

RFdiffusion (latest code on Oct 25, 2023)

Webpage

<https://github.com/RosettaCommons/RFdiffusion>

Version

latest code on Oct 25, 2023

Installation

RFdiffusion and its model params

```
$ git clone https://github.com/RosettaCommons/RFdiffusion.git 20231025
$ cd 20231025
$ mkdir models && cd models
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/6f5902ac237024bdd0c176cb93063dc4/Base_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/e29311f6f1bf1af907f9ef9f44b8328b/Complex_base_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/60f09a193fb5e5ccdc4980417708dbab/Complex_Fold_base_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/74f51cfb8b440f50d70878e05361d8f0/InpaintSeq_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/76d00716416567174cdb7ca96e208296/InpaintSeq_Fold_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/5532d2e1f3a4738decd58b19d633b3c3/ActiveSite_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/12fc204edeae5b57713c5ad7dcb97d39/Base_epoch8_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/f572d396fae9206628714fb2ce00f72e/Complex_beta_ckpt.pt
$ wget http://files.ipd.uw.edu/pub/RFdiffusion/1befcb9b28e2f778f53d47f18b7597fa/RF_structure_prediction_weights.pt
```

python env (miniforge)

```
$ sh Miniforge3-Linux-x86_64.sh
...
[...] >>> /apl/RFdiffusion/20231025/miniforge3
...
$ ./miniforge3/bin/conda shell.bash hook > ./conda_init.sh
$ ./miniforge3/bin/conda shell.csh hook > ./conda_init.csh

$ ./apl/RFdiffusion/20231025/conda_init.sh
$ conda install cudatoolkit=11.7.1 pytorch==1.13.1 torchvision==0.14.1 torchaudio==0.13.1 pytorch-cuda=11.7 -c pytorch -c nvidia
$ conda install -c dgteam/label/cu117 dgl
$ cd env/SE3Transformer/
$ pip install --no-cache-dir -r requirements.txt
$ python setup.py install
$ pip install hydra-core pyrsistent
$ cd ../../
$ pip install -e .
```

Notes

- This version may not work with pytorch 2.x? 1.13.1 was used.
- In RCCS job script, explicit GPU specification like "export CUDA_VISIBLE_DEVICES=0" seems to be necessary.
 - (Normally, this may not be necessary. This additional requirement may be caused by the GPU resource management mechanism in our system.)