Setting up ESMFold on CARC

Note: Recommend using Xena machine as it is equipped with GPUs

1) Load the appropriate modules onto the machine, notably conda (if it is not already active) and cuda. For me the commands are:

```
module load gcc/8.3.0-wbma
module load cuda/11.6.2-jeoh
```

Notes for step 1)

If conda is not active you can load it with:

```
module load miniconda3/latest
```

Or check available versions with:

```
module spider conda
```

To view the available cuda versions do:

```
module spider cuda
```

To view the dependencies for a certain cuda version do

```
module spider cuda/<version>
```

One of the dependencies for ESMFold (openfold) is not compatible with certain versions of cuda. I would recommend using the version of cuda I specified here unless you know openfold is compatible with your version.

2) Create a conda environment for ESMFold with the following command:

```
conda create -n esmfold python==3.9
```

Notes for step 2)

Python==3.9 is required because of some dependencies of esmfold that are not compatible with higher versions (this may change at a future date).

3) Activate your created conda environment:

```
conda activate esmfold
```

4) Install PyTorch with GPU support from this site https://pytorch.org/get-started/locally/ . Make sure to install using the cuda version you loaded in step 1). For me the command looks like this:

```
conda install pytorch torchvision torchaudio
pytorch-cuda=11.6 -c pytorch -c nvidia
```

5) CARC uses GPUs that are fairly old and (by default) not supported by PyTorch. To account for this, we can install older binaries from https://github.com/nelson-liu/pytorch-manylinux-binaries/releases using pip. This will allow us to use our older GPUs on new versions of PyTorch. For me the command looks like this:

```
pip install torch==1.13.1+cu116 -f
https://nelsonliu.me/files/pytorch/whl/torch_stable.ht
ml
```

6) Using the steps available at https://github.com/facebookresearch/esm , install ESMFold and its dependencies. For me the following 3 commands accomplish this:

```
pip install "fair-esm[esmfold]"

# OpenFold and its remaining dependency
pip install 'dllogger @
git+https://github.com/NVIDIA/dllogger.git'

pip install 'openfold @
git+https://github.com/aqlaboratory/openfold.git@4b410
59694619831a7db195b7e0988fc4ff3a307'
```

7) You should now have successfully installed ESMFold!