AlphaFold2 Short Course November 11 2024

```
#get on A100 testing partition
sinteractive --partition=atesting_a100 --gres=gpu:1 --
ntasks=8 --time=30:00

#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

#use precomputed MSAs to run model inference (time saving
measure for purpose of workshop)
cd /projects/$USER
#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 outputs
cat timings.json
etc.
```

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