MDANSE practical

- cd /PATH/TO/…/Data-Miguel/Practice_MDANSE/**Case2**
- Copy (from http://mdanse2018.essworkshop.org → 8. Dropbox:26th_Wednesday:Practical_H_MDANSE) the following files: python-netcdf4_1.2.2-2_amd64.deb, scripts.tar.gz and ref_data.tar.gz
- Install the python module to read netCDF files (the standard output used by MDANSE):
  - sudo dpkg –I python-netcdf4_1.2.2-2_amd64.deb
  - sudo apt-get install –f

MDANSE practical 2

- Start with case 2. Main goals/pitfalls:
  - Learn about subtleties converting Lammps trajectories
  - Problems when trying to compare to neutron and x-ray diffraction data
  - Analysis of MDANSE output, e.g. msd (no fitting or “secondary” analysis tools in MDANSE, so you need to write your own programs, e.g. python, Matlab, etc.)

MDANSE practical 3

- Suggest to continue with Case 5: Benzene crystal. Main pitfalls:
  - Use alias to convert correctly DL_POLY trajectories
  - No strong Bragg peaks in calculated S(Q), even if system is crystalline. S(Q) calculated as FT from g(r) with r_{max} = 1 nm → Similar to measure a nanocrystal!
  - M.s.d. of atoms vs m.s.d. of molecular center of mass
  - EISF and $F_{self}(Q,t)$ of a molecular crystal. How close are we to the theoretical 6-site jump model?

MDANSE practical 4

- Suggestions to keep working at home (when given, you need to edit the Python scripts and correct the paths there before running them):
  - Cases 5b and 6b: Compare the density of states of benzene using a flexible and a rigid model
  - Case 3: Subtleties converting Gromacs trajectories and manipulating PDB input files requested by MDANSE.
  - Case 1: Simplest case (monatomic liquid) for testing. The system is small (864 atoms), but the trajectory contains 25000 frames, so some analysis (in particular the dynamic incoherent structure factor) will take some time.