







AlphaFold 3

/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif

0. ????


alphafold3 Google DeepMind   json

- data pipeline:


(multi-sequence alignment, msa)  (templates)
 json 

- inference:  msa  templates  json  mmcif
 confidence score

  [github](#)  apptainer  alphafold3

 [term of use](#)

 Google DeepMind 

1. ????



```
path_to_af3db="/fsb/data/alphafold/3"
path_to_af3container="/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif "

io_dir=</path/to/your/input/and/output>
weights_dir=<path/to/directory/containing/your/af3-weights>

RUN_ALPHAFOLD="apptainer run --nv --bind
```

```

${path_to_af3db}:/databases,${io_dir}:/host_iopath,${weights_dir}:/af3_weights
${path_to_af3container} python run_alphafold.py"

```

```

[[ ${path_to_af3db} ]]]] alphafold3]]]]] [${io_dir}]

]]]]]]]]]]]]]]]]]] [${weights_dir}] ]]]]] alphafold3]]]]]]]]]]]]]]]]]]

```

run_alphafold.py [github](#)

$$\begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline \end{array} \quad \left(\begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline \end{array} \right)$$

```

${RUN_ALPHAFOLD} --help

```

input.json \${io_dir} alphafold3

```

${RUN_ALPHAFOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/

```

```

input.json name ${io_dir} data pipeline json
confidence score log stderr (
python logging )
documentation output
documentation

```

2. ???data pipeline?inference

The diagram illustrates the data flow between a CPU and a GPU. On the CPU side, data enters a 'data pipeline' (represented by a row of 8 boxes), then moves to an 'inference' block (a row of 5 boxes). On the GPU side, data enters a 'data pipeline' (a row of 2 boxes) and then moves to a 'cpu' block (a row of 2 boxes). Arrows indicate the direction of data flow: from the CPU's data pipeline to its inference block, from the CPU's inference block to the GPU's data pipeline, and from the GPU's data pipeline to its cpu block.

```

[ ] [ ] [ ] [ ] [ ] [ ] [ ] [ ]
bool [ ] [ ] [ ] [ ] [ ]
--run data_pipeline [ ] --run inference

```

☐ True.

	:
	:

- data pipeline (cpu job)

```

${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
  --json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
  --run_inference=False

```

- inference (gpu job)

```

${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
  --json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
  --run_data_pipeline=False

```

```

##### msa templates#####
alphafold3##### msa templates#### json##### --
run_data_pipeline=False##### msa templates## json
##### DeepMind-input documentation##### msa templates##### json
##### msa templates## json##### Mb####

```

3. ?????????

```

##### ${RUN_ALPHAFAOLD} --help #####
run_alphafold.py ##### 3#####

```

- `--input_dir` `--json_path` ##### `input_dir`
`input_dir`##### `json`#####
- `--jackhmmmer_n_cpu` `--nhmmmer_n_cpu` ##### `cpu cores`#####
- ##### `random seed`##### `alphafold3` `random seed`
`input.json`

4. ???????????????

data pipeline##### inference#### gpu#####

- 2PV7##### homomer#### 298
- 1AKE##### homomer#### 214

83a100ib 734090d A100 (memory 40 G) 4090d
(memory 24 G) inference. 722080tiib 72rtxib . GPU
[performance documentation](#) alphafold3 A100(80G),
A100(40 G) H100 4090

data pipeline inference

- 8 cpu cores 300 msa templates 1.5-2 h
msa templates 10 s
- alphafold3 5
100 s inference

performance [performance documentation](#)

5. ?????????

2PV7 RMSD=4.410 (: Angstrom)
A:B - A:B RMSD 4 RMSD 3.012, 2.759, 2.971,
2.740. alphafold3 alphafold2. 2 subunits DockQ
0.499>0.23 docking

1AKE 1AKE RMSD=18.176 4AKE RMSD=26.791
alphafold2-multimer subunits DockQ=0.019<<0.23
Alphafold3 4090d
A100

“ dockQ (Mirabello & Wallner, 2024, Bioinformatics) subunits
0-1 <0.23 >0.8