

Practical F: Build a triple-axis spectrometer!



MDANSE 2018

**Simulation of Inelastic
Neutron Scattering
using McStas and
material dynamics models**

Sept. 24th – 28th 2018

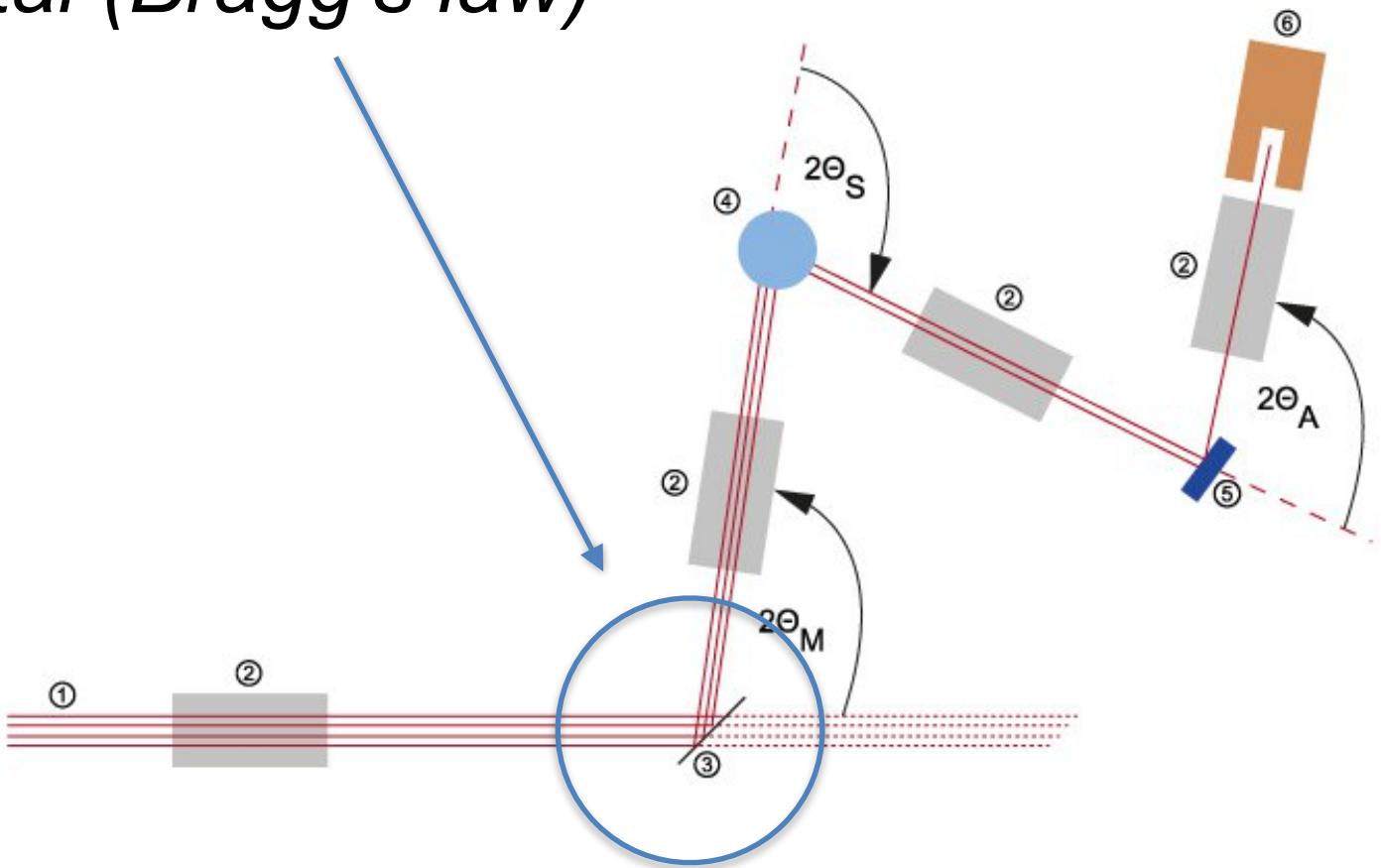
Puerto de la Cruz – Tenerife

(c) A. Martí (2012)

TAS essentials



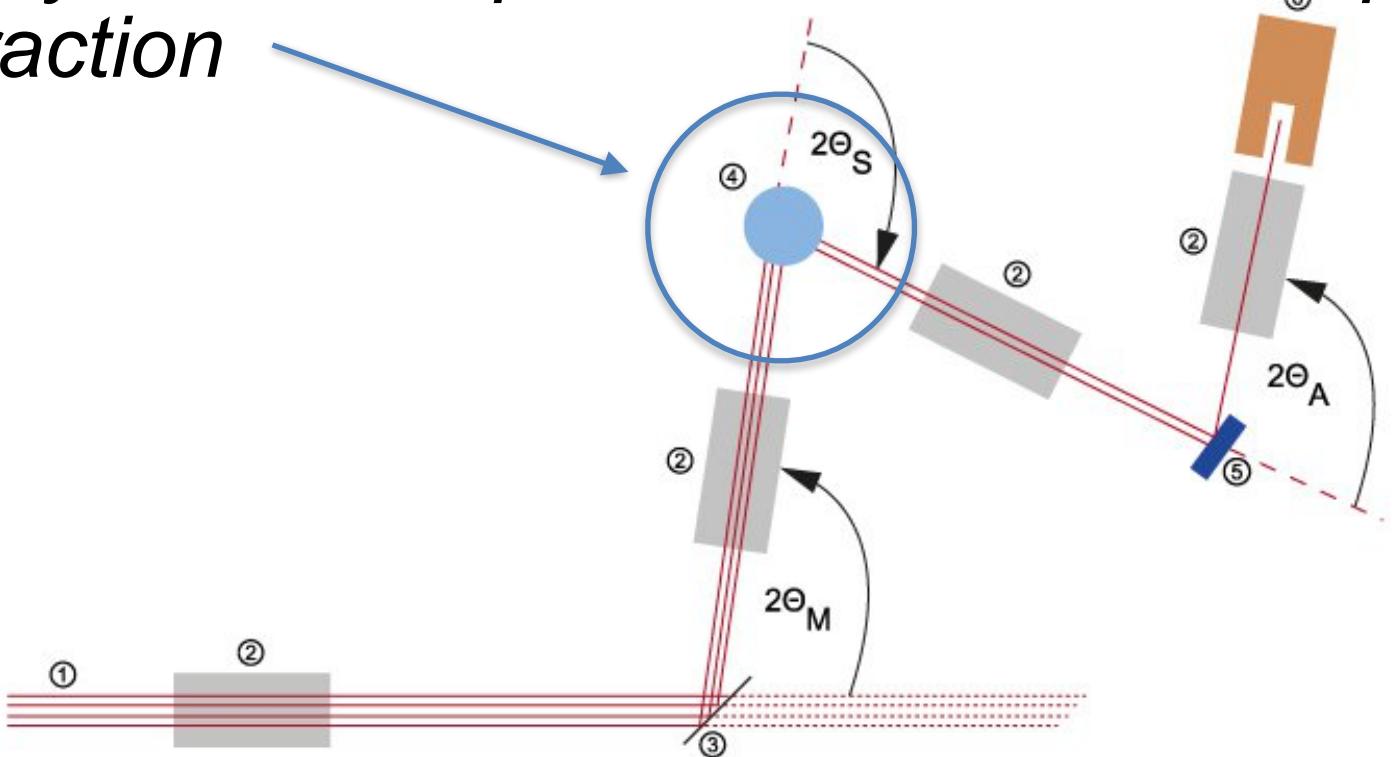
- | Spectrometer with 3 “axes”
- | 1. Define incoming beam k_i by a monochromator crystal (Bragg’s law)



TAS essentials



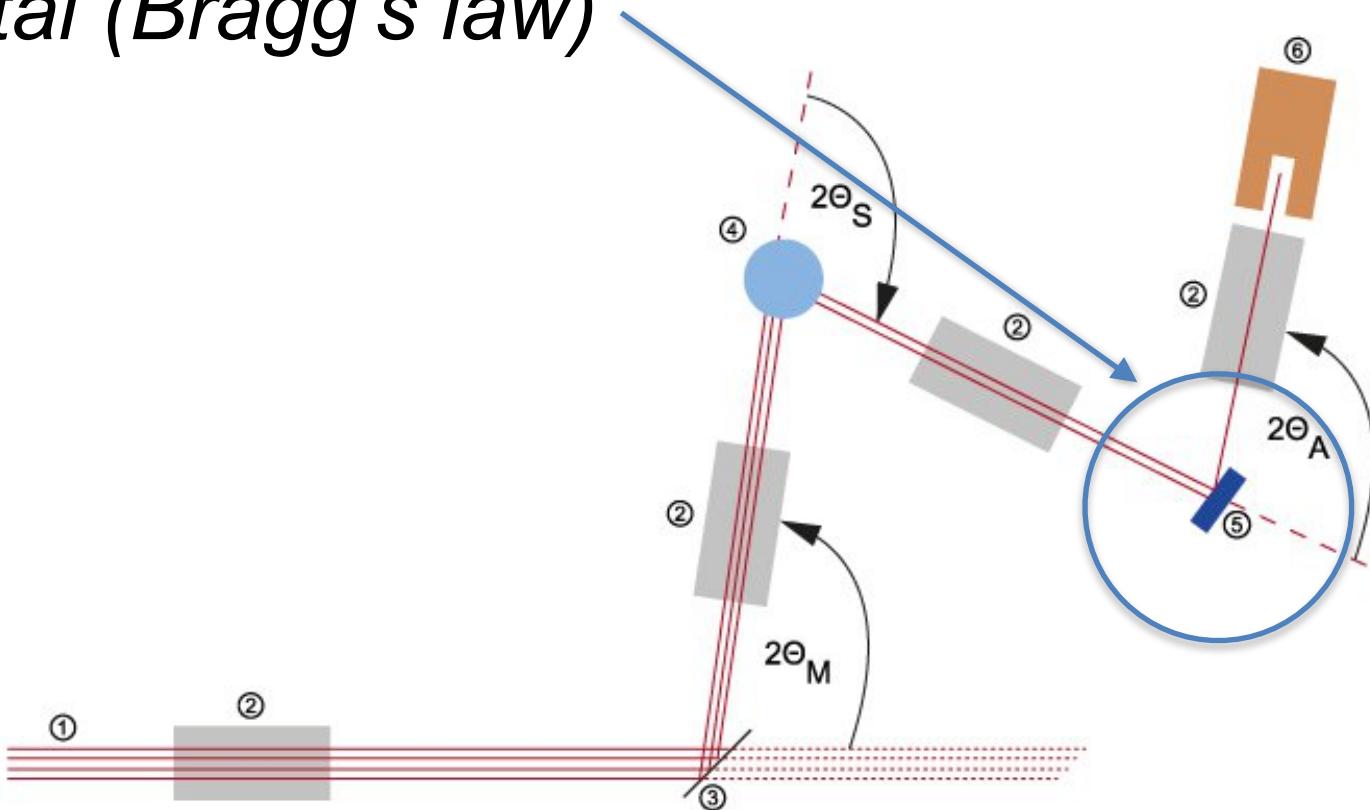
- | Spectrometer with 3 “axes”
- | 2. A ‘sample-axis’ for zooming in on structural and dynamical aspects of the beam-sample interaction



TAS essentials



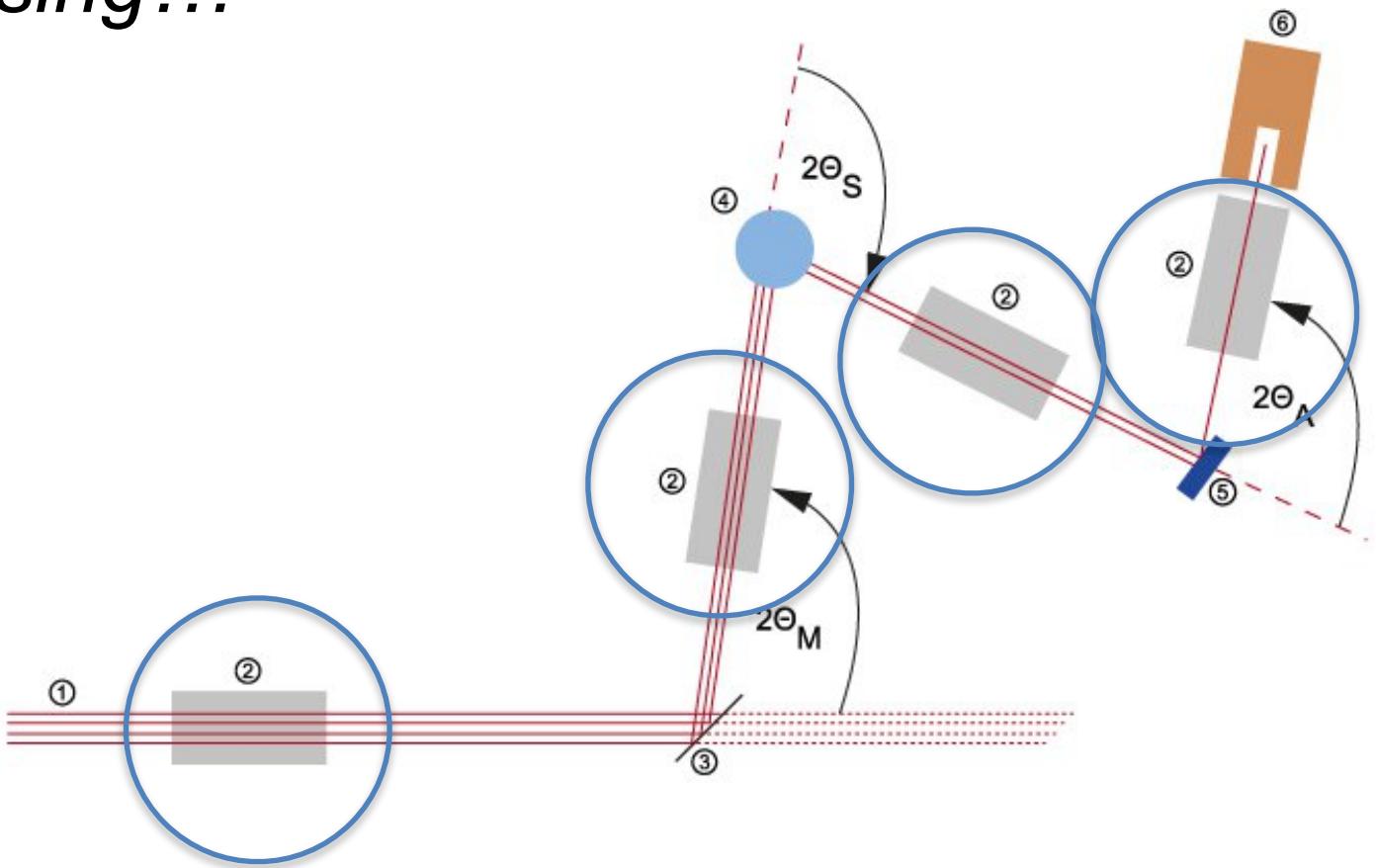
- | Spectrometer with 3 “axes”
- | 3. Define outgoing beam k_f by an analyser crystal (Bragg’s law)



TAS essentials



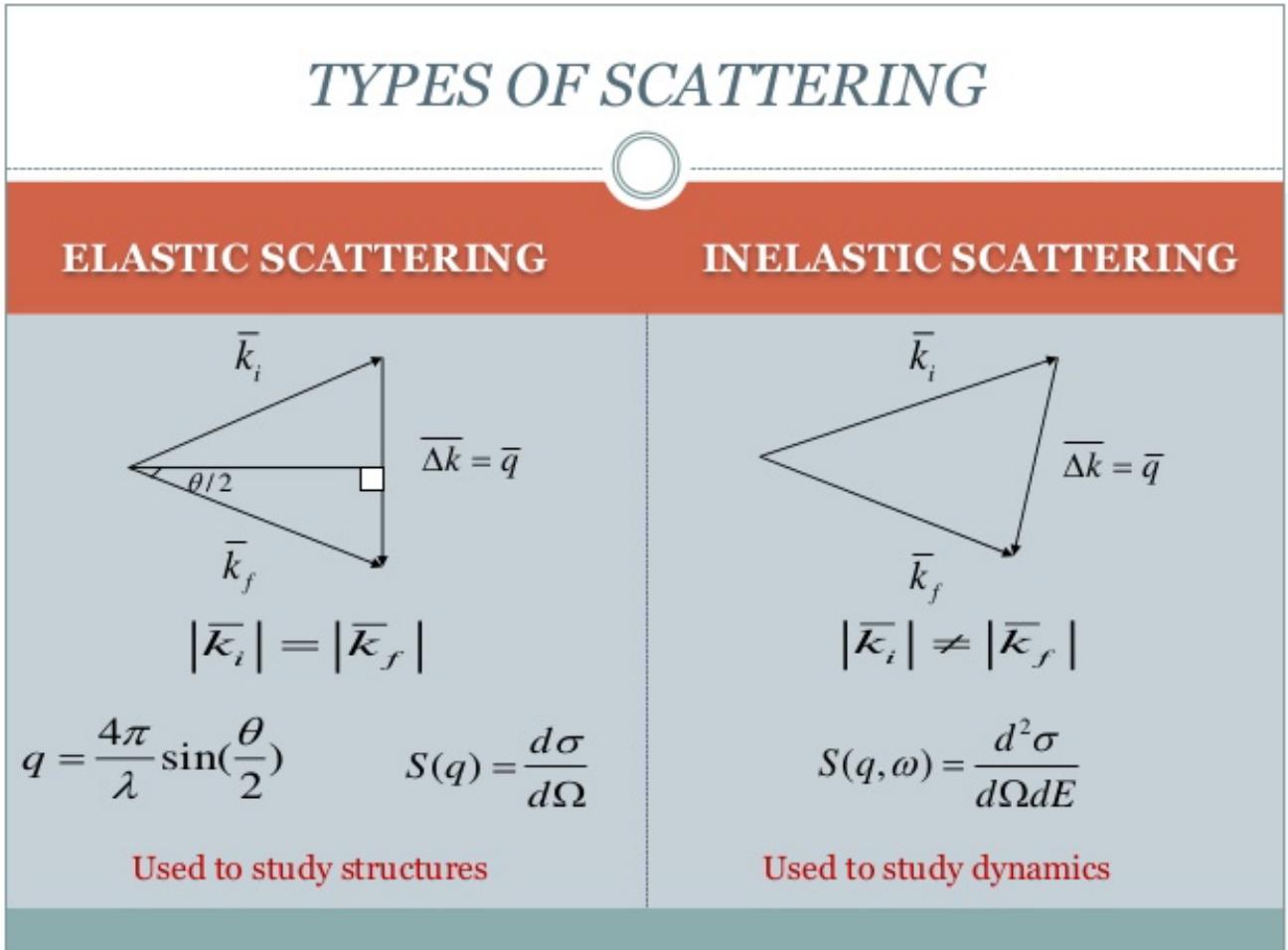
- | Spectrometer with 3 “axes”
- | As a start we will not add collimation or consider focusing...



TAS essentials



... with these 3 axes, we can study momentum-energy-transfer in the sample-beam interaction



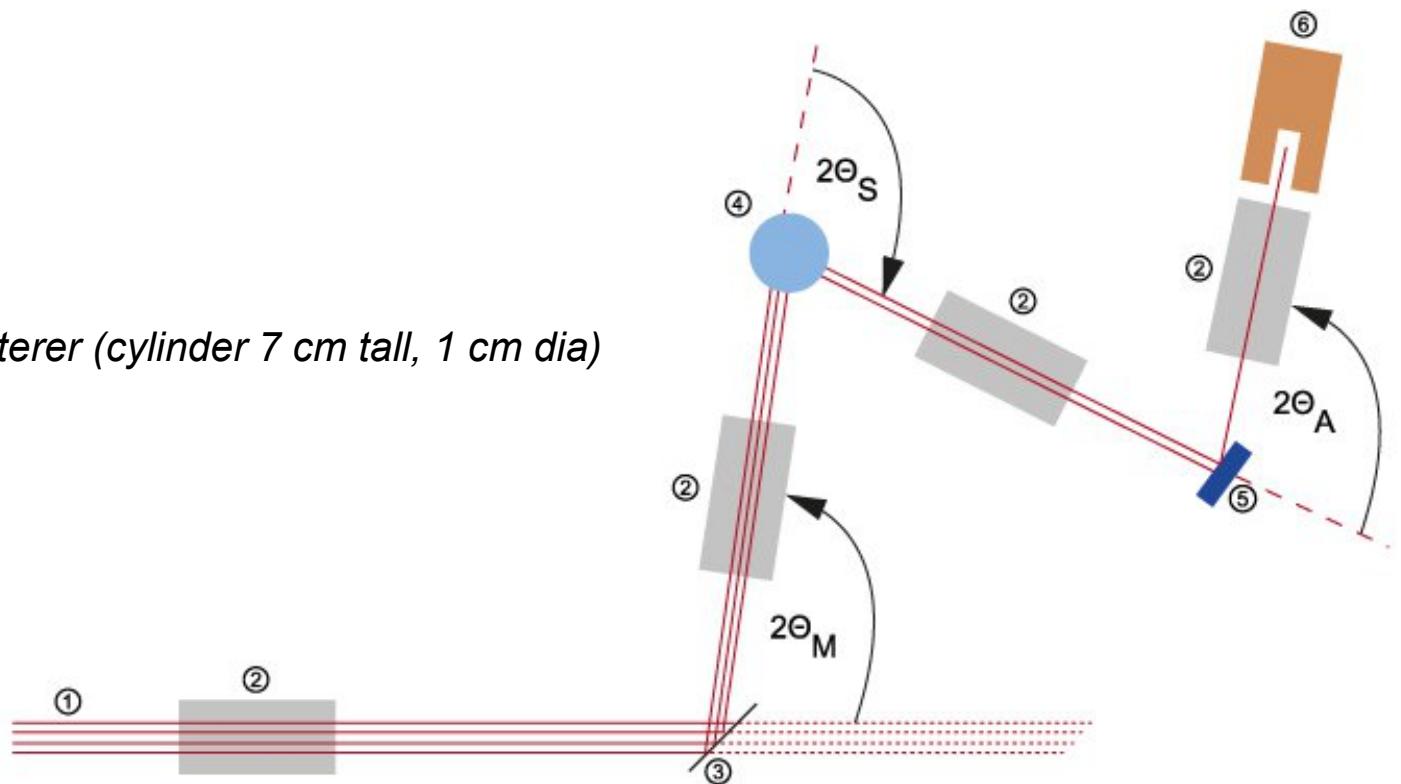


Task 1: build a simple, non-optimised TAS (5 min)

- Assume “thermal” source, e.g. parameters of ILL Thermal tube in Source_gen
 - Hint: use the mcdoc utility!

“Reactor-face” TAS

- Mono:
 - @ 3 m
 - 10x10 cm mono, PG002
 - No focusing
- Sample pos:
 - Start with Incoherent scatterer (cylinder 7 cm tall, 1 cm dia)
 - 2 m from mono
- Analyser
 - @ 1m from sample
 - 10x10 cm mono, PG002
 - No focusing
- Detector
 - PSD



- You can of course use other monitors along the way if you wish
- Recommendation: Use Arm's for the rotation (in- and out-going)
- Recommendation: Use rotation-angles of (A1,A2) (A3,A4) (A5,A6)

Once built, perform scan



- | Set up for 2\AA neutrons at both ana and mono
- | Perform a “rocking curve” i.e. A1 scan
- | Go Go Go!!
- | Clock is ticking!!





Let's cheat a little: template TAS

- | *Lots of work done for you, including:*
- | *Reciprocal space calculator
(from original TASmad code)*
- | *Automatic focusing options for both Mono
and Ana*





Plus special features for this course:

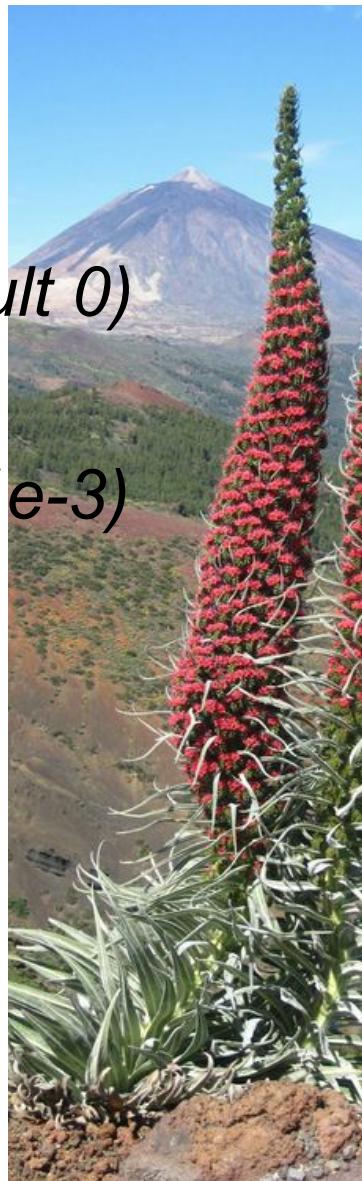
1. New samples added, with parameters

a. Single crystal related:

- SX: Flag to indicate use of Single_crystal (default 0)
- mosaic: SX mosaicity in arc minutes (default 30)
- delta_d_d: SX lattice spacing variation (default 1e-3)
- Eplus: additive energy term (SX is elastic only)

b. Res_sample related:

- RES: Flat q/E resolution mode (default 0)





Run a scan

YOU DO THIS



- Download [this BCC structure](#) to your working folder*



- Perform an elastic scan around (100):*

```
mcrun templateTAS.instr QH=1.9,2.1 QK=0 QL=0 SX=1 Sqw_coh=BCC_fake.lau -N21 -n1e4
```



- And an energy-scan (no inelastic contribution from sample)*

```
mcrun templateTAS.instr QH=2 QK=0 QL=0 EN=-1,1 SX=1 Sqw_coh=BCC_fake.lau -N21 -n1e4
```



- Reduce mosaic and delta_d_d to “very small” values to mimic a delta function. Use to estimate elastic resolution.*



Run a simulation, e.g.

`mcrun templateTAS.instr QH=2 EN=0 RES=1`

Use the command line util `mcreplot.pl` to look at the resolution ellipsoid

