Stripping and analysis of MD simulations

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To analyze MD simulations

1. Remove the water (right now the files are really big and we only care about the protein)
2. Do analysis on the “stripped” (without water) file

AmberTools can do both things

To strip the simulations:

1. Copy `cpptraj.input, run_strip.slurm` from `/net/dali/home/mscbio/structbio/struct_MD/analysis` to the directory you ran the simulations in
2. The setup is very similar to running the simulations (open the files, change names, `sbatch run_strip.slurm`)
3. This will produce a file called `xxxNAMExxx_50ns_stripped.pdb` this is the file you use to do analysis
4. You should copy this file to your local computer and look at it in pymol (or equivalent) to make sure nothing insane happened
    1. The protein should just like wiggle around not a huge amount of visual motion/unfolding

AmberTools can do both things

To analyze simulations

- There are lots of ways to calculate the things necessary for this assignment I am going to give 2 possible ways

1. Using cpptraj directly (same manor as stripping)
2. Using a python package (pytraj)

(1) Cpptraj

- https://amberhub.chpc.utah.edu/cpptraj/
- Copy `analysis.cpptraj, run_analysis.slurm` from `/net/dali/home/mscbio/structbio/struct_MD/analysis` to working directory
- The commands in this file will calculate the rmsd of all the residues (:1-123) without the hydrogens (&!@H=) in reference to the first frame and the 10th frame
- The output will be put into .dat files that you can then use to plot using your favorite method

(1) Cpptraj

- You also need to calculate some dihedral angles (multidihedral) and the SASA (surf)
- All the commands have a similar set up as rmsd, but look at the docs to be sure
  - command [<dataset name>] [<mask>] [out <filename>]

(2) Pytraj

- https://amber-md.github.io/pytraj/latest/index.html
- https://amber-md.github.io/pytraj/latest/analysis.html
- Python front-end of cpptraj, easily installed via conda locally, it is already on the cluster
- Has very similar commands: rmsd, multidihedral, molsurf

(2) Pytraj example

- Copy `jupyter.slurm, analysis_pytraj.ipynb` from `/net/dali/home/mscbio/structbio/struct_MD/analysis` to working directory
- If you `sbatch jupyter.slurm` and then open `sbatch.jupyter` it gives instructions for opening a jupyter notebook via the cluster
- The example in this is for calculating RMSD from the first frame and the 100th frame

You could also use

- VMD
- Pymol
- Or just write scripts to calculate these things, its up to you ☺