#!/bin/bash --norc

#SBATCH --account=csb\_gpu\_acc

#SBATCH --partition=a6000x4

#SBATCH --partition=batch\_gpu

#SBATCH --constraint=csbtmp

#SBATCH --mail-user=add your VU email address here

#SBATCH --mail-type=BEGIN,END,FAIL

#SBATCH --nodes=1

#SBATCH --ntasks=16

#SBATCH --gres=gpu:nvidia\_rtx\_a6000:1

#SBATCH --mem=24G

#SBATCH --time=change walltime based on needs (usually 4:00:00 or more for our AF2.3.2)

#SBATCH --job-name=af232-mlt-test

#SBATCH --output=af232-mlt-test.log

# 11/14/23 Alphafold2 installation and scripts

# Jarrod Smith [jarrod.smith@vanderbilt.edu](mailto:jarrod.smith@vanderbilt.edu)

#script modified by Sai Medury to run on Rocky9 Jun25

# Set your input/output data path

CALCDIR=specify the calcdir for your project

# Your input fasta should be in the directory above:

FASTA=name of FASTA file (should reside in calcdir)

# Where is the AF2 miniconda environment

AF2\_MINICONDA=/sb/apps/alphafold232/miniconda3

# Where is the AF2 Inference data

AF2\_DATADIR=/csbtmp/alphafold-data.230

# Where is the AF2 Git?

AF2\_REPO=/sb/apps/alphafold232/alphafold

cd $CALCDIR

#Look at the driver and GPUs

nvidia-smi

echo -n "Running on "

echo $SLURM\_JOB\_NODELIST

# Activate CSB Alphafold2 miniconda environment

source $AF2\_MINICONDA/bin/activate af232

export LD\_LIBRARY\_PATH=$AF2\_MINICONDA/envs/af232/lib:$LD\_LIBRARY\_PATH

python $AF2\_REPO/run\_alphafold.py \

--fasta\_paths=$FASTA \

--max\_template\_date=9999-12-31 \

--data\_dir=$AF2\_DATADIR \

--output\_dir=$CALCDIR \

--uniref90\_database\_path=$AF2\_DATADIR/uniref90/uniref90.fasta \

--mgnify\_database\_path=$AF2\_DATADIR/mgnify/mgy\_clusters\_2022\_05.fa \

--uniref30\_database\_path=$AF2\_DATADIR/uniref30/UniRef30\_2021\_03 \

--bfd\_database\_path=$AF2\_DATADIR/bfd/bfd\_metaclust\_clu\_complete\_id30\_c90\_final\_seq.sorted\_opt \

--template\_mmcif\_dir=$AF2\_DATADIR/pdb\_mmcif/mmcif\_files \

--pdb\_seqres\_database\_path=$AF2\_DATADIR/pdb\_seqres/pdb\_seqres.txt \

--obsolete\_pdbs\_path=$AF2\_DATADIR/pdb\_mmcif/obsolete.dat \

--uniprot\_database\_path=$AF2\_DATADIR/uniprot/uniprot.fasta \

--use\_gpu\_relax \

--model\_preset=multimer