

AlphaFold2

Korištenje

Dostupne verzije i pripadajući moduli:

Verzija	Modul
2.1.1	bioinfo/alphafold2/2.1.1
2.0.1	bioinfo/alphafold2/2.0.1

Primjer skripte za opis poslova:

alphafold2.sge

```
#$ -N alphafold2
#$ -pe gpu 1
#$ -l cores=5
#$ -cwd

module load bioinfo/alphafold2/2.0.1

GPUDEVICE=$(cat $TMPDIR/gpu)

run_alphafold.sh -d $ALPHAFOLDDB -o dummy_test -m model_1 -f example/query.fasta -t 2020-05-10 -a $GPUDEVICE -n 5
```



Napomena

Aplikacija je instalirana i konfigurirana u Python virtualnom okruženju kojeg korisnik može proširiti sa svojim proizvoljnim Python aplikacijama. Nakon učitavanja modula, korisnik dodatne aplikacije instalira s:

```
conda create --prefix $LOCALPKGS python=3.8
conda install --prefix $LOCALPKGS potrebni-python-pkg
ili
pip install --prefix $LOCALPKGS potrebni-python-pkg
```

Instalacija

Aplikacija je pripremljena koristeći miniforge Conda installer slijedeći upute s: https://github.com/kalininalab/alphafold_non_docker

Izvorni kod aplikacije: <https://github.com/deepmind/alphafold>

Naredbe instalacije

```
source miniforge3/bin/activate
conda create --prefix /apps/virtenv/alphafold2 python=3.8
conda activate /apps/virtenv/alphafold2
conda install -y -c conda-forge openmm==7.5.1 cudnn==8.2.1.32 cudatoolkit==11.0.3 pdbfixer==1.7
conda install -y -c bioconda hmmer==3.3.2 hhsuite==3.3.0 kalign2==2.04
conda install -y -c conda-forge pandas
pip install absl-py==0.13.0 biopython==1.79 chex==0.0.7 dm-haiku==0.0.4 dm-tree==0.1.6 immutabledict==2.0.0
jax==0.2.14 ml-collections==0.1.0
numpy==1.19.5 scipy==1.7.0 tensorflow==2.5.0
pip install --upgrade jax jaxlib==0.1.69+cuda111 -f https://storage.googleapis.com/jax-releases/jax_releases.
html
wget -c https://github.com/deepmind/alphafold/archive/refs/tags/v2.0.1.zip
unzip v2.0.1.zip -d /apps/virtenv/alphafold2/alphafold-2.0.1/
cd /apps/virtenv/alphafold2/lib/python3.8/site-packages/
patch -p0 < ../.././alphafold-2.0.1/docker/openmm.patch
cd /apps/virtenv/alphafold2/alphafold-2.0.1/alphafold/common
wget -q https://git.scicore.unibas.ch/schwede/openstructure/-/raw/7102c63615b64735c4941278d92b554ec94415f8
/modules/mol/alg/src/stereo_chemical_props.txt
cd /apps/virtenv/alphafold2/alphafold-2.0.1/
wget -c https://raw.githubusercontent.com/kalininalab/alphafold_non_docker/main/run_alphafold.sh
```

Preuzimanje potrebnih baza

```
scripts/download_alphafold_params.sh alphafold_data
scripts/download_bfd.sh alphafold_data
scripts/download_mgnify.sh alphafold_data
scripts/download_pdb70.sh alphafold_data
scripts/download_small_bfd.sh alphafold_data
scripts/download_uniclust30.sh alphafold_data
scripts/download_uniref90.sh alphafold_data
scripts/download_pdb_seqres.sh alphafold_data
scripts/download_small_bfd.sh alphafold_data
```