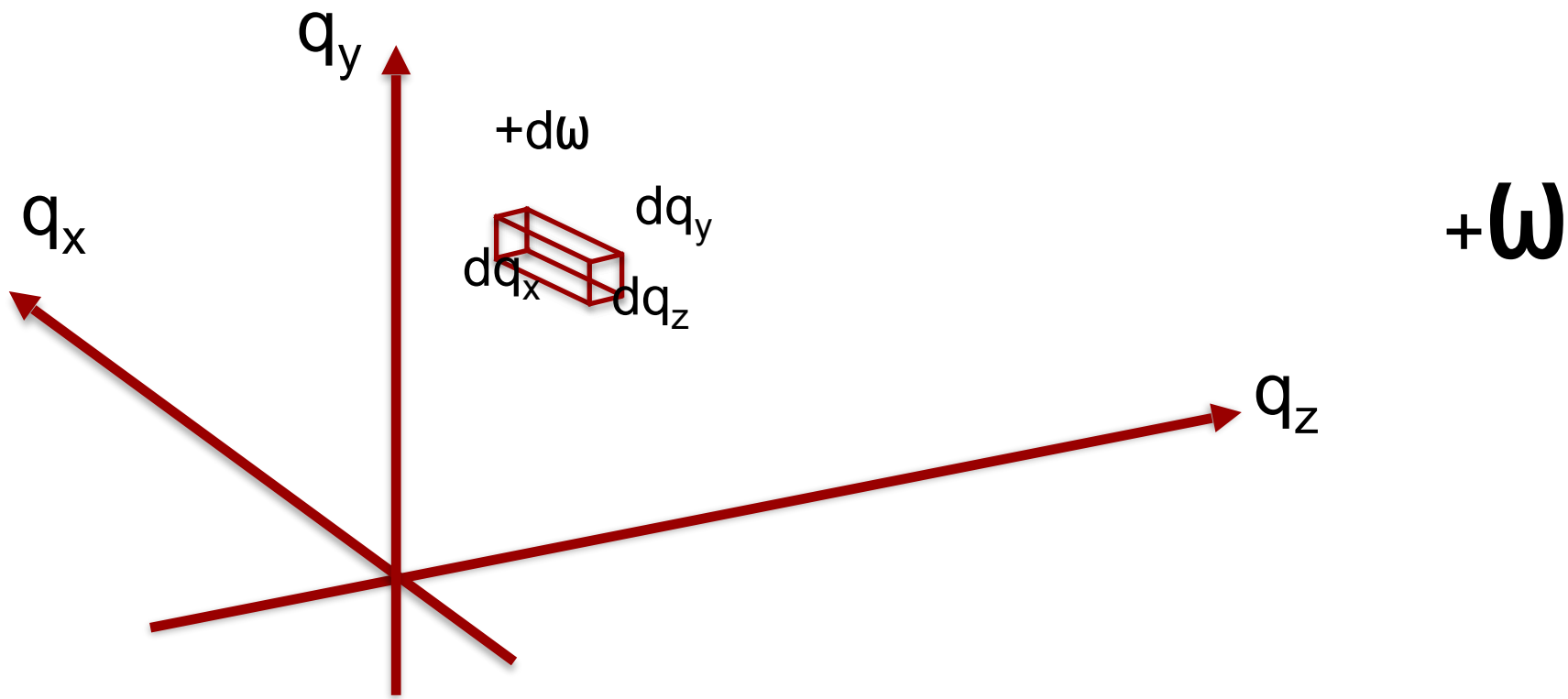
- Rb liquid in time of flight
- Coherent and incoherent

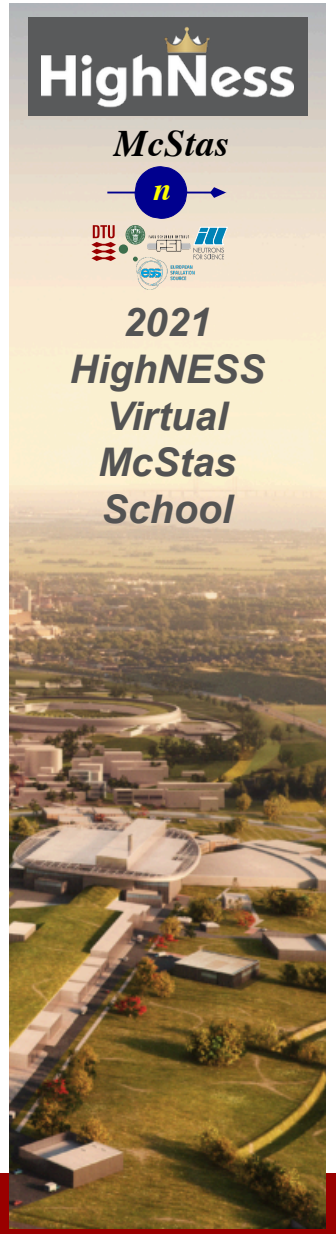




Inelastic scattering in McStas

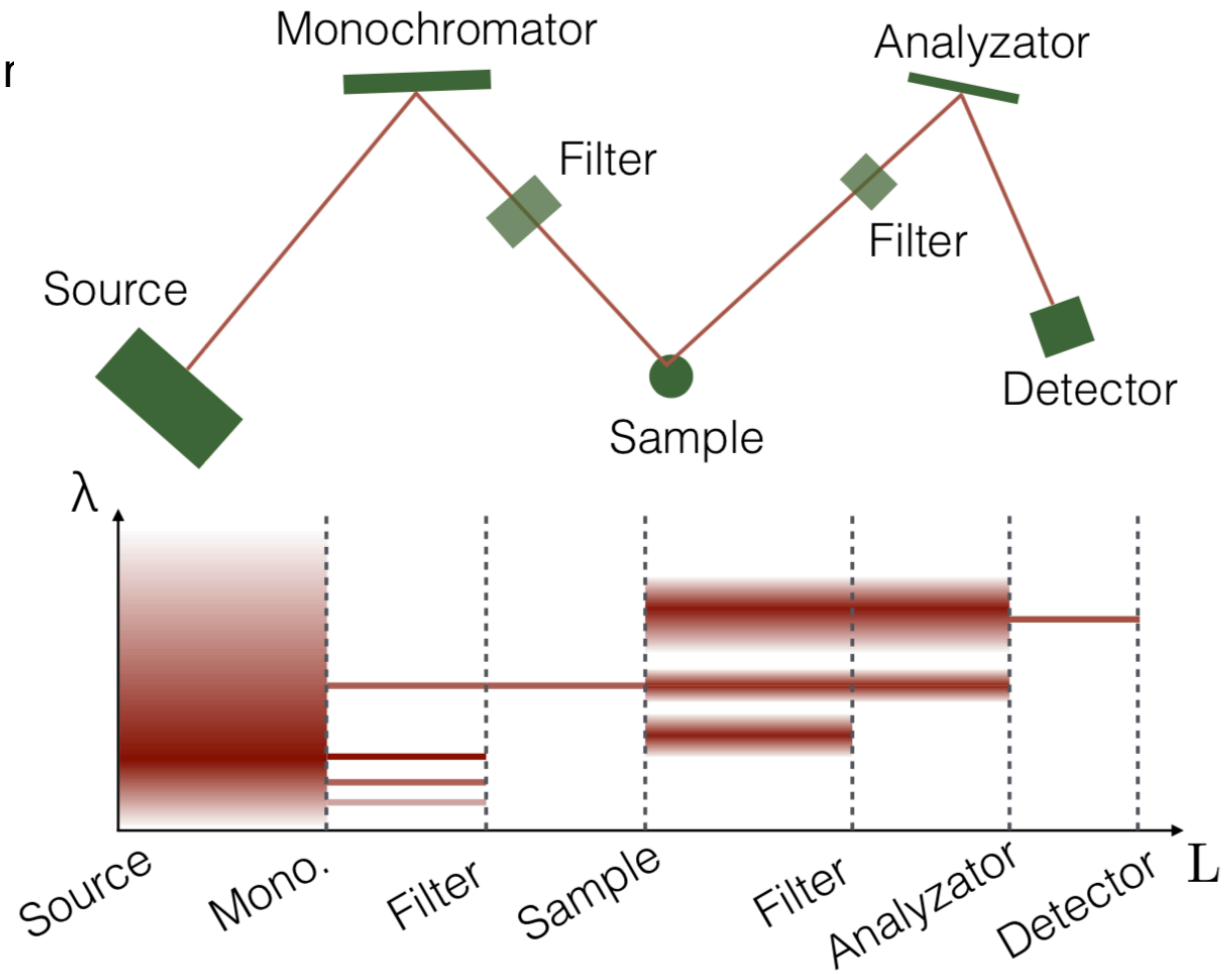
- Monte carlo sampling issues
- Need to sum over large amount of possible final states to find cross section
- Need large amount of rays to sample all the options

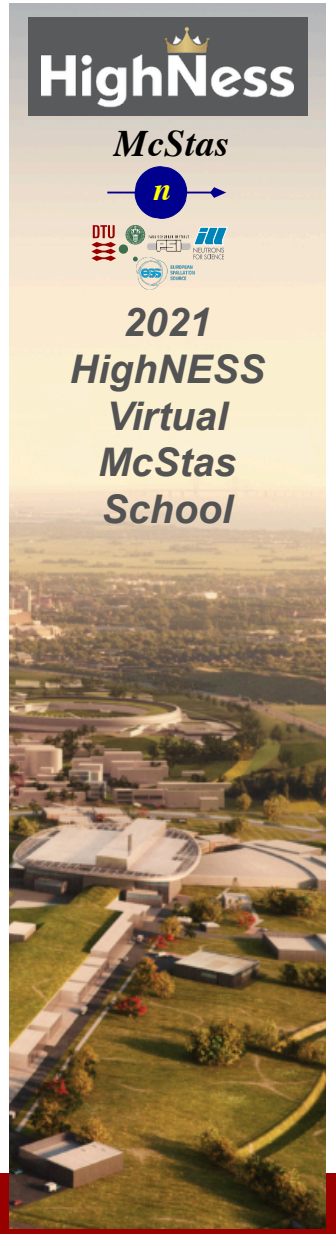




TAS

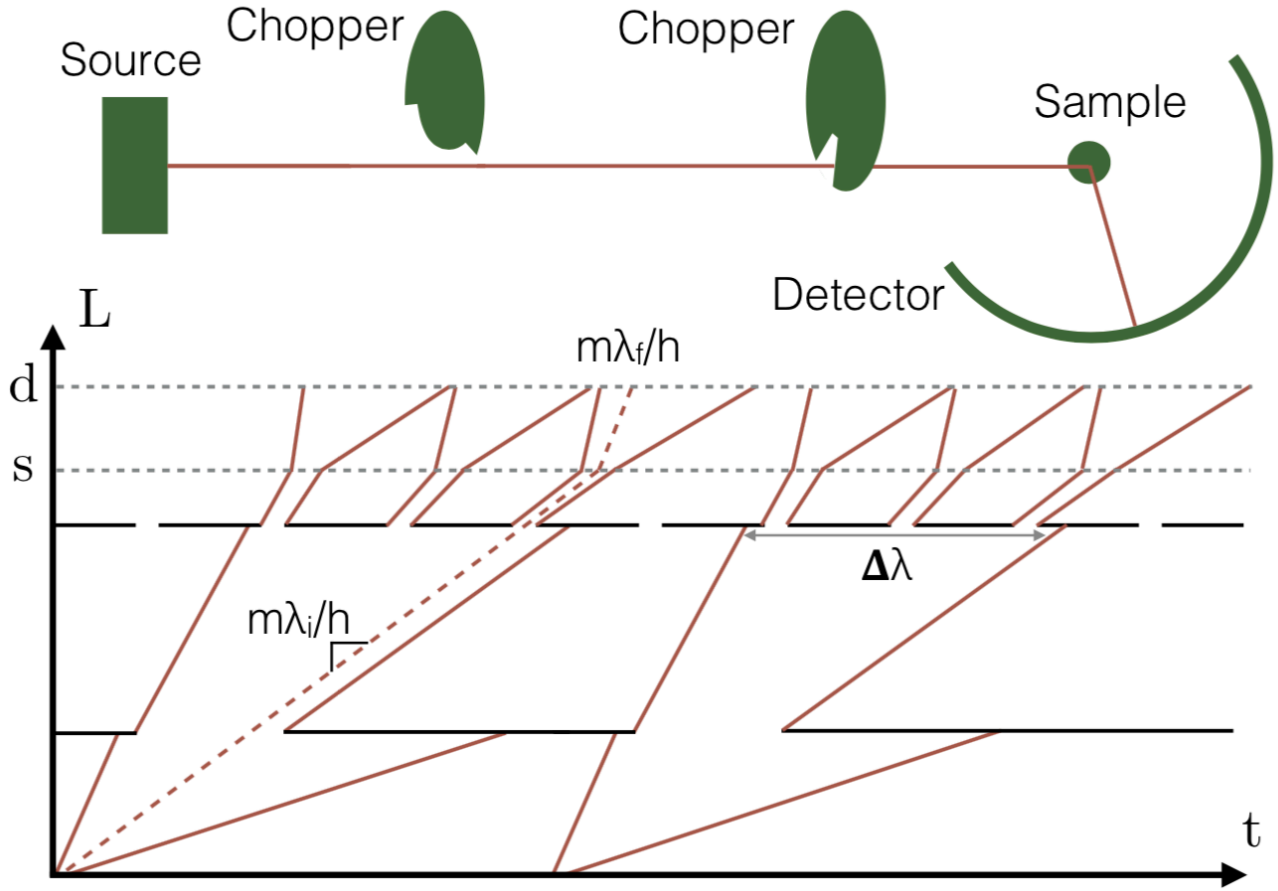
- Only a small fraction of neutrons arrive, r

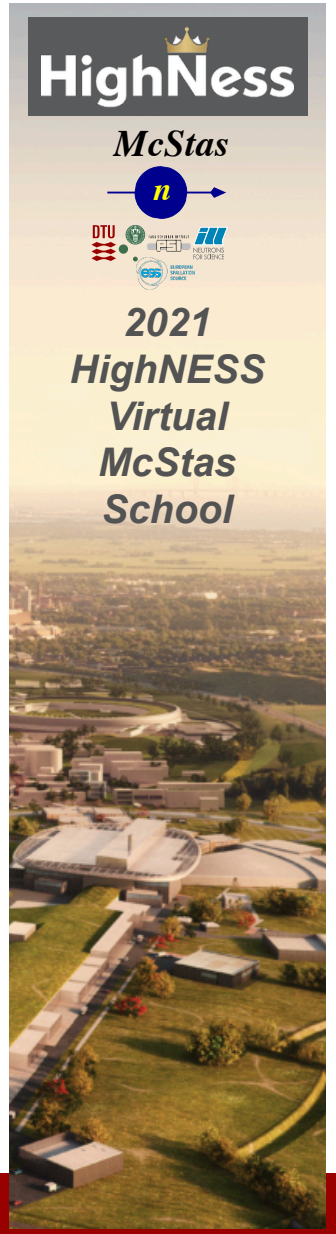




Chopper spectrometers

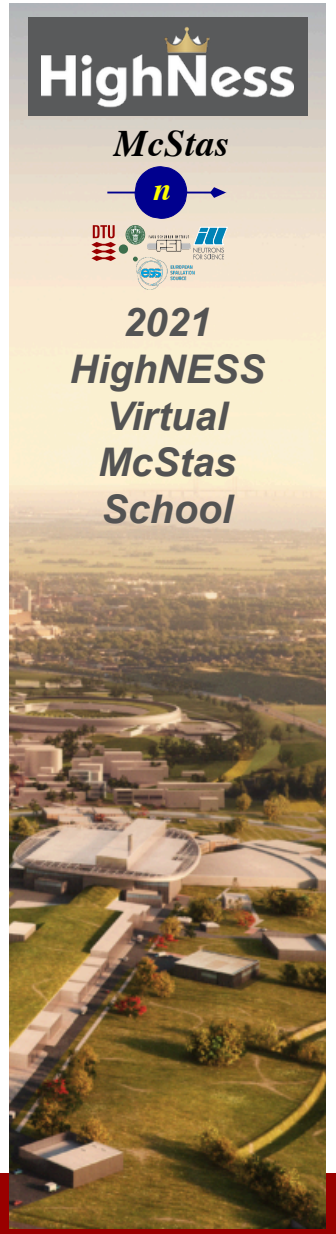
- Only a small fraction of neutrons arrive





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)



Exercise

- Use provided TAS instrument to scan the phonon dispersion
- Requires that you work in folder containing components from the zip file
- Further explanation on github