

Exposure Grouping by Beam Shift for data processing in RELION

- Create a new directory and clone the repository
git clone https://github.com/DustinMorado/EPU_group_AFIS
- Load the appropriate module (for Hormel institute user)
Module load Miniconda3/py39_23.1.0
- Activate your conda environment
Conda activate
- Then run the following command

```
python /path/to/EPU_group_AFIS/EPU_Group_AFIS.py \  
  --xml_dir /path/to/xml_directory \  
  --n_clusters 1 \ # Set to 1 for Global CTF estimation  
  --apix PIXEL_SIZE \ # Replace with your pixel size (e.g., 0.85)  
  --mtf_fn /path/to/MTF.star \  
  --voltage 300 \  
  --cs 2.7 \  
  --q0 0.1 \  
  --ftype FILE_TYPE \ # Use 'tiff' or 'mrc'  
  --movie_dir /path/to/movie_directory \  
  --output_fn /path/to/output/movies.star \  
  --quiet
```

- Above command will generate a scatter plot based on image shift values (count and type in command line).
- Check the output file to ensure that the grouping has been performed correctly and according to the number of unique exposure groups specified.
- You can import this output file into **RELION** for further processing.

