| script in **CsCl/** | Explanation | # Plots |
|---|---|---|
| **AutoCCA_84-run_v5.py** | Calculate the Auto-Correlations with 'Loki' and plot, including the mean intensity pattern, Fourier-coefficients, detector masks AC, subplot of; mean intensity patter, detector mask's AC and AC of polar images. Data loaded from CXI-file. | -plot 'single' : 17<br>-plot 'subplot' : 1<br>-plot 'all' : 18 |
| **CCA_RadProf_84-run_v2.py** | Calculate the Radial Profile, from CXI-file, with 'Loki' and the Auto-Correlation. Plot the result including som e of the diffraction patterns. | subplots : 2 |
| **CrossCA_84-run_v7.py** | Calculate and plot the Cross-Correlations from CXI-file. Plots of Fourier Coefficients for selected q_2 values (from command line) and CC of detector mask and cos(psi) with psi as the reciprocal space angle. | 5 |
| **fix_all_pdb_for_condor.py** | Add the missing columns 77-78 in the PDB-files. Condor requires these columns. | |
| **Plot_diffraction.py** | Plots 3 diffraction patterns from CXI-file. | subplot : 1 |
| **RadProf_84-run_v2.py** | Load one CXI-file and calculate the Radial profile. plot together with with the mean intensity pattern. There are multiple options for the subplots, e.g. 2 radial profile plots; one of the second half of the profile and one of the entire profile. | subplot : 1 |
| **run-CsCl-w-condor-in-terminal.py** | Python script for Command Line Arguments to pass to 'simulate_CsCl_84-X.py' | |
| **simulate_CsCl_84-X.py** | Simulate diffraction experiment with Condor . | |
| **test_gnoise_asics.py** | Load the detector mask and then locate the ASICs or Tiles. Generate normal distributed noise per ASIC (or Tile) and plot. | subplot : 1 |
| **CrossCA_84-run_qvsq.py** | Read in 42 (current Davinci cluster limit) cross-correlations from 'Segments…' files generated by **CrossCA_84-run_v7.py** and plot 2D maps of the correlations for 3 different Fourier coefficients and stores the summed correlations in a hdf5-file. **CrossCA_84-run_qvsq-fqc.py** reads sets of 42 summed correlations and calculates the FQC [Kurta2017]. | subplot : 1 |
| **run_CCA_slurm.sh** | Slurm script for the Davinci-cluster: runs **RadProf_84-run_v2.py** | |
| **run_sim_slurm_new.sh** | Slurm script for the Davinci-cluster:<br>runs the Condor simulation script, **simulate_CsCl_84-X.py**, for each PDB-file in designated folder (in parallell). | |
| **run_plot_diff_slurm.sh** | Slurm script for the Davinci-cluster: runs **Plot_diffraction.py** | |
| **run_2loop_loki_slurm.sh** | Slurm script for the Davinci-cluster:<br>runs **AutoCCA_84-run_v5.py** or **CrossCA_84-run_v7.py** for each CXI file in designated folder. Runs all calculation in parallel, one job for each CXI-file. After no more jobs are queued, runs the plot version of the script which reads all the separate calculations (storesd in HDF5-files), sum and plot the result. | |
| script in **CsCl/test_result** | | |
| **CCA_cxi_84-X_v3.py** | Load a CXI-file. Plot some the diffraction patterns in a subplot (intensity, amplitude and pattersson), calculate CCA with 'Loki' or 'CXILT14' and plot the results. Option to make one quadrant noisy (3 options /implementations of noise). | 1-14 |
| **run_CCA_84_script.py** | Python script for Command Line Arguments to pass to 'CCA_cxil_84-X_v3.py'. | |
| **read_CXI_84-119_v3.py** | Load a CXI-file and plot. Several plotting options. | 6 |