AlphaFold 2.2.0 (2022/3/11)

Webpage (source code)

https://github.com/deepmind/alphafold

Version

2.2.0 (2022/3/11; alphafold params were also downloaded on 2022/3/11. Other databases are the same as 2.1.1 case.)

Installation

- The same procedure as 2.1.1 case was employed.
    - AlphaFold params were newly downloaded. (download_alphafold_params.sh)

Update of script

Wrapper script was updated to support new features.

run_alphafold22x_rccs.sh

- default AlphaFold code and database setting were updated.
- Options added
    - -g (re-enabled)
        - This is necessary when you want to perform relaxation of the predicted structures using GPU. (You don't need to specify number of GPUs etc.)
    - -R
        - skip running MSA tools and use precomputed one. NOTE: this will not check if sequence/db/conf have changed. (--use_precomputed_msas=True of run_alphafold.py)
    - -s [seeds per model]
        - number of seeds per model for multimer system. (default: 5) (Number of models (usually 5)) * (number of seeds; this param) predictions will be performed. MSA time will not be affected by this param. (--num_multimer_predictions_per_model=(num) of run_alphafold.py)
    - -S
        - skip relaxation of predicted structure (default: do relaxation) (--run_relax=False of run_alphafold.py)

Notes

- Calculation may be very slow if disk load is high...