

AlphaFold 3

Disclaimer: this page is provided for experimental support only!

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The project home page where you can find the latest information [there](#).

Using AlphaFold 3 through a container

The Apptainer/Singularity container for AlphaFold 3 is available at

`/dcsrsoft/singularity/containers/alphafold-v3.sif` .

As stated on the Github page, it is possible to test AlphaFold 3 with the following JSON input (named `fold_input.json`):

```
{
  "name": "2PV7",
  "sequences": [
    {
      "protein": {
        "id": ["A", "B"],
        "sequence":
"GMRESYANENQFGFKTINSDIHKIVIVGGYGKLGGLFARYLRASGYPIILDREDWAVAESILANADVIVSVPINLTLETIERLKPYL
TENMLLADLTSVKREPLAKMLEVHTGAVLGLHPMFGADIASMAKQVVVRCDGRFPERYEWLLEQIQIWGAKIYQTNATEHDHNM
TYIQALRHFSTFANGLHLSKQPINLANLLALSSPIYRLELAMIGRLFAQDAELYADIIMDKSENLA VIETLKQTYDEALTFFENNRQG
FIDAFHKVRDWF GDYSEQFLKESRQLLQQANDLKQG"
      }
    }
  ],
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 1
}
```

To ease the use of AlphaFold 3, we have downloaded:

- the databases to `/reference/alphafold3/db`

- the model to `/reference/alphafold3/model`

Here an example of Slurm job that can be used to run Alphafold 3 with the above JSON file:

```
#!/bin/bash -l

#SBATCH --time 2:00:00
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --partition gpu
#SBATCH --gres gpu:1
#SBATCH --gres-flags enforce-binding
#SBATCH --cpus-per-task 8
#SBATCH --mem=64G

dcsrsoft use 20241118
module load apptainer
export APPTAINER_BINDPATH="/scratch,/work,/users,/reference"

mkdir -p output
apptainer run --nv /dcsrsoft/singularity/containers/alphafold-v3.sif --json_path=fold_input.json --
output_dir=output --model_dir=/reference/alphafold3/model --db_dir=/reference/alphafold3/db
```

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