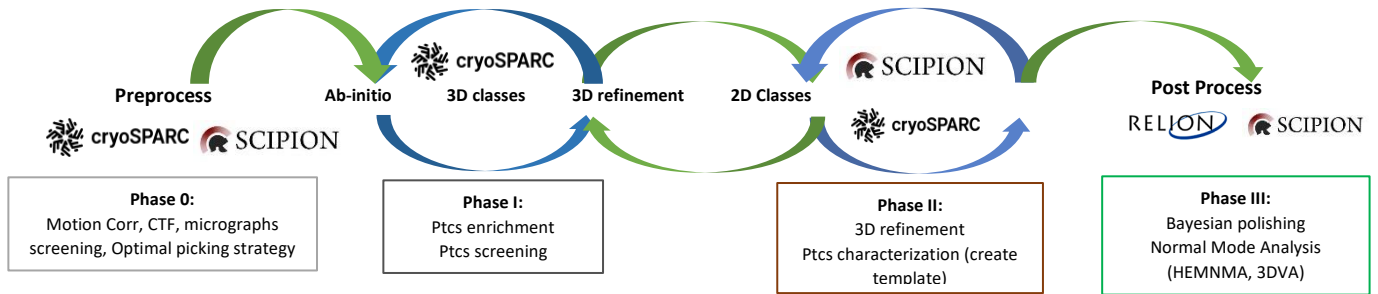Remi RUEDAS
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From Cryosparc to star file (Relion or Scipion)

How to convert the files from Cryosparc to Relion of 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 mrcs
      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 "_data_optics" 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 :

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:

Relion jobs

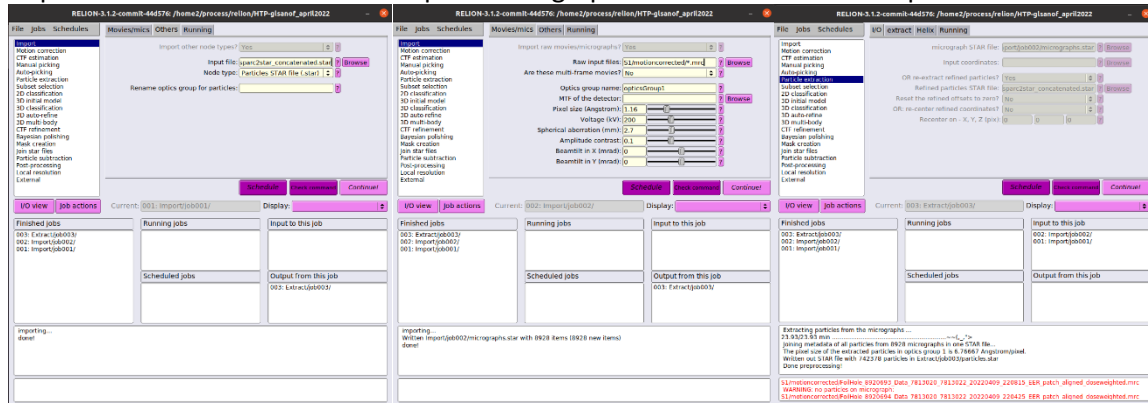**Import Particles**   **Import Micrographs**   **Re-extract particles**

Cryosparc to Scipion

Same as previously.