

ESMFold

(Protein Structure Prediction)

Build conda environment that contains all the Python packages (3-5 minutes):

```
cd ESMFOLD
module load miniconda3
module load python/3.12.5
module load cuda

#Takes about 3-5 minutes
conda env create -f esmfold_gpu.yml
```

If YML file does not work, you can load the packages individually:

```
cd ESMFOLD
module load miniconda3
module load python/3.12.5
module load cuda

conda create -n esmfold_gpu_workshop python=3.10
source activate esmfold_gpu_workshop

conda install numpy=1.23.5
conda install pytorch torchvision torchaudio cudatoolkit=11.3 -c pytorch -c
nvidia
pip3 install transformers==4.30.0
pip3 install biopython
pip3 install accelerate
pip3 install requests
pip3 install tqdm
pip3 install intel-openmp
```

ESM-variant

(Protein Variant Effect Prediction)

Build conda environment that contains all the Python packages (3-5 minutes):

```
cd ESMVariant
module load miniconda3
module load python/3.12.5
module load cuda

#To download the latest version of esm-variants
git clone https://github.com/ntranoslab/esm-variants.git

#Takes about 3-5 minutes
conda env create -f esmvariant_gpu.yml
```

If YML file does not work, you can load the packages individually:

```
cd ESMVariant
module load miniconda3
module load python/3.12.5
module load cuda

#To download the latest version of esm-variants
git clone https://github.com/ntranoslab/esm-variants.git

conda create --name esmvariant_gpu_workshop
source activate esmvariant_gpu_workshop
pip3 install tqdm numpy pandas biopython torch fair-esm
```

RFDiffusion

(Protein Binder Prediction)

Build conda environment that contains all the Python packages):

```
module load miniconda3
module load python/3.12.5
module load cuda

cd RFDiffusion

#Clones the repo and moves the contents directly into this folder for
simplicity
git clone https://github.com/RosettaCommons/RFdiffusion.git && mv
RFdiffusion/* ./

conda env create -f rfdiffusion_env.yml
source activate SE3nv

#Installs the SE3 Transformer
cd env/SE3Transformer
pip install --no-cache-dir -r requirements.txt
python setup.py install

#Navigate back to the home directory
cd ../../

#Install the rfdiffusion module from the root of the repository
pip install -e . # install the rfdiffusion module from the root of the
repository

conda install foldseek=8.ef4e960
conda install pdb-tools
conda install -c conda-forge biopython
conda install pandas

conda deactivate
```