this note is for Week3-VMD results of 50 ns simulation

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Part 1 – commands to open VMD

open desktop in greene—open terminal

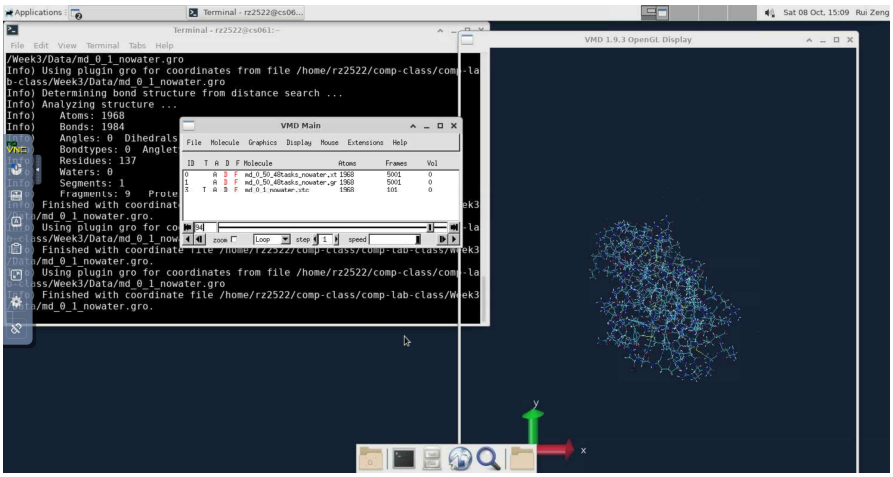
module load vmd/1.9.3

vmd

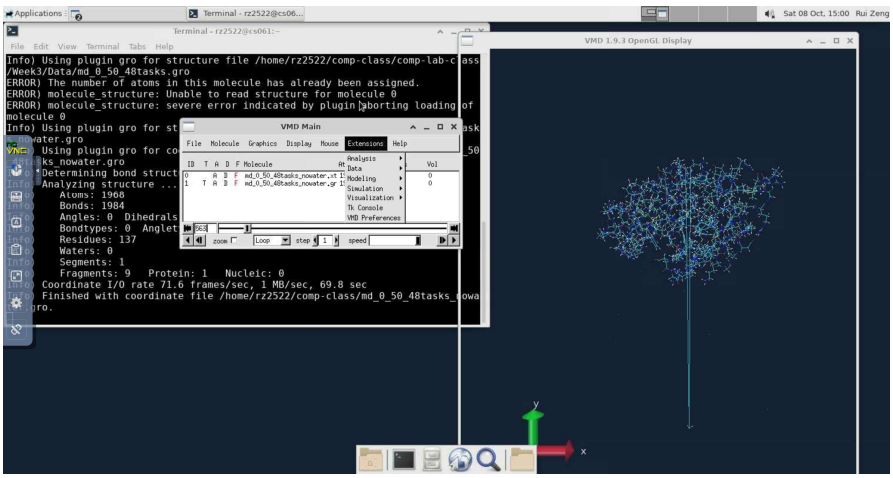
load file

 # Part 2 – VMD results for 1 ns and 50 ns (no water)

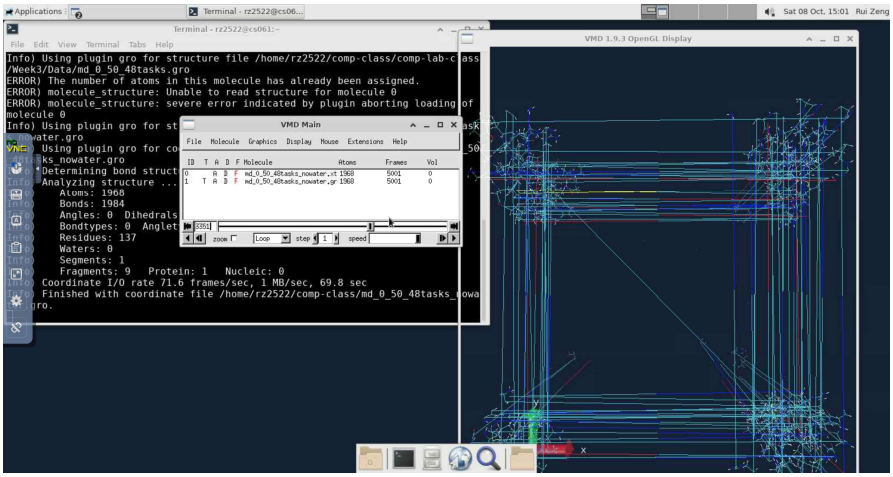
 # for the whole process of 1 ns, the molecule looks fine



 # after ~5 ns, some atoms in the molecule collide with the boundaries



 # from ~5 ns to 50 ns, the whole simulation becomes much disordered



Part 3 – Notes about file size

For 50 ns simulation, there would be 5001 frames, and for each frame there are 1968 atoms (remove water, or 1963 atoms if remove all solvents), so if the gro file contains 5001 frames, the final size of gro file would be ~420 MB.

The only way to avoid large file when removing water is to generate **a gro file which only contains one frame (~133 KB).**

command

mpirun -np 1 gmx_mpi trjconv -s [file name].gro -f [file name].xxx -o [output file name].gro

If the '.xxx' in -f option is '.gro' or '.cpt', the output gro file would only contain 1 frame

Large_file_error: If the '.xxx' in -f option is '.xtc', then the output gro file would contain 5001 frames

Another kind of large_file_error: If use mdtraj.remove_solvent(), and save as gro file, the gro file would contain 5001 frame and be >400 MB