Practical:

Single crystals and powders

2019 CSNS McStas School

Agenda

- *Laue Camera*
- *Use and modify the diffractometer*
  - *PSI_DMC*

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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
```

Laue Camera

Now add a guide

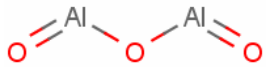
Insert → Optics → Guide

```
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
```

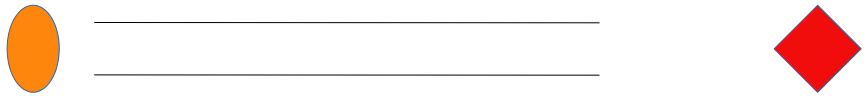
Laue Camera

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, order=1)
AT (0, 0, 20.5) RELATIVE PREVIOUS
```

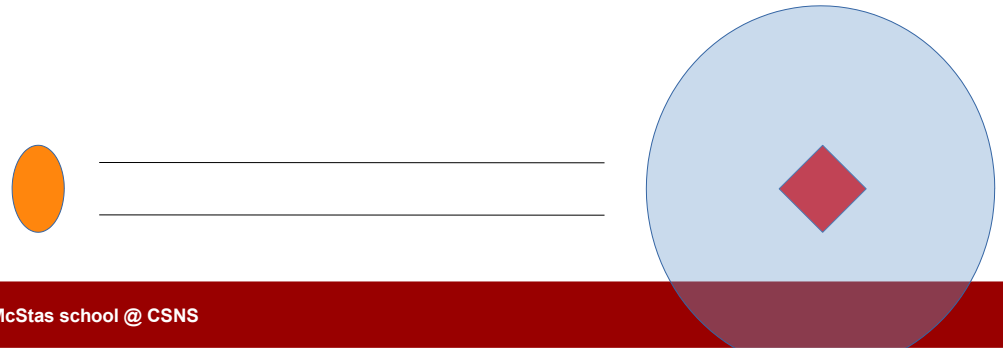


Laue Camera

Add *the* ideal Laue Camera Monitor – covering 4π

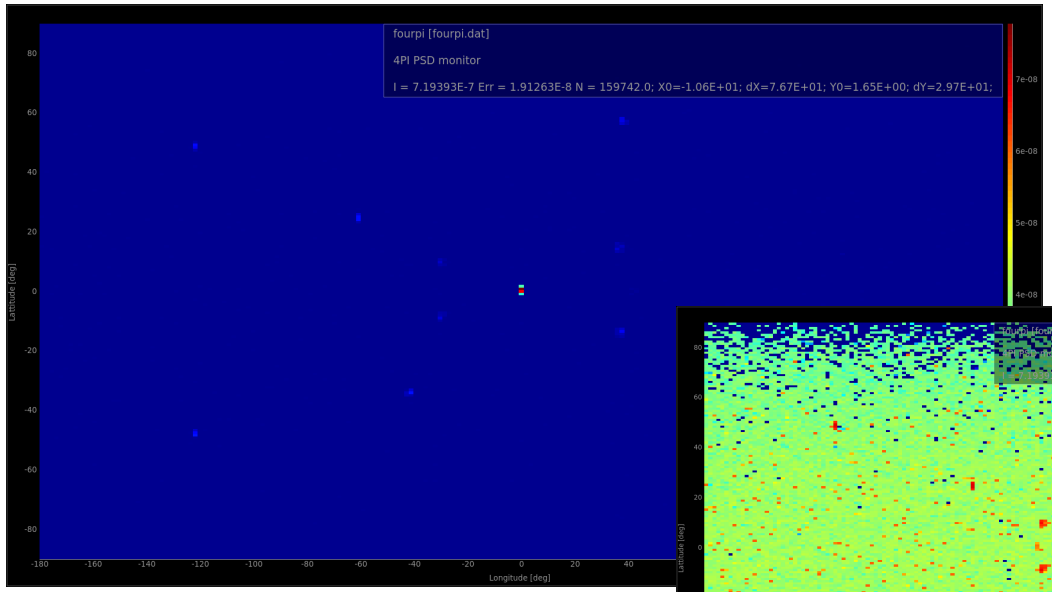
Insert → Monitors → PSD_monitor_4PI

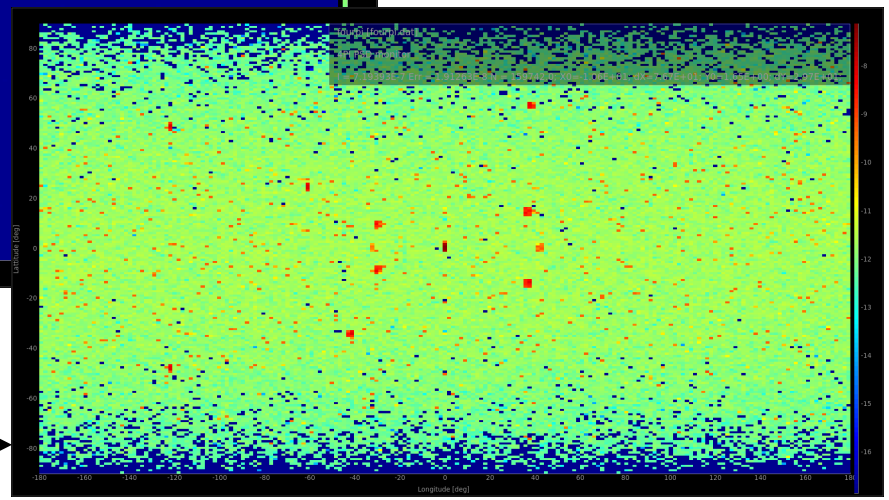
```
COMPONENT fourpi = PSD_monitor_4PI(
    radius=1, filename="fourpi.dat", nx=201, ny=201)
AT(0,0,0) RELATIVE PREVIOUS
```



Laue Camera

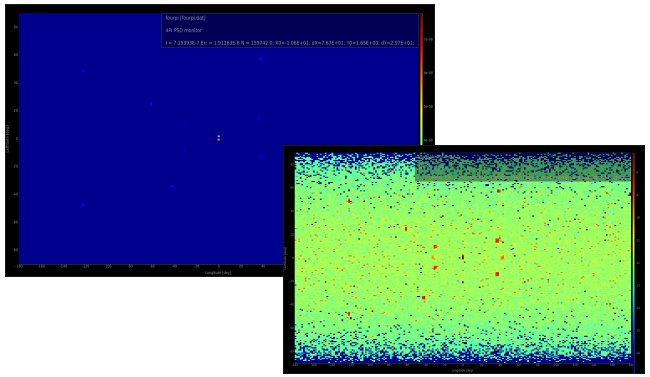
Run your simulation (you can safely increase the number of rays to 10^7 - the ncount) – you should get something like:





Press L for logarithmic

Laue Camera



The coherent scattering is not much stronger than the incoherent “background”. Let’s use EXTEND and WHEN to make a monitor which only senses the coherent signal.

- In the DECLARE section of your instrument – declare a variable of `type char;`
- Add an EXTEND-block to the end of the Single_crystal component:
- `EXTEND`
- `%{`
- `  myvar = hkl_info.type;`
- `%}`
- Add another 4-PI monitor and insert `WHEN` (myvar==99) in front of the AT keyword. (99 is the ascii-code for ‘c’)
- Think of a possible way to only monitor incoherent scattering… HINT: type==’i’ for incoherent

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?
  - Add a set of arms before the sample to add Y, Z, Y rotations (Eulerian cradle). Make the rotation angles input parameters.
  - 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

PowderN and More

- *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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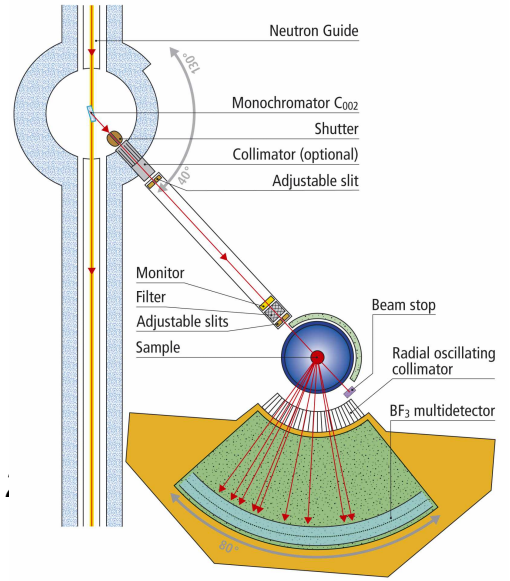
PowdersN and more



- *Let's use the PSI_DMC instrument as a starting point. We will now make the simulation randomly choose between two powders. The instrument file can be found in the McStas distribution. (File → New from template → PSI → PSI_DMC)*

1) *Add another powder in the same spot as the one already there. Look in the mcstas data directory for sample .laz-files*
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 – Do you get what you expect?*
6) *What would you change to make the mixing factor !=0.5?*
7) *Use a similar technique to the Laue camera to make the detector only catch scattering from one sample.*

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PowderN and More

- *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, but leave the second PowderN sample in place).*

2) *Change the y-position and size of the samples to be:* `+-sample_height/4.0` *and* `sample_height/2.0` *respectively*

3) *Add the statement* `GROUP samples` *after the AT at both samples. (N.b. "samples" 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 and More

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

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

Do you remember why this can be?

2) *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. Note that the McStas definition of scattered includes many things (guide-wall reflections etc.)*

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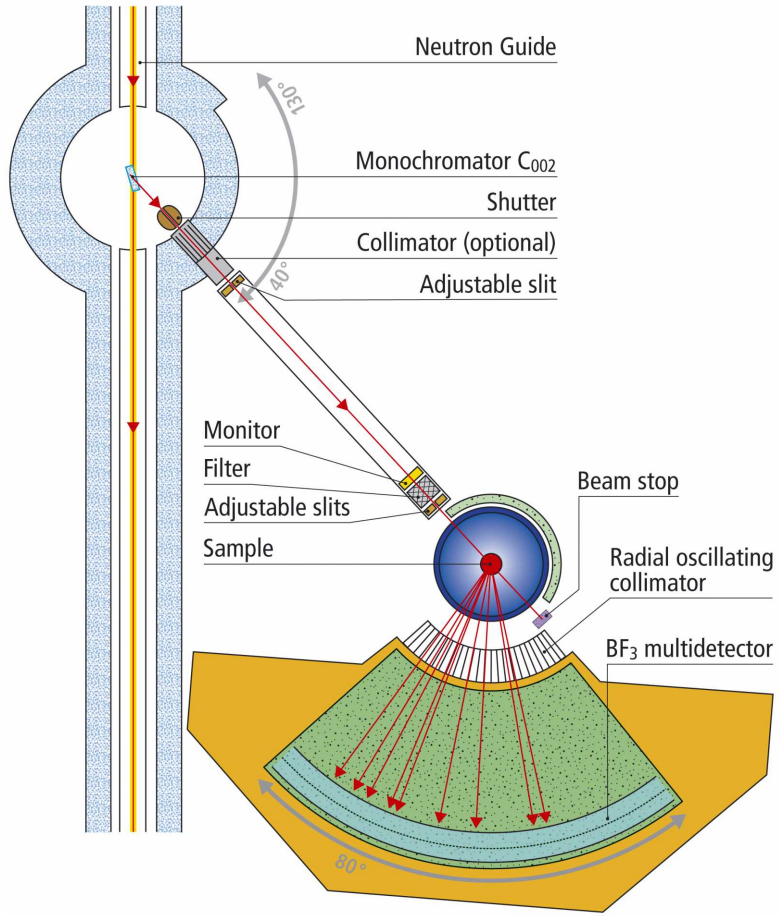
PowderN and More



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.

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
```

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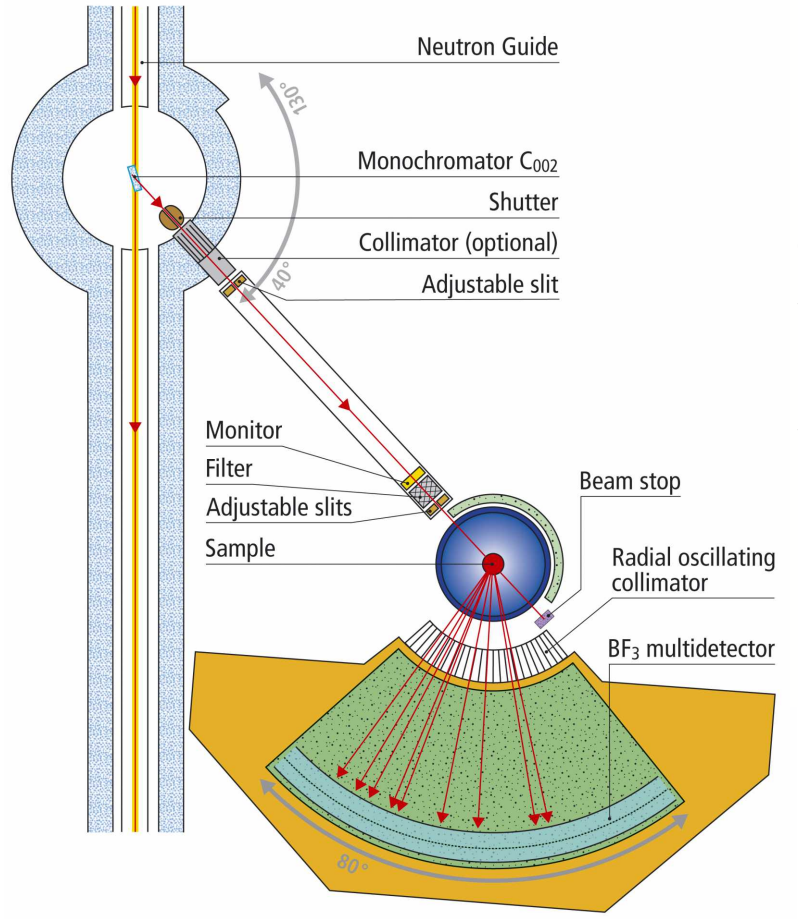
PowderN and More



Insert more detector banks to modify DMC to become more like a Laue camera (catch more of the crystal signal). New banks could be above and below and on the other side of the sample. You will need to use a `GROUP` for this.

Increase the mosaicity of the crystal to scatter more of the beam. This can be done to an extent – think about what limits it, and how you could extract such limits from the simulations.

Using the WHEN keyword we can make a “sample changer”. Can you think of how?

HINT: similar to the earlier exercise with a mix of two crystals.