McStas: dynamics in single crystals

Sample overview reminder: Currently, SX + inelastic not so easy…

	McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
5	Single_crystal *McStas team*	Bragg spots, tabular input (lau). "Perfect imperfect" single crystal with mosaicity / lattice variation	Single crystal and MX diffraction	✓	✓	✓ (Bragg spots)	✗	✓	✓

Single_crystal is elastic only….

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10	Phonon_simple *McStas team / Kim Lefmann*	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	✗	✗	✗	✓ (phonon, at this point FCC lattice only)	✗	✗

Phonon_simple is inelastic only…. (and BCC only…)

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14	Spot_sample *Garrett Granroth, SNS/ORNL*	Resolution-oriented sample component Dirac delta-functions in (Q and energy)	Inelastic scattering	✗	✗	✓	✓	✗	✗

Spot_sample is “not a material”, provides

δ-functions in Q,ω only

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15	Union components, Mads Bertelsen, NBI/KU	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, ...)

Union components allow to combine features of Single_crystal and Phonon_simple + adds phonon polarisation

DTU ess EUROPEAN SPALLATION SOURCE

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17	"4D S(\vec(Q),\omega)" Duc Le - soon at ISIS STFC?	Ala Isotropic_Sqw, but with crystal lattice	Elastic and inelastic experiments with crystals	✅	✅	✅	✅	✅	?¿?

Contribution from Duc Le, ISIS STFC is not in the code tree yet: It is unfortunately McStas 2.0 specific.
Provides a "4D equivalent" of Isotropic_Sqw - and has flat sampling in that 4D-space: relatively slow, big files, requires lots of statistics

But - could we do a hack maybe?

- *How about using Monte Carlo to choose between the different components? :-)*
- *I.e.:*
- *0.3 x*
- *+*
- *0.7 x*

5	Single_crystal *McStas team*	Bragg spots, tabular input (lau). "Perfect imperfect" single crystal with mosaicity / lattice variation	Single crystal and MX diffraction	✓	✓	✓ (Bragg spots)
10	Phonon_simple *McStas team* / *Kim Lefmann*	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	✗	✗	✓ (phonon, at this point FCC lattice only)

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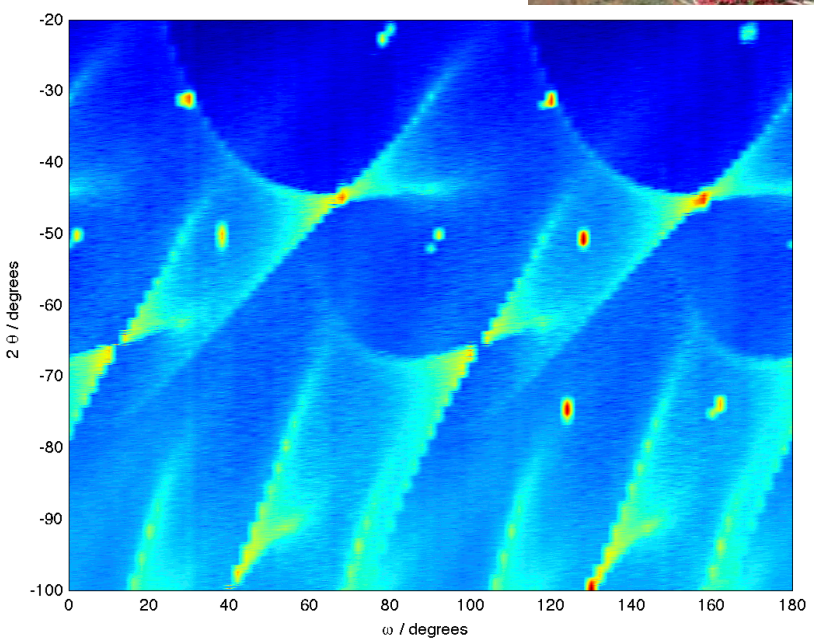
… there is a hack, recipe:

```
INITIALIZE %{
  declare select_sample;
%}

Arm ()
…
EXTEND %{
  select_sample = rand01();
%}

COMPONENT SX= Single_crystal(…)
WHEN (select_sample < 0.3)
…
COMPONENT Phonon = Phonon_simple(…)
WHEN (select_sample >= 0.3)
…
```



In this exercise you will have access to an instrument that uses this type of hack

The instrument is found on the DropBox:

Magnon_bcc_visualisation.instr

and needs the .lau and .comps also found there:

BCC_fake.lau
Magnon_bcc.comp
Sqq_w_monitor.com

!! PLEASE COPY FILES ACROSS – WORKING DIRECTLY IN /media/sf_Shared_folder CAN CAUSE ISSUES !!

(For the time being, skip the TAS_Magnon.instr instrument)

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New, purely inelastic component from Kim Lefmann 2018.

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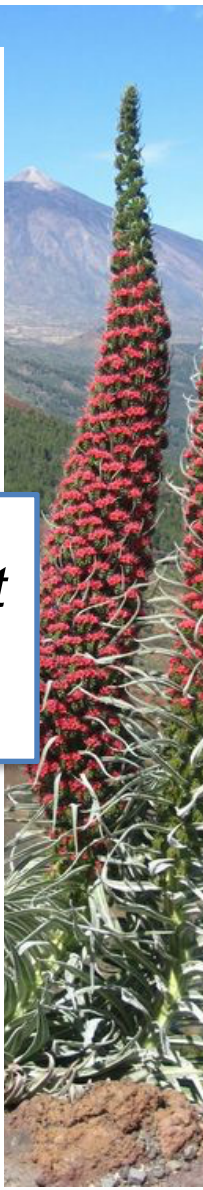

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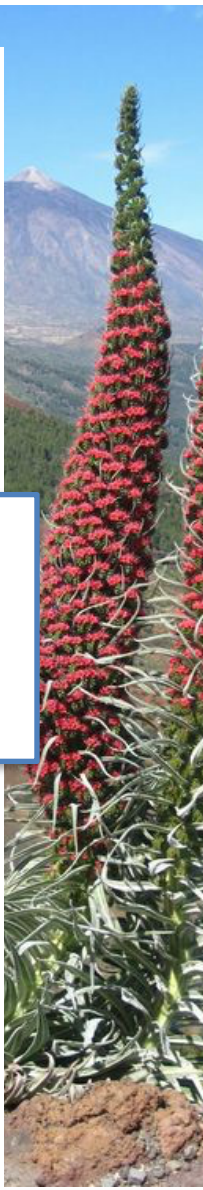
Magnons are related to spin-waves, but there are subtle differences - Sylvain? :-)

(For the time being, skip the TAS_Magnon.instr instrument)

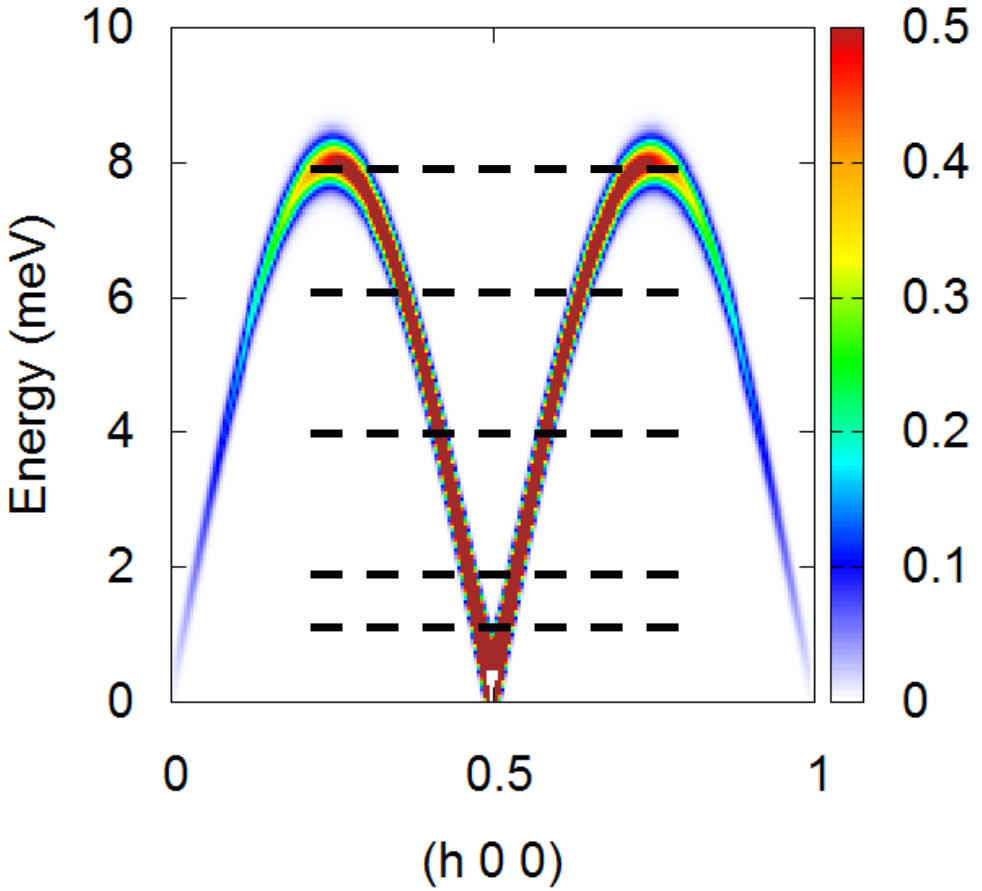


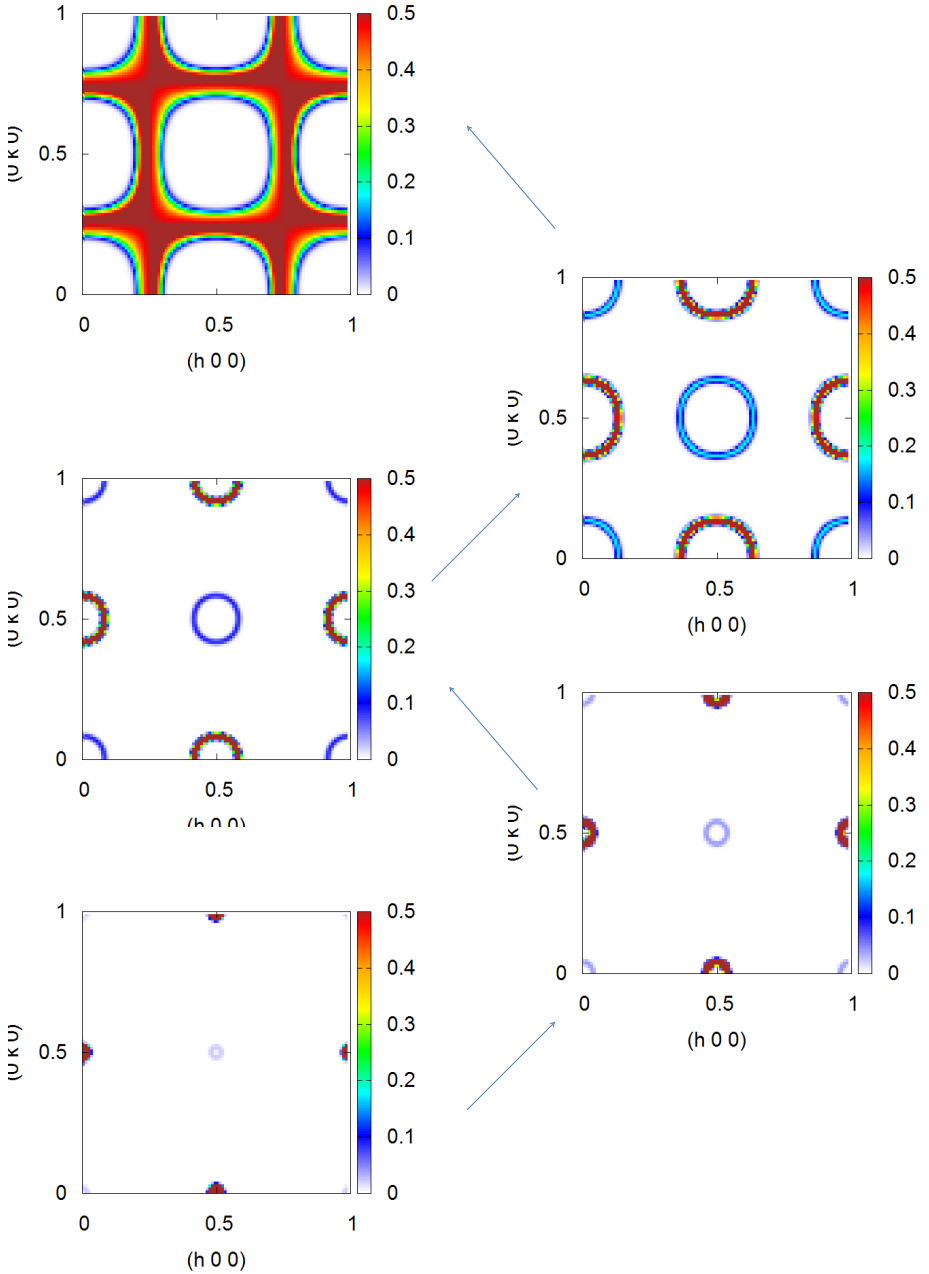
SPIN WAVES = MAGNONS

MORE GENERALY

MAGNONS : $\Delta S = 1$ EXCITATIONS

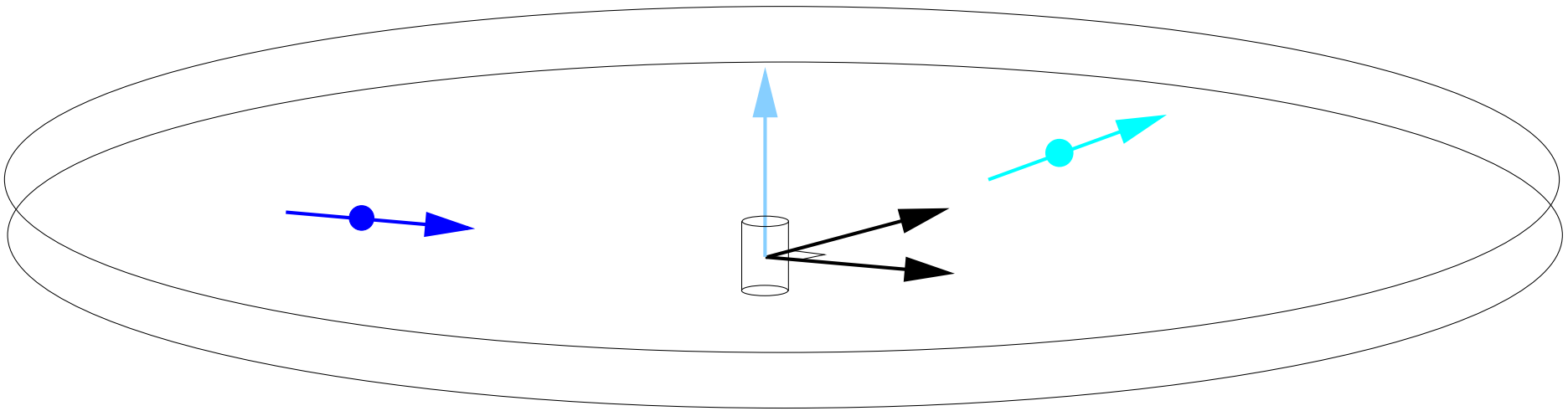
« Slicing a cone »





Instrument contents

- *White-beam source*
- *Selection between Single_crystal and Magnon_bcc.comp*
- *A “scattering-plane” inelastic monitor that “cheats” by directly measuring*
  k_i and k_f



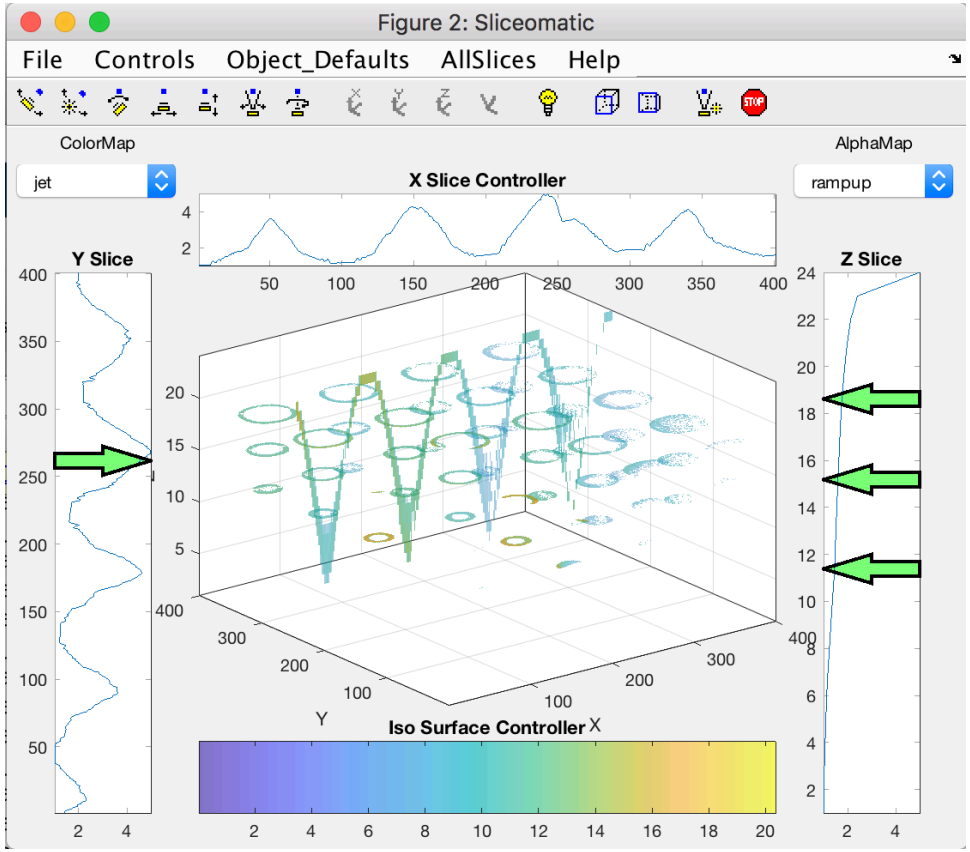
Tasks:

1. Locate the instrument file, compile and visualise “as usual”
2. In terminal run mcdoc Magnon_bcc_visualisation.instr
3. In terminal run mcdoc Magnon_bcc.comp and check how comp is used in the instrument file
4. In terminal run mcdoc Sqq_w_monitor.comp check how comp is used in the instrument file
5. Run a long simulation (1e7-8) and plot the results (log)

Tasks - 2

5. Load and view in Matlab / iFit using:

- *– use the loadvol.m script from the DropBox*
- *Vol=loadvol('your_datadir');*



Optional exercise

6. If you are longing for some more TAS :-)

Try modifying TAS_Magnon.instr for the same Single_crystal and Magnon_bcc setup as found in the visualisation instrument

Make it work and do some nice scans :-)

Optional exercise

- *7. Try including a Phonon_simple instead of the Magnon_bcc component - use either of the previous instruments*