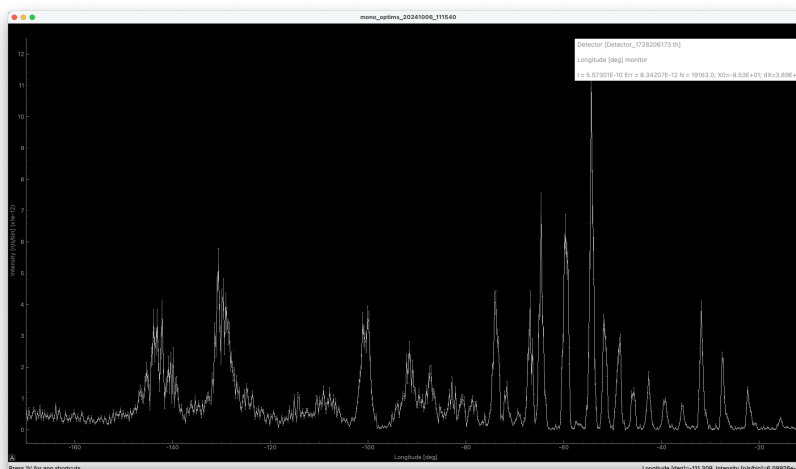


A powder diffractometer

Based on the output of the earlier exercises, we will now assemble a powder diffractometer.

TASKS

1. Find back your solution to the monochromator exercise or take one of those provided
2. Using mcdoc and the PDF information, add **PowderN** to the sample position. Sample geometry should be a cylinder of **radius=0.005** and **yheight=0.07**. Sample definition can be one of your choice, but a good candidate is **reflections=Na2Ca3Al2F14.laz**
3. Next, add a banana-shaped detector (cylindrical cut) by using **Monitor_nD** of radius 1.2 m and height 30 cm, measuring a diffractogram using **options="banana theta bins=640 limits=[-170 -10]"** - positioned AT (0,0,0) RELATIVE your sample
4. Run a simulation with **1e7** neutron rays, hopefully you have arrived at something that resembles this as a diffraction pattern. In existence, but not too

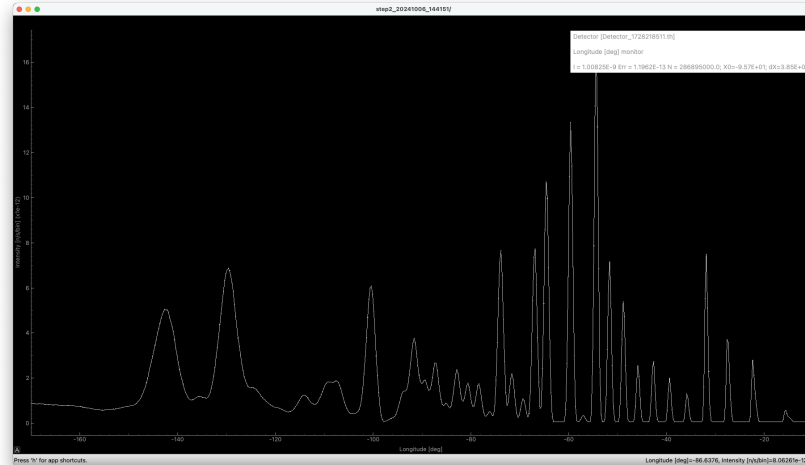


pretty...

(produced using this instrument)

5. We should now optimise a bit:
 - Assign only a tiny fraction of stats to “direct beam”, set **p_transmit=1e-6**
 - Assign just 3% to incoherent scattering **p_inc=0.03**
 - Let us use a **d_phi** limitation, corresponding to detector height / detector radius ~14 deg.
 - Let us only scatter to the negative side (detector only in place there) **tth_sign=-1**
 - Use a **SPLIT** of ~ 800, corresponding to the number of dspacings available in the reflection file

6. Rerun with MPI (auto will run on all available cores) and $1e7$ rays, much bet-



ter:

(produced using this instrument)

7. **Bonus task:** Use `mcdocto` add a radial collimator in between sample and detector
8. **Bonus task:** Add a flag (similar to e.g. `coll_in` to enable/disable your radial collimator
9. **Bonus task:** Use `NeXpy` and `NeXus` output to fit a selected peak. Do you see an improved resolution by adding the radial collimator?