

# Practical E, Diff., Laue Cam.



**MDANSE 2018**

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

Sept. 24<sup>th</sup> – 28<sup>th</sup> 2018

Puerto de la Cruz – Tenerife

(c) A. Martí (2012)





# First things first

Move the ASE python environment  
out of the way

Issue the following command in a terminal  
in your home directory.

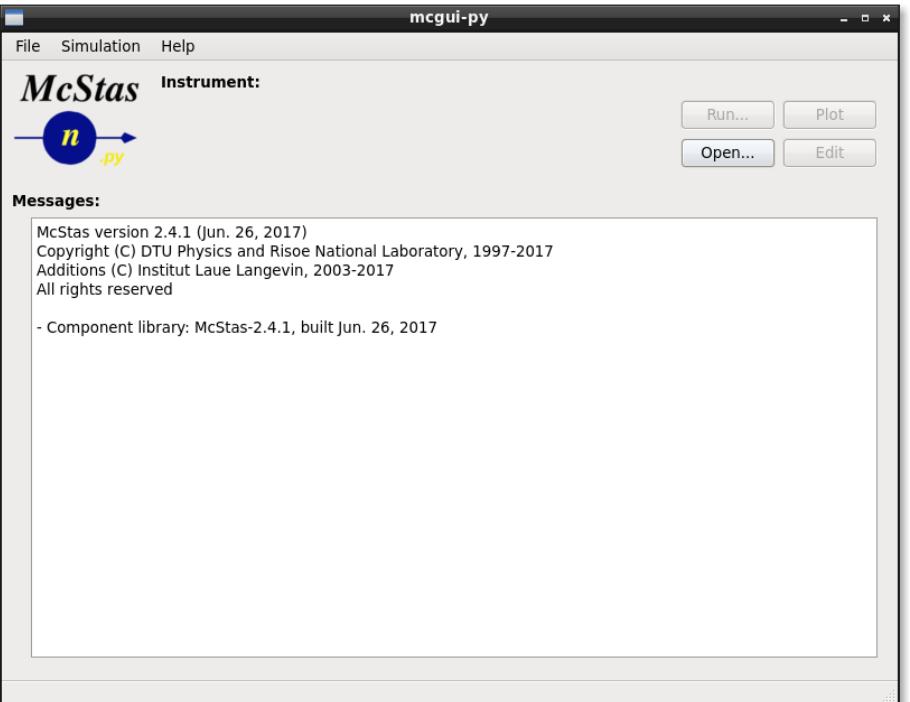
“mv miniconda3 miniconda3\_gone”





# Second things second

- Try to run “**mcstas-2.4.1-environment**” (tab completion works!)
- In this new shell run “**mcgui**” (tab completion does not work)
- You should now have:





# Agenda

- ★ *Laue Camera*  
*Build along in 4 steps!*
- ★ *Diffractometer*
  - *PSI\_DMC*
- ★ *Laue Camera revisited*





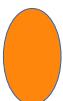
# Build along Laue Camera

First insert a source

File → New Instrument

Insert → Sources → Source\_simple

```
// insert components here (e.g. Insert -> Source -> ...)  
COMPONENT source_simple = Source_simple(  
    radius=0.05,  
    dist=5,  
    focus_xw=0.02,  
    focus_yh=0.05,  
    lambda0=2,  
    dlambda=1.9)  
AT (0, 0, 0) RELATIVE PREVIOUS
```



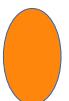


# Build along Laue Camera

Now add a guide

Insert → Optics → Guide

```
COMPONENT guide = Guide(  
    w1=0.02, h1=0.05, w2=0.02, h2=0.05, l=20, m=1)  
AT(0,0,2) RELATIVE source_simple
```



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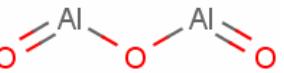




# Build along Laue Camera

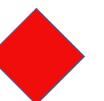
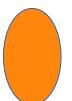
Add a sample – in this case a standard crystal

Insert → Samples → Single\_crystal



```
COMPONENT single_crystal = Single_crystal(
    reflections="Al2O3_sapphire.lau",
    yheight=0.05, radius=0.01, mosaic=1, delta_d_d=1e-4,
    az=4.757, ay=0, az=0, bx=2.3785, by=0, bz=-3.364,
    cx=0, cy=12.9877, cz=0,
    p_transmit=0.1)
```

```
AT (0, 0, 0) RELATIVE PREVIOUS
```



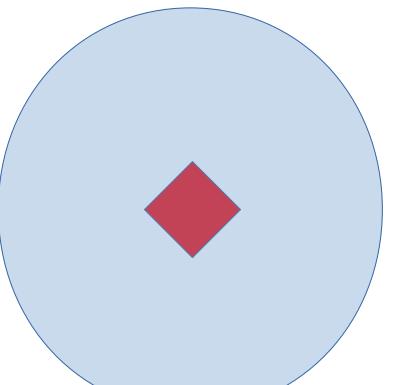
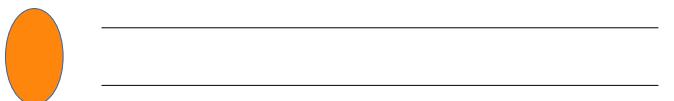


# Build along Laue Camera

Add *the* ideal Laue Camera Monitor – covering  $4\pi$

Insert → Monitors → PSD\_monitor\_4PI

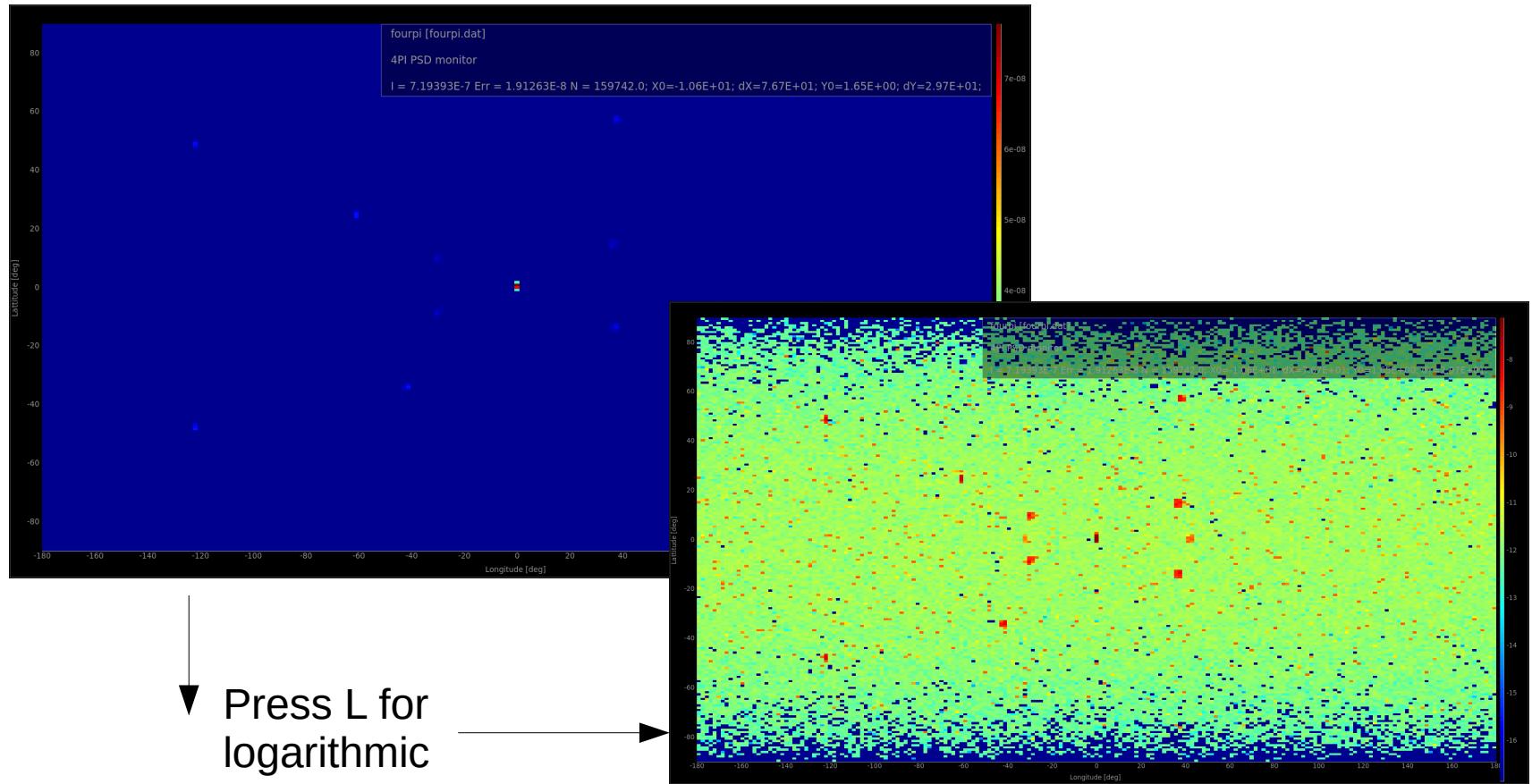
```
COMPONENT fourpi = PSD_monitor_4PI(  
    radius=1, filename="fourpi.dat", nx=201, ny=201)  
AT(0,0,0) RELATIVE PREVIOUS
```





# Build along Laue Camera

Run your simulation (you can safely increase the number of rays to  $10^7$  the ncount) – you should get something like:





# Build along Laue Camera

*Play around with this example instrument:*

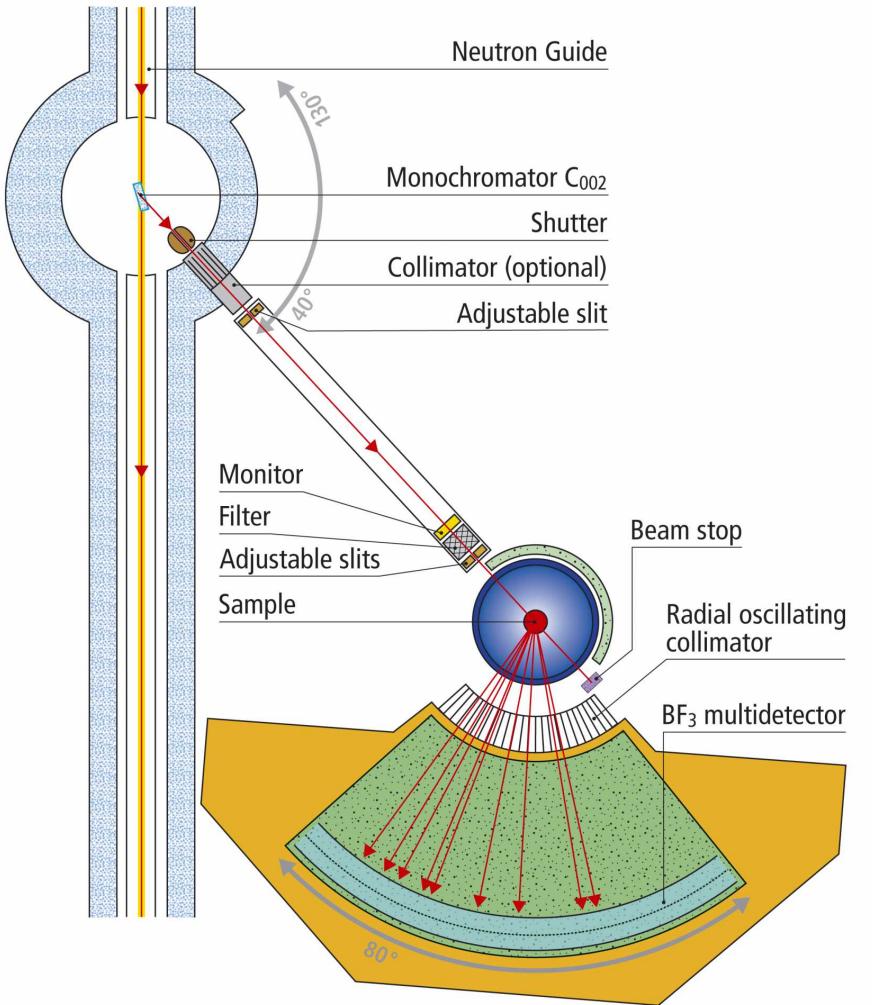
- Add an `Arm` components before the sample to allow rotation around the Y-axis.
- Add “**SPLIT 20**” before the sample **COMPONENT** statement. What happens?
- Try to extend this to Y, Z, Y rotation (Eulerian cradle).
- Insert a different crystal instead e.g. “**Al.lau**”. i.e. change the crystal unit cell parameters and the reflection list.
- Insert a powder sample instead





# Real Instruments

## PSI DMC



File → New from  
Template → PSI\_DMC

Run the instrument with  
it's default parameters.

Now we'll try to insert a  
Single crystal instead of  
the default Powder.

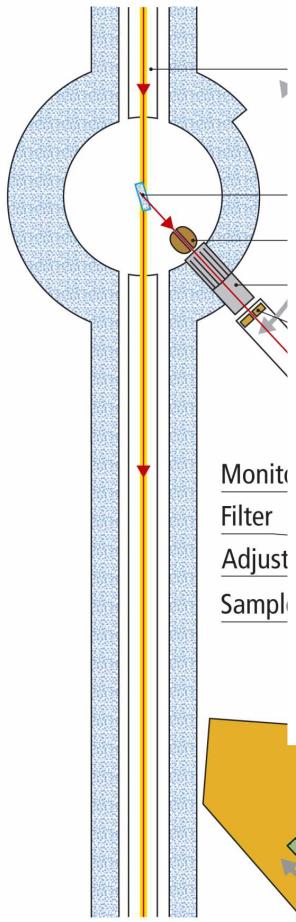




# Real Instruments

PSI DMC

Increase the height of the detector and make it resolve the signal along y.



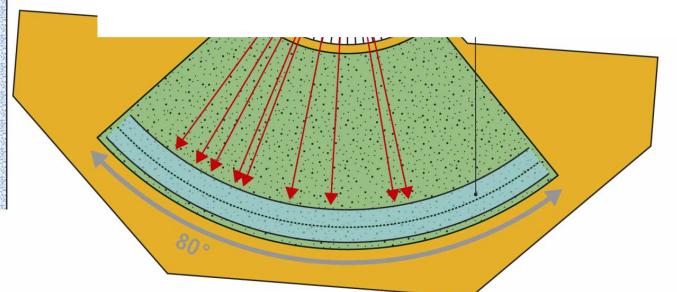
Set:

**Options="banana, theta y auto limits bins=20", yheight=0.3**

In the detector.

...and change the sample to be e.g. an Aluminium crystal.

```
COMPONENT single_crystal = Single_crystal(
    reflections="Al.lau",
    yheight=0.05, radius=0.01, mosaic=1, delta_d_d=1e-4,
    az=4.0495, ay=0, ax=0, bx=4.0495, by=0, bz=0,
    cx=0, cy=4.0495, cz=0,
    p_transmit=0.1)
AT (0, 0, 0) RELATIVE PREVIOUS
```





# TOPAZ and SENJU

Take a look at a couple of “real” instrument simulations of Laue Cameras: they both resides in the Dropbox under  
“25th\_Tuesday/Practical\_E\_McStas\_Diffraction, Laue”

1. SNS TOPAZ
2. J.PARC SENJU (aka. BL18)

Here you need to also copy a datafile for the J-PARC source  
“source\_BL18.txt”

Surgeon General's Warning:  
There are lots of COMPONENTS here

