alphafold2_on_alpine

```
#RMACC Symposium 2024: AlphaFold2 on Alpine

##log in with your training account ID, e.g.,
ssh user0030@tlogin1.rc.colorado.edu

##get on GPU node using the reservation
sinteractive --partition=aa100 --gres=gpu:1 --ntasks=8 --time=30:00 --reservation=rmaccsymp

##view and load the AlphaFold module
module whatis alphafold
ml alphafold

##explore pre-set variables, look at alphafold options
run_alphafold
ls $CURC_AF_DBS
ls $CURC_AF_EXAMPLES
cat $CURC_AF_EXAMPLES/dummy.fasta
cat $CURC_AF_EXAMPLES/multimer.fa
echo $TMPDIR

##navigate to your project space
cd /projects/$USER

##use precomputed MSAs to run model inference (time-saving measure for purpose of workshop)

###copy precomputed MSAs from examples dir
cp -r /curc/sw/install/bio/alphafold/examples/runs/dummy .

###the model inference and relaxation should take about 10-15 minutes to complete
run_alphafold -d $CURC_AF_DBS -o /projects/$USER -f $CURC_AF_EXAMPLES/dummy.fasta -t
2020-05-14 -m "monomer" -g true -p true

###while it's running, open another terminal window and ssh into the GPU your job is running
on
squeue -u $USER
ssh <nodename>, e.g. ssh c3gpu-c2-u11

###look at GPU activity
watch -d -n 20 nvidia-smi

##when AlphaFold is finished look at timings outputs
cat timings.json
```