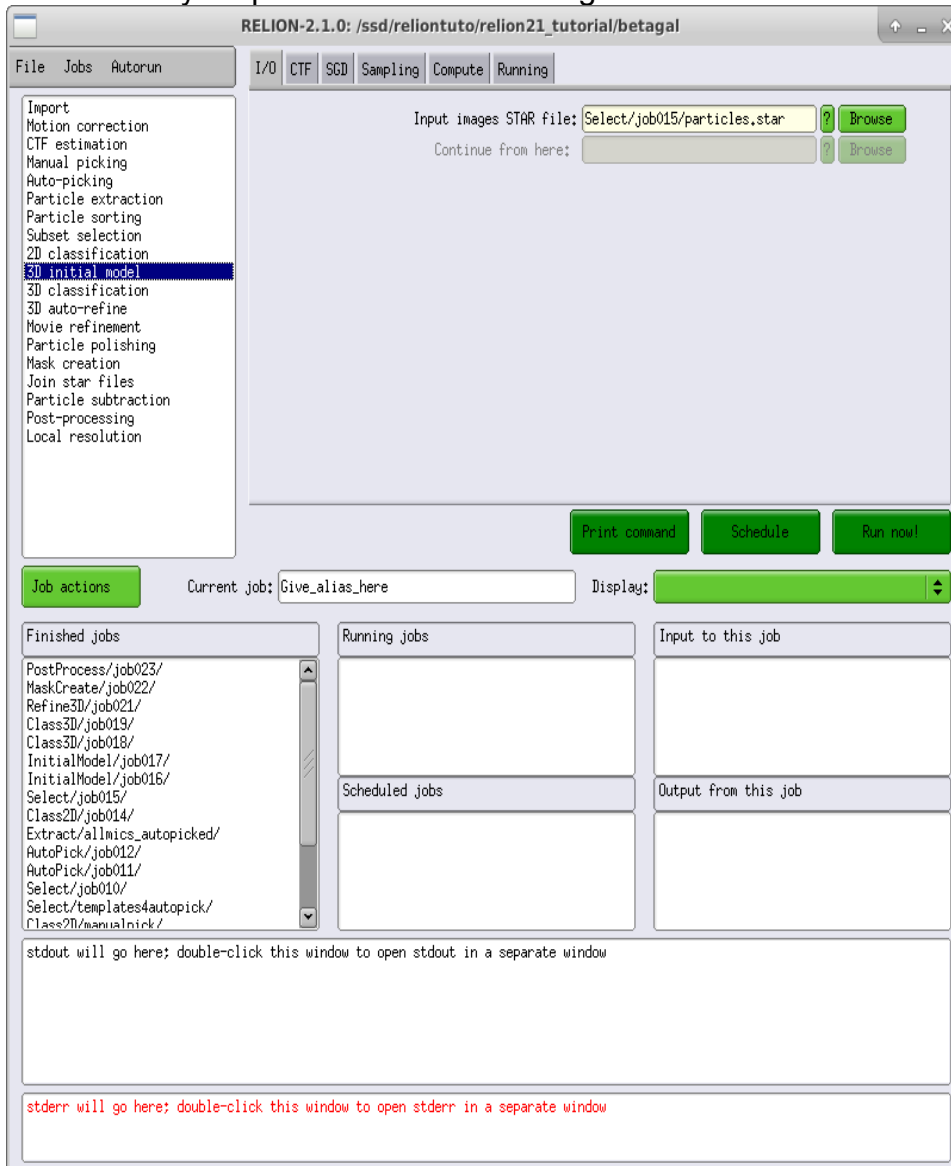


3D initial model in RELION 2.1

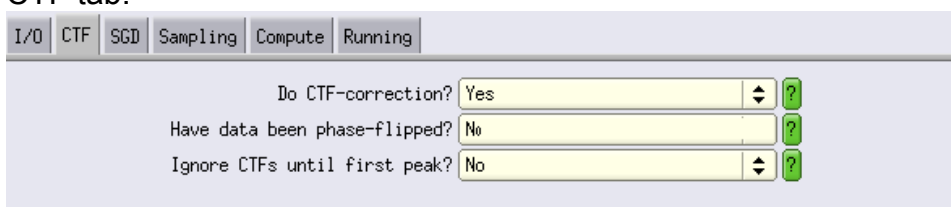
If you do not have the selected particles after 2D Classification, copy them from the precalculated results to the working directory:

```
#>cp -r PrecalculatedResults/Select/job015 Select/job015
```

Then select your particles.star file in the gui:



CTF tab:



SGD tab:

I/O CTF SGD Sampling Compute Running

Mask diameter (A): 200 ?

Symmetry: D2 ?

Number of iterations: 3 ?

SGD subset size: 200 ?

Write-out frequency subsets: 10 ?

Limit resolution SGD to (A): 20 ?

SGD increased noise variance half-life: -1 ?

Sampling tab:

I/O CTF SGD Sampling Compute Running

Angular sampling interval: 15 degrees ?

Offset search range (pix): 6 ?

Offset search step (pix): 2 ?

Compute tab:

I/O CTF SGD Sampling Compute Running

Use parallel disc I/O? Yes ?

Number of pooled particles: 3 ?

Pre-read all particles into RAM? Yes ?

Copy particles to scratch directory: ?

Combine iterations through disc? No ?

Use GPU acceleration? No ?

Which GPUs to use: ?

Running tab:

I/O CTF SGD Sampling Compute Running

Number of MPI procs: 1 ?

Number of threads: 1 ?

Submit to queue? No ?

Queue name: openmpi ?

Queue submit command: qsub ?

Standard submission script: /s4-linux/vlion/none/bin/qsub.csh ? Browse

Minimum dedicated cores per node: 1 ?

Additional arguments: ?

If your run takes too long you can copy the precalculated run to the running directory and use these results:

```
#>cp -r PrecalculatedResults/InitialModel/job016 InitialModel/job016
```

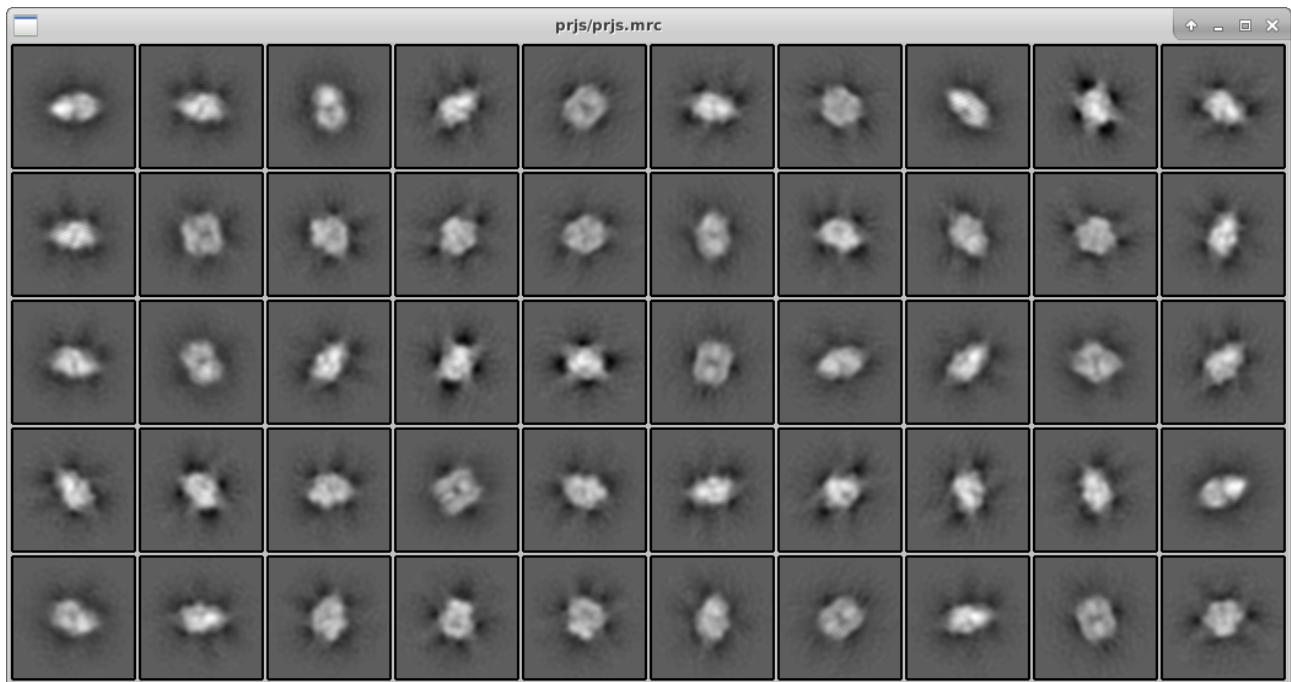
```
#>cp -r PrecalculatedResults/InitialModel/job017 InitialModel/job017
```

Visual inspection of the correspondence between 2D projections and the experimental images.

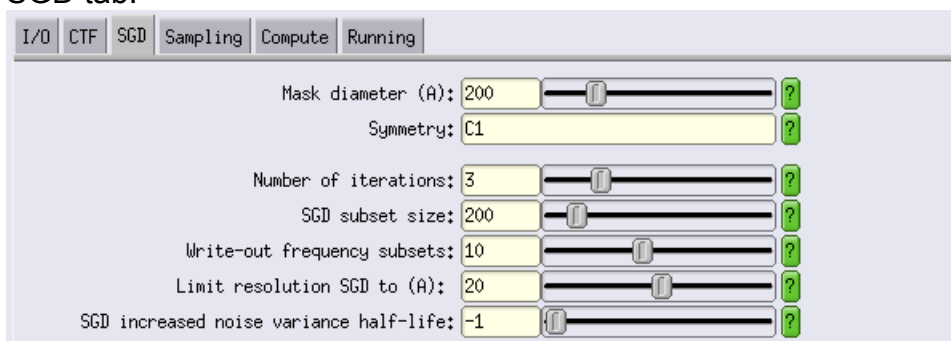
```
#>cd InitialModel/symC1 (or cd InitialModel/job016 )  
#>mkdir Projections  
#>relion_project --i run_it003_class001.mrc --o Projections/proj --nr_uniform 50  
#>relion_display --i Projections/proj.star
```

Or alternatively (with bsoft):

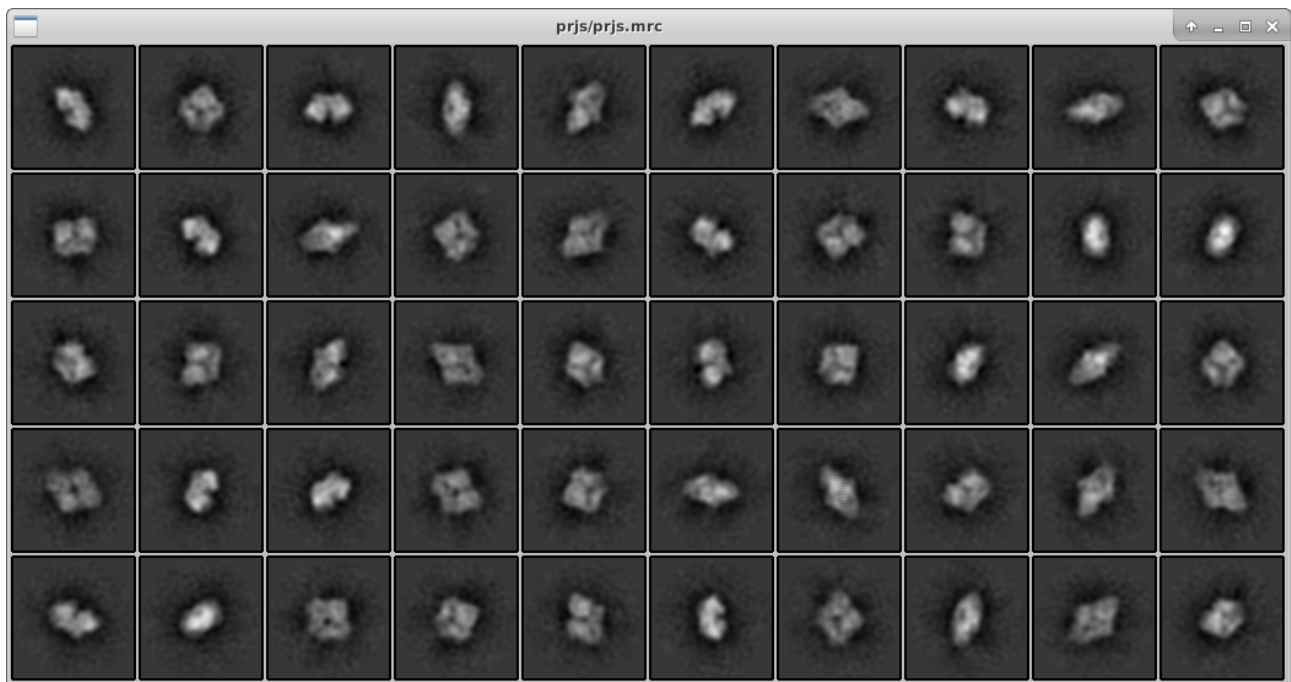
```
#>bproject -origin 50,50,50 -random 50 run_it003_class001.mrc #>Projections/prjs.mrc  
#>relion_display --i Projections/prjs.mrc --gui
```



If you repeat the initial model creation process by changing only the symmetry to C1 in the SGD tab:



you should get a different (better) result:



Now, let's use Chimera to align the apparent symmetry axes parallel to the XYZ axes.

```
#>chimera InitialModel/job017/run_it003_class001.mrc;
```

Use the duplicate option under the File menu of the Volume viewer.

Deactivate map #1 on the Model Panel;

Rotate map #0 to have it's symmetry axis parallel to the XYZ axes;

Save this model as InitialModel/symC1/inimodel.mrc

Check the result of the alignment by imposing D2 symmetry on the resulting map:

```
#>relion_image_handler --i inimodel.mrc --o inimodel_symD2.mrc --sym D2
```

The output map should be similar to the input map:

```
#>chimera inimodel.mrc inimodel_symD2.mrc
```