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=Your_email
#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_Your_Result_Directory \
    --fasta_paths=Your_Sequence_File.fasta \
    --max_template_date=2020-05-14 \
    --db_preset=full_dbs \
    --
bfd_database_path=$AF/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sort
ed_opt \
    --
uniref30_database_path=$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 --mail-type=ALL
#SBATCH --mail-user=Your_email
#SBATCH --cpus-per-task 2
#SBATCH --gres=gpu:a3g.20gb:1
#SBATCH --mem=100G
#SBATCH -p gpu
#SBATCH -t 8-00:00:00

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_Your_Result_Directory \
    –fasta_paths=Your_Multiple_Sequence_File.fasta \
    --max_template_date=2020-05-14 \
    --db_preset=full_dbs \
    --
bfd_database_path=$AF/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sort
ed_opt \
    --
uniref30_database_path=$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*