

A How to run the network

- (1) Install like Isonet (<https://github.com/IsoNet-cryoET/IsoNet>). Meaning install Tensorflow, then the other dependencies:

```
pip install -r requirements.txt
```

Then add environment variables:

```
source source-env.sh
```

Ultimately check that it is properly installed by running:

```
isocare.py check
```

- (2) Now we create the folder for our project. In there, create 2 more folder: "tomoset_odd" and "tomoset_even" and copy the odd and even tomograms into the respective folder (Make sure to rename both tomograms to have the same name).
- (3) Now we want to create the star files of the odd and even tomograms, for that, we run

```
isocare.py prepare_star tomoset_odd
--output_star tomo_odd.star --pixel_size 10.8
```

and

```
isocare.py prepare_star tomoset_even
--output_star tomo_even.star --pixel_size 10.8
```

- (4) We now extract the odd and even subtomograms respectively by running

```
isocare.py extract tomo_odd.star
--subtomo_star subtomo_odd.star
--subtomo_folder subtomo_odd
```

and

```
isocare.py extract tomo_even.star
--subtomo_star subtomo_even.star
--subtomo_folder subtomo_even
```

- (5) Now to start the refine step using the odd and even subtomograms, we run the following command:

```
isocare.py refine subtomo_odd.star
--subtomo_star_even subtomo_even.star
--gpuID 0 --iterations 15
--epochs 13
--steps_per_epoch 200
```

– you can change the number of iterations to what you want. in our testing, the network usually finished between 5 and 12 iterations, depending on the tomogram and difficulty to learn. Main optimisation happens in the choice of epochs and steps per epoch, just like in cryoCARE.

- (6) After comparing the different outputs of each iteration we can now predict using our favourite prediction by running:

```
isocare.py predict tomo_odd.star  
—star_file_even tomo_even.star  
—model ./results/model_iter05.h5 —gpuID 0
```

- We suggest checking the real space and fourier space of the subtomogram predictions. they are a good indicator of how the final prediction will go