

Parallelfold

Korištenje

Dostupne verzije i pripadajući moduli:

Verzija	Modul
2.1.1	bioinfo/parallelfold/2.1.1

Parallelfold je modificirana skripta Alphafolda i služi za raščlanjivanje CPU(MSA and template searching) i GPU(prediction model) dijela.

Primjer pokretanja CPU dijela:

cpu_parafold.sge

```
#!/bin/bash
#$ -N parafold2
#$ -pe p28-mpi 10
#$ -cwd

module load bioinfo/parallelfold/2.1.1

run_alphafold.sh -d $ALPHAFOLDDB -o output -f -i fasta/actin_gallus1.fasta -p monomer_ptm -t 2021-12-15 --
usegpu=False
```

Bitan je flag `--usegpu=False` koji naznačuje da se ne koristi GPU neko isključivo CPU i `-f` koji zaustavlja alphafold nakon kreiranja feature.pkl u output direktoriju.

Nakon CPU dijela treba pokrenuti GPU dio za dalje. Pokreće se isti job u istom direktoriju, feature.pkl mora biti prisutan u output folderu za GPU dio.

Primjer GPU dijela:

gpu_parafold.sge

```
#!/bin/bash
#$ -N parafold2
#$ -pe gpu 1
#$ -l cores=5
#$ -cwd

module load bioinfo/parallelfold/2.1.1

GPUDEVICE=$(cat $TMPDIR/gpu)

cuda-wrapper.sh run_alphafold.sh -d $ALPHAFOLDDB -o output -i fasta/actin_gallus1.fasta -p monomer_ptm -t 2021-12-15 -a $GPUDEVICE -n 5
```

Vizualizacija rezultata PLLDT i PAE

Primjer korištenja:

visualisation.sge

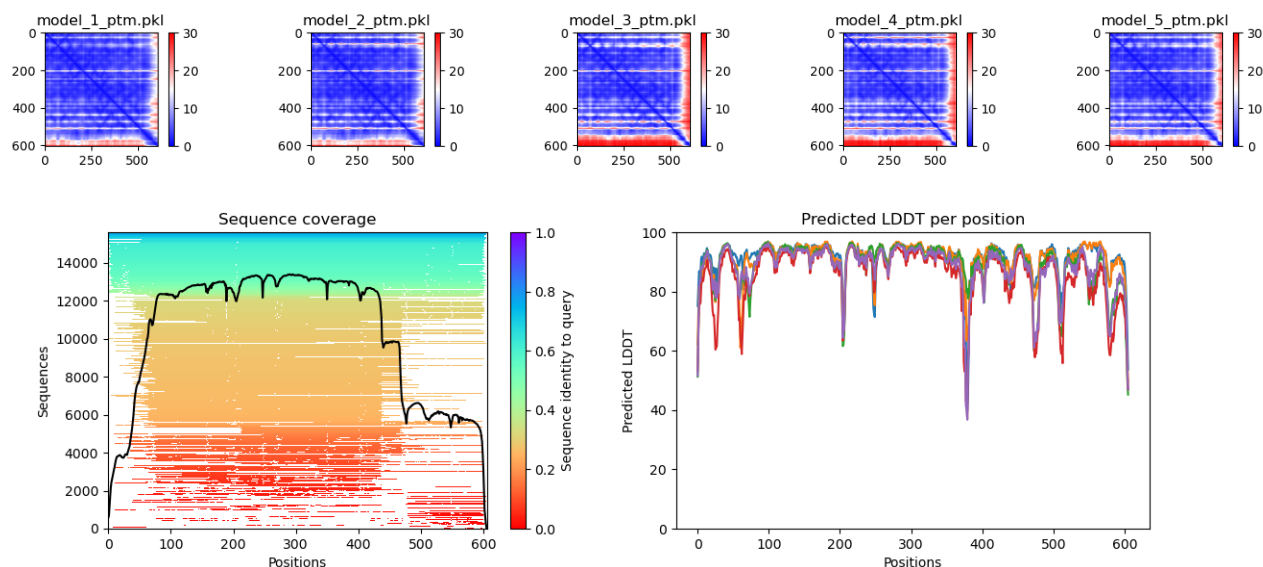
```
#!/bin/bash
#$ -N PLLDT_PAE
#$ -pe *mpisingle 2
#$ -cwd

module load bioinfo/parallelfold/2.1.1

run_visualisation.sh -i output/Canis_Lupus_dehydrogenase_sub_5/ -o my_outputs -n Canis
```

Potrebna je putanja do direktorija sa rezultatima za pojedini uzorak (-i), putanja do direktorija gdje će biti stvorene slike(-o), potrebno je i napisati prefix za imena slike(-n)

Rezultati:



Instalacija

Prerequisites

```
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
```

Install and patch

```
git clone https://github.com/Zuricho/ParallelFold.gitcd /apps/virtenv/parallelfold2.1.1/lib/python3.8/site-packages/
patch -p0 < ../../ParallelFold/docker/openmm.patch
wget -q https://git.scicore.unibas.ch/schwede/openstructure/-/raw/7102c63615b64735c4941278d92b554ec94415f8/modules/mol/alg/src/stereo_chemical_props.txt
```

