RoseTTAFold

`/fs00/software/rosettafold/1.1.0`

注意: `apptainer` 默认会 bind用户的 `home` 目录，如果用户本来就有 `RoseTTAFold` 或者 `folding` 的 conda 环境则可能会发生冲突。用户可通过添加 `--no-home` 选项避免此问题。

```
#BSUB -J RoseTTAFold
#BSUB -q gpu
#BSUB -n 8
#BSUB -gpu num=1

###### Configurie Numpy threads  ######

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
export MKL_NUM_THREADS="$LSB_DJOB_NUMPROC"

###### Definition ######

ROSETTAFOLD_DATADIR=/fsb/data/rosettafold      # path to RoseTTAFold data (host)
ROSETTAFOLD_IMAGE=RoseTTAFold-1.1.0.sif        # path to RoseTTAFold image (host)
ROSETTAFOLD_APPDIR=/app/RoseTTAFold            # path to RoseTTAFold working directory (container)

###### Database ######

UNIREF30_DB=$ROSETTAFOLD_DATADIR/UniRef30_2020_06
BFD_DB=$ROSETTAFOLD_DATADIR/bfd
PDB100_DB=$ROSETTAFOLD_DATADIR/pdb100_2021Mar03

###### Example ######

RUN_ROSETTAFOLD="apptainer run --bind $UNIREF30_DB:$ROSETTAFOLD_APPDIR/UniRef30_2020_06 \
                --bind $BFD_DB:$ROSETTAFOLD_APPDIR/bfd \
                --bind $PDB100_DB:$ROSETTAFOLD_APPDIR/pdb100_2021Mar03 \
                --nv $ROSETTAFOLD_IMAGE"
```

```
# For monomer structure prediction (e2e)
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_e2e_ver.sh $ROSETTAFOLD_APPDIR/example/input.fa
output/

# For monomer structure prediction (pyrosetta)
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_pyrosetta_ver.sh $ROSETTAFOLD_APPDIR/example/input.fa
output/

# For complex modeling
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network/predict_complex.py \
        -i $ROSETTAFOLD_APPDIR/example/complex_modeling/paired.a3m \
        -o output/ -Ls 218 310

# For PPI screening using faster 2-track version (example input and output are at example/complex_2track)
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network_2track/predict_msa.py \
        -msa $ROSETTAFOLD_APPDIR/example/complex_2track/input.a3m \
        -npz output/complex.npz -L1 218
```

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