The final project will combine elements of many of the subjects you learned in MolSim 2020. Good luck!

Download the structure for Trp-cage protein, (1L2Y.pdb) and do the following:

1) **Forcefields.** Generate a topology file for your system using AMBER99SB-ILDN and TIP3P waters. Then, generate the input configuration by creating a box around your protein (at least 1.0 nm from the box edge) and add solvent and counterions (so that the system charge is zero)

2) **Simulation Parameters.** Run energy minimization, then equilibrate your system in NPT over 1 ns to 1 bar and 300K using Berdensen barostat, and a velocity rescale thermostat.

   ***Submit plots of Temperature vs Time, and Pressure vs Time to verify that your system is equilibrated.**

3) **Parallel Computing**. Take the equilibrated system and run 1ns of NPT (at 1bar and 300K) using the following different CPU settings (remember you can adjust the number of cores (ranks) and open MP used for a simulation by setting -ntomp and -np in your mdrun flags, respectively)
   a. -np 2 -ntomp 1
   b. -np 4 -ntomp 1
   c. -np 6 -ntomp 1
   d. -np 2 -ntomp 2
   e. -np 4 -ntomp 4

   *** Submit a scaling plot. A scaling plot contains ns/day on one axis and the amount of resource on the other. (*You can use np * ntomp to use a single value for comparing resource, or you can make multiple plots. Just make sure you have all 5 data points displayed on a plot*)**

4) **Trajectory Analysis**. Take the equilibrated system and run two production simulations using the settings you determined to be the most efficient in #3.
   a. Run 10 ns of NVT (turn pressure scaling off) at 500K
   b. Run 10 ns of NVT (turn pressure scaling off) at 273 K

   *** Plot data from 500K run, and the 300K on the same plots. Generate the following 4 plots: 1) Temperature vs. Time, 2) Pressure vs. Time, 3) Protein RMSD (using c-alpha) vs. Time, and 4) Water Density vs. Time**

5) **VMD/Visualization.** Submit a rendered image (using tachyon or snapshot) for the final frame of the 273K and 500K run.