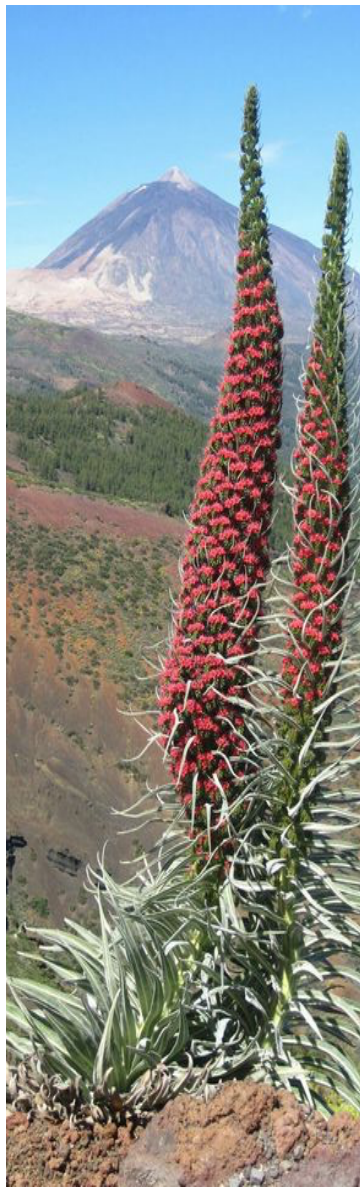
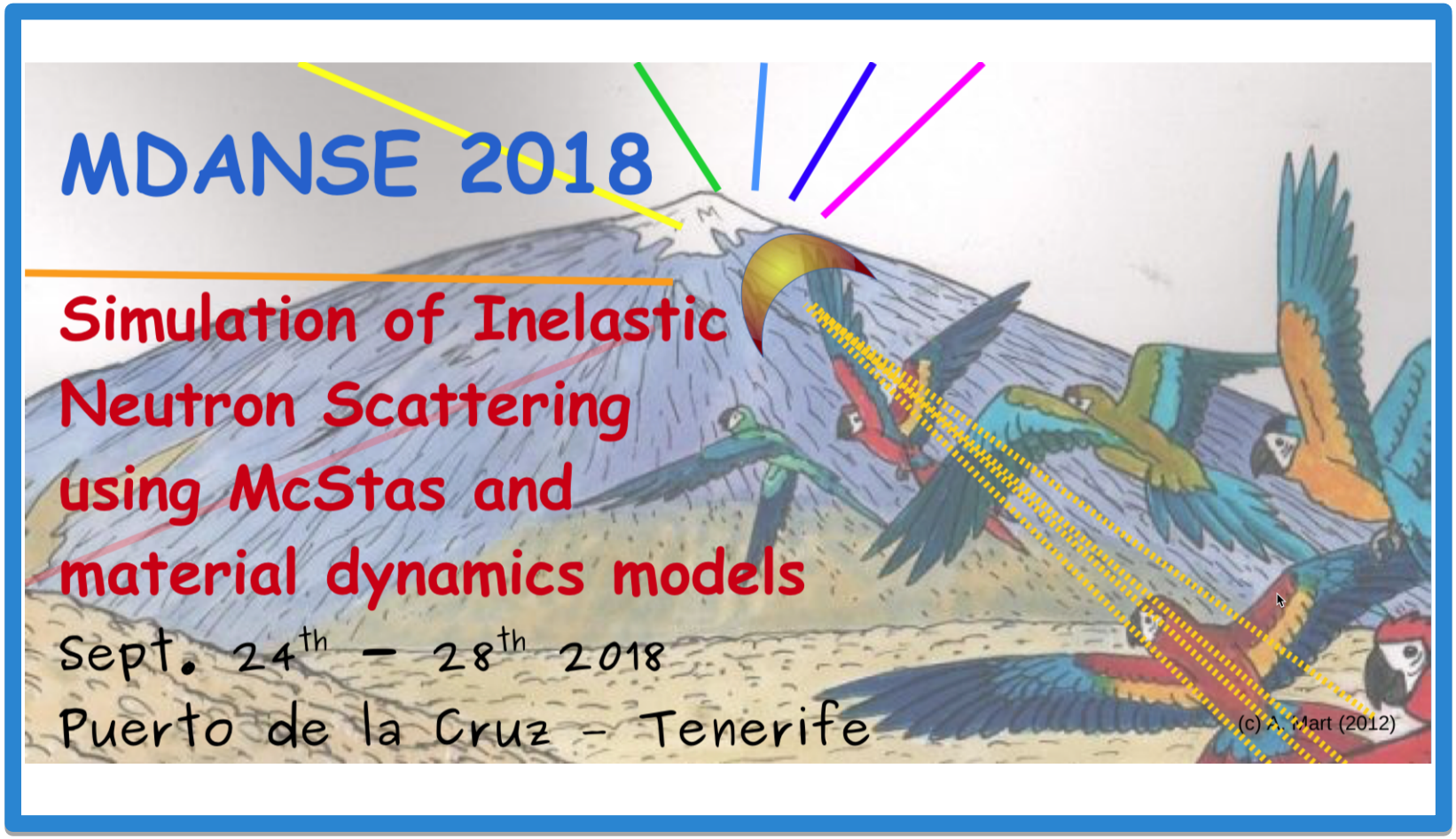
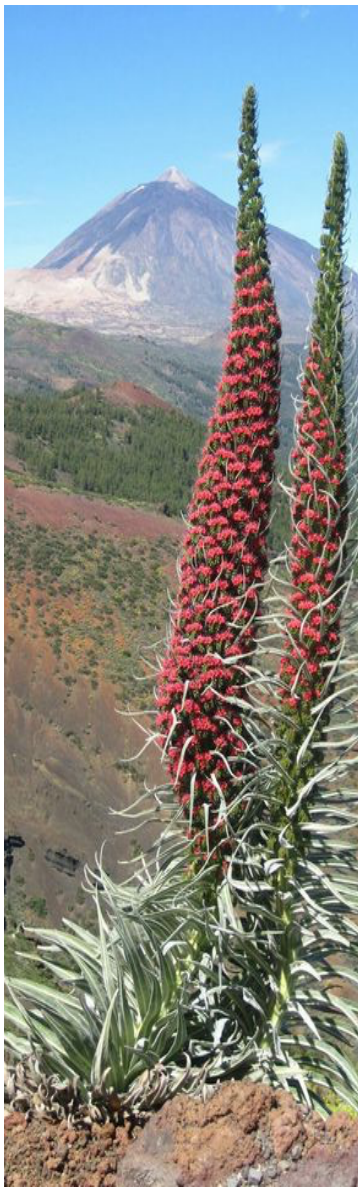
Practical J, McStas samples





Agenda

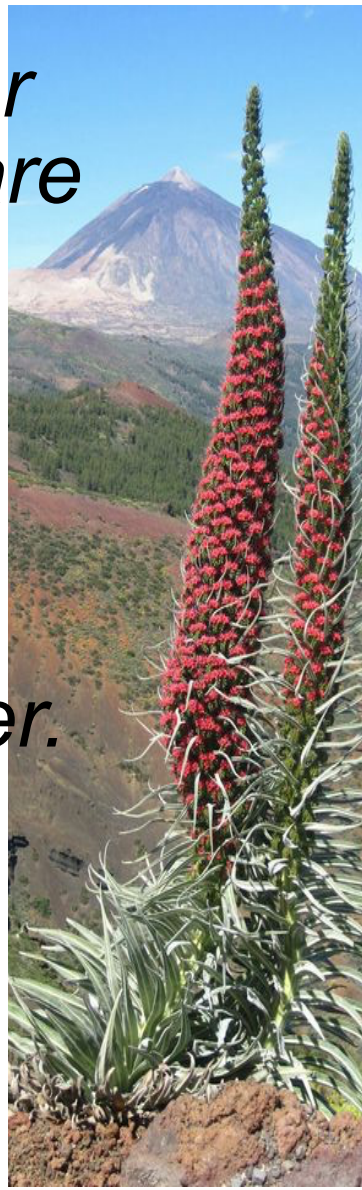
- *Structure*
  - *PowderN*
  - *Single_crystal*
  - *Union*
- *Small angle scattering*
- *Connections to other pieces of software*



PowderN exercise

In this exercise we will try to put two powder samples together in a few ways and compare the results.

1) *Two samples in the same spot, and stochastically choose between them*
2) *Two samples stacked vertically*
3) *Two samples where one is behind the other.*



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PowderN exercise

Let's use the PSI_DMC instrument as a starting point. We will now make the simulation randomly choose between two powders.

1) *Add another powder in the same spot as the one already there.*

2) *Add* `double r;` *inside the* `DECLARE` *section of the instrument file.*

3) *Add an Arm in front of the first one, and add to it an* `EXTEND`*-block. Add the following code in it:* `r=rand01();`

4) *Now add the following before the AT on the two powders.* `WHEN(r<0.5)` *and* `WHEN(r>0.5)` *respectively.*

5) *Run the instrument again – Do you get what you expect?*

6) *What would you change to make the mixing factor !=0.5?*

PowderN exercise

Let's change this to have two samples on top of each other.

1) *Make a new copy of the instrument (or remove the edits you did before, leaving the second Powder sample in place).*
2) *Change the y-position and size of the samples to be +- height/2.0 and height/2.0 respectively*
3) *Add the statement* `GROUP sample` *after the AT at both samples. (N.b. sample is a name chosen arbitrarily. It has to be different than the component names though.)*
4) *Run a simulation – is there any difference to the previous result? Why/Why not?*

PowderN exercise

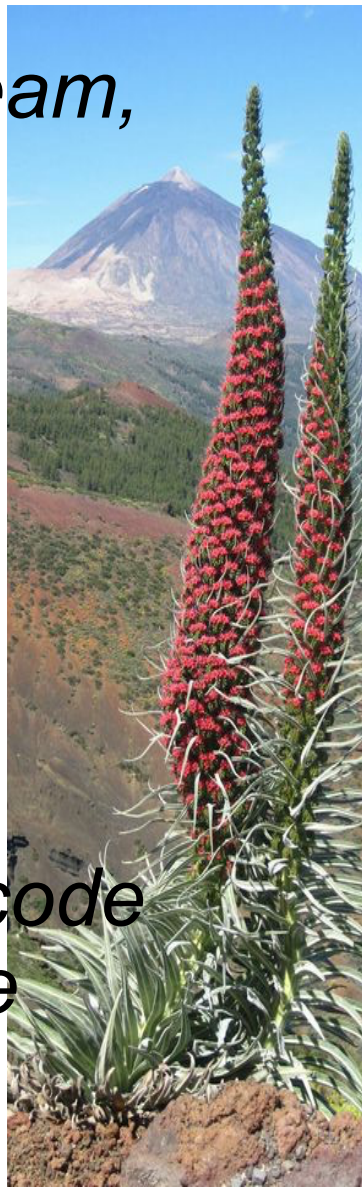
Move samples around such that one is in front of the other.

1) Run a simulation – Do you still see the signatures of both samples?

2) Do you remember why this can be?

3) How can we get around this?

Intermission:
A quick trick to remove the direct beam



- *If your monitor also can be hit by the direct beam, "swamping" the signal, you can do this:*

  Add the following code just after your sample code:

```
EXTEND
%{
  if (!SCATTERED){ABSORB;}
%}
```

- *This will terminate all rays which the sample-code has not flagged as scattered. Bear in mind the McStas definition of scattered includes many things (guide-wall reflections etc.)*

SANS models

- *Get a new instrument: We'll use the ISIS_SANS2d*
- *We'll explore some of the SANS-options that exist in McStas.*
- *The SANS2D-model does not include a sample, nor detector at present, so we'll add that in. Add Ls2d and RR to your* **DEFINE INSTRUMENT** *line in the top of the file to be able to scan them.*

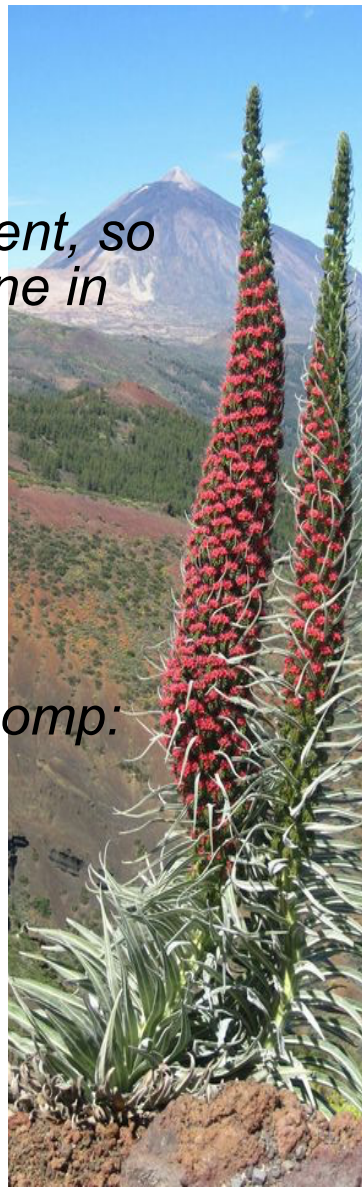
1) *Add a PSD_monitor to replicate the detector:*

```
COMPONENT detector_front = PSD_monitor(
  nx = 200, ny = 200, filename = "PSD.dat",
  xwidth = 1, yheight=1, restore_neutron=1)
AT(0,0,Ls2d) RELATIVE sample.
```

2) *Add a sample – First we'll use the the standard SANS_spheres comp:*

```
COMPONENT sample = SANS_spheres(
  xwidth=0.01, yheight=0.01, zdepth=0.001,
  focus_xw=1, focus_yh=1, target_z=Ls2d,
  R=RR, Delta_rho=0.6)
AT (0, 0, 0.2) RELATIVE psd4
```

Now run a simulation to see what you get.



SANS models

- *Now we shall explore the possibilities that SasView_models can give us. Change the sample to a SasView_models.comp. Keep the target parameters but change the last line to:*

  `model_index=51, model_pars={1,7,50}`

- *The model_index indeicates which of a large number of models scatterung fucntions) the sample is using. You can use mcdoc to find out which, and what the parameters mean. Try to generate a picture similar to the one before.*

- *Try a couple of the other SasView_models.*

  `ex. model_index=23, model_pars={50,0.2}`

SANS models

- *2D SANS images are all fine – but wouldn't it be better if we could let the computer do the radial integration for us?*

  recipe: Insert another monitor – for instance a **`Monitor_nD`** *with* **`options="radius ..."`**

  or an instance of **`SANSQ_monitor`**

- *Remember to use* **`mcdoc`** *– it's your friend!*

Union exercise

- *Start the McStas GUI (“**mcgui**”) and “**Open**” (a copy) of “**Union_test_absorption_image.instr**”*
- *Run the instument as is – to get a starting pt.*

  This is an image of a sample stick inside a cryostat.
  The compilation step takes a bit of time so be patient.
- *Open the instrument file and, by looking at the definition of the Al-material, change the cryostat drum material to be made of Iron. (Tip: take a peek at the data file “Fe.laz”. It resides inside “/usr/share/mcstas-2.4.1/data”)*
- *Try to add a sample that diffracts strongly (NaCaAlF?) and see if you can catch some powder diffraction on a detector. You may have to add a new monitor with a different size and shape to see it.*