

Using AlphaFold2 on IGBMC HPC

- Connect to IGBMC hpc through SSH `ssh login@hpc.igbmc.fr`
- Go to your alphafold folder (`/shared/mendel/projects/xxx/cryoem/alphafold/` for instance)
- Generate/edit the sequence fasta file (`sequence.fasta`)

```
>ID_OF_THE_SEQUENCE  
AMINO_ACID_SEQUENCE
```

If you want to generate a multimer structure you must provide a sequence for each polypeptide (2x the same sequence with **ID_1** and **ID-2** for a homodimer, and so on)

Generate/edit the slurm script (username, fasta file) and name it `xxx.sh`

- for a monomer

```
#!/bin/bash  
#SBATCH --mail-type=ALL  
#SBATCH --mail-user=username@igbmc.fr  
#SBATCH --cpus-per-task 2  
#SBATCH --gres=gpu:a3g.20gb:1  
#SBATCH --mem=50G  
#SBATCH -p gpu  
  
module load alphafold/2.3.2  
AF=/shared/genomes/alphafold2/2023-04-28  
  
srun run_alphafold.sh \  
  --data_dir=$AF/ \  
  --output_dir=$(pwd)/ap_out \  
  --fasta_paths=sequence.fasta \  
  --max_template_date=2020-05-14 \  
  --db_preset=full_dbs \  
  --  
bfd_database_path=$AF/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_opt \  
  --  
uniref30_database_path=$AF/uniclust30/uniclust30_2018_08/uniclust30_2018_08 \  
 \  
  --uniref90_database_path=$AF/uniref90/uniref90.fasta \  
  --mgnify_database_path=$AF/mgnify/mgy_clusters_2018_12.fa \  
  --template_mmcif_dir=$AF/pdb_mmcif/mmcif_files \  
  --obsolete_pdbs_path=$AF/pdb_mmcif/obsolete.dat \  
  --use_gpu_relax=True \  
  --model_preset=monomer \  
  --pdb70_database_path=$AF/pdb70/pdb70
```

- for a multimer

```
#!/bin/bash

#SBATCH -p gpu
#SBATCH --gres=gpu:a3g.20gb:1
#SBATCH --cpus-per-task=10
#SBATCH --mem=50G
#SBATCH --mail-user=username@igbmc.fr
#SBATCH --mail-type=ALL

module load alphafold/2.3.2

mkdir -p /tmp/username

AF=/shared/genomes/alphafold2/2023-04-28

srun run_alphafold.sh \
  --data_dir=$AF/ \
  --output_dir=$(pwd)/ap_out \
  --fasta_paths=TOP2A_HUMAN_DIMER.fasta \
  --max_template_date=2020-05-14 \
  --db_preset=full_dbs \
  --
bfd_database_path=$AF/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_opt \
  --
uniref30_database_path=$AF/uniclust30/uniclust30_2018_08/uniclust30_2018_08 \
  \
  --uniref90_database_path=$AF/uniref90/uniref90.fasta \
  --mgnify_database_path=$AF/mgnify/mgy_clusters_2018_12.fa \
  --template_mmcif_dir=$AF/pdb_mmcif/mmcif_files \
  --obsolete_pdbs_path=$AF/pdb_mmcif/obsolete.dat \
  --use_gpu_relax=True \
  --model_preset=multimer \
  --pdb_seqres_database_path=$AF/pdb_seqres/pdb_seqres.txt \
  --uniprot_database_path=$AF/uniprot/uniprot.fasta
```

Run the script:

```
sbatch xxx.sh
```

You will get one email when the job start and a second one when its complete (or crashed). You can also follow it with *squeue*

From:
<https://bsi.inscog.eu/> - BSI wiki

Permanent link:
<https://bsi.inscog.eu/doku.php?id=alphafold2&rev=1710322204>

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