Steps for MSA cluster generation

1. Make folder for project. For example, make a folder names cluster_MSA_afv2
    1. *Mkdir cluster_MSA_afv2*
2. Upload fasta file to “cluster_MSA_afv2”
    1. *Vi test_models.fasta*
3. Upload the python scripts (pipeline_CFB) to current folder
    1. *Scp –r Downloads/pipelineCFB* vmischley@login.expanse.sdsc.edu:/expanse/lustre/projects/was136/vmischley/***cluster_MSA_afv2***
4. Move the submit script for MSA generation (CFS_submit_script.slurm) to folder that you want the MSA folder to be created
    1. *Cp pipeline_CFB/CFS_submit_script.slurm ./*
5. Edit CFS_submit_script.slurm. Change the name of the fasta file and change the name of the MSA folder. For example, change fasta file to test_models.fasta
    1. *Vi CFS_submit_script.slurm*
6. Run CFS_submit_script.slurm. This generates the MSAs. It will take between 24-48 hours. This will generate an MSA folder.
    1. *Sbatch CFS_submit_script.slurm*
7. Once the MSA folder is generated, run run_batch_pipeline.py . This will rename the MSAs and will split the MSAs into jobs that will take 48 hours to complete. It will also create the submit scripts for you. Three arguments: location of MSA folder (use full path) number of recycles and version of AF.
    1. *Python pipeline_CFB/run_batch_pipeline.py /expanse/lustre/projects/was136/vmischley/cluster_MSA_afv2/test_models_MSA 12 alphafold2_multimer_v2*
8. Change into the model folder where all of the submit scripts are
    1. *Cd models*
9. Submit all of the submit scripts
    1. *Sbatch 1_CFB_test_models_MSA_1_submit.slurm*
10. Check that all of the models completed within 48 hours by looking at the log.txt files
    1. *Vi models/test_models_afv3_1_models/log.txt*

11. Run move_af.py to copy only pdb files and .json files into one folder (optional). Input argument is path to model folder. If using move_af.py you must run an interactive node, or else you run out of memory

1. *srun --partition=debug --pty --account=was138 --nodes=1 --ntasks-per-node=4 --mem=32G -t 00:30:00 --wait=0 --export=ALL /bin/bash*
2. *Python move_af.py /expanse/lustre/projects/was136/vmischley/cluster_MSA_afv2/test_models*

12. After completion, download folder