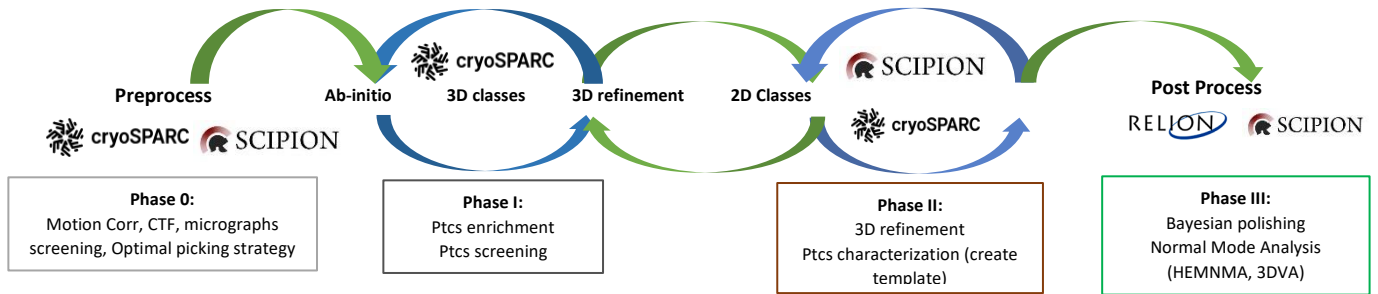


From Cryosparc to star file (Relion or Scipion)

How to convert the files from Cryosparc to Relion or Scipion. Including the command line.



Last phase of the data processing, use the particles and the refined map obtained in Cryosparc into Relion (Bayesian Polishing). Or go to Scipion to better characterize the particles.

Cryosparc to Relion

1. Recreate the same folder structure than in cryosparc. ie Folder tree of cryosparc.

```
remi_ruedas@CRYOEM-DATA-RR:/home2$ ls process/relion/HTP-glsanof_april2022/  
default_pipeline.star Extract Import J15 J73 S1
```

There **J15** contain the particles path (soft link using `ln -s`) and **J73** will contain the `.star` file and the `.mrc` map/mask.

2. Download the cryosparc files containing the information about particles location and put them in the corresponding (Two files `passthrough_particles.cs` & `particles.cs`), the map (`.mrc`) and the mask (`.mrc`):

```
cp insert/path/to/J73/P8_J73_passthrough_particles.cs /destination/to/relion/  
cp ~/J73/cryosparc_P8_J73_008_particles.cs /destination/.../  
cp ~/J73/cryosparc_P8_J73_008_volume_map.mrc /destination/.../  
cp ~/J73/cryosparc_P8_J73_008_volume_mask_refine.mrc /destination/.../
```

3. Convert `.cs` to `.star` (under `pyem` environment):

- a. Activate `pyem`:
`unset PYTHONPATH`
`conda activate pyem`

```
" . ~/miniconda3/etc/profile.d/conda.sh "
```

- b. Convert `.cs` to `.star`. **Merge `particles.cs` with `passthrough_particles.cs`!** Done automatically by `csparc2star` .

```
~/pyem/csparc2star.py P8_J73_passthrough_particles.cs  
cryosparc_P8_J73_008_particles.cs output_name.star
```

(Explain the command:

```
csparc2star.py name_of_input1 name_of_input2 name_of_output)
```

4. Edit .star with sed to have the right mrc files-names (under pyem):

Control by

- a. Change files format of the particles to mracs

```
sed -i 's/particles.mrc/particles.mrcs/g' from_csparc.star  
or using vi
```

```
:%#.mrc#.mrcs#
```

- b. If the folder structure was recreated, no need to edit the path to particles of the star file to make them point to the right path.

- c. Convert *.mrc of the symbolic link of the particles

```
rename 's/\.mrc$/\.mrcs/' *.mrc
```

5. Edit the optic group "_rlnOpticsGroup" table of the ****.star file using vi.

```
#Edit .txt with vi:
```

```
vi name.txt
```

```
insert mode : i
```

```
visual mode : esc
```

```
quit and save : MAJ+ZZ
```

```
quit without save : MAJ+ZQ
```

```
"
```

```
_rlnOpticsGroupName #1
```

```
[...]
```

```
opticsGroup1 [...]
```

```
"
```

The value associated to each column have to be edited because the introduction of the _rlnOpticsGroupName will shift the column by +1.

6. How the final star file should look :

```
data_optics
loop
_rlnOpticsGroupName #1
_rlnVoltage #2
_rlnSphericalAberration #3
_rlnAmplitudeContrast #4
_rlnOpticsGroup #5
_rlnImageSize #6
_rlnImagePixelSize #7
_rlnImageDimensionality #8
opticsGroup1 200.000000 2.100000 0.100000 2 280 1.160000 2

data_particles
loop
_rlnImageName #1
_rlnMicrographName #2
_rlnCoordinateX #3
_rlnCoordinateY #4
_rlnAngleRot #5
_rlnAngleTilt #6
_rlnAnglePsi #7
_rlnOriginXAngst #8
_rlnOriginYAngst #9
_rlnDefocusU #10
_rlnDefocusV #11
_rlnDefocusAngle #12
_rlnPhaseShift #13
_rlnCtfBfactor #14
_rlnOpticsGroup #15
_rlnRandomSubset #16
_rlnClassNumber #17
000110315/extract/FolHole_8872758_Data_7813020_7813022_20220409_122333_EER_patch_aligned_doseweighted_particles.mrcs S1/motioncorrected/FolHole_8872758_Data_7
813020_7813022_20220409_122333_EER_patch_aligned_doseweighted.nrc 1636 299 -80.785301 117.127998 37.685295 -10.708249 -2.486750 25039.371094 24960.152344 264.255
554 0.000000 0.000000 2 1 1
000159015/extract/FolHole_8872758_Data_7813020_7813022_20220409_122333_EER_patch_aligned_doseweighted_particles.mrcs S1/motioncorrected/FolHole_8872758_Data_7
813020_7813022_20220409_122333_EER_patch_aligned_doseweighted.nrc 732 1060 -39.929344 120.731674 -146.279343 30.399248 -3.197250 25076.250000 24997.031250 264.25
554 0.000000 0.000000 2 2 1
000159015/extract/FolHole_8872758_Data_7813020_7813022_20220409_122333_EER_patch_aligned_doseweighted_particles.mrcs S1/motioncorrected/FolHole_8872758_Data_7
813020_7813022_20220409_122333_EER_patch_aligned_doseweighted.nrc 192 1714 -127.068985 144.281876 -19.263432 -9.490249 0.659750 25190.791016 25111.572266 264.255
554 0.000000 0.000000 2 2 1
```

7. Start Relion import the start files with import job import particles star files:

- a. Import particles using particles.star file
- b. Import micrographs classical way to generate a micrograph.star file
- c. Re-extract particles as a control of the correct link between particles and micrographs

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- d. Perform 2D classes and check if everything is fine! (If relion is able to find particles and work with them.)
- e. Usually I re-run a refine 3D before going to further post-process step

Supplementary information

Soft link to the particles:

Path to cryosparc dataprocessing files

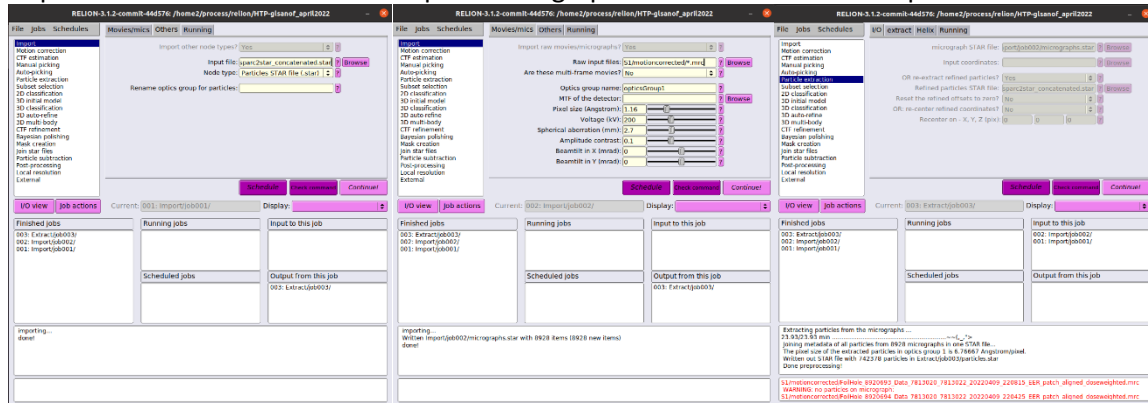
```
lru@remi:~$ ln -s /home2/process/P22/315/extract/FoIHole_9974335_Data_7813020_7813022_20220410_19_2240_EER_patch_aligned_doseweighted_particles.mrc -> /home2/process/P22/315/extract/FoIHole_9974335_Data_7813020_7813022_20220410_19_2231_EER_patch_aligned_doseweighted_particles.mrc
```

Relion jobs

Import Particles

Import Micrographs

Re-extract particles



Cryosparc to Scipion

Same as previously.