this note is for Week3-VMD results of 50 ns simulation
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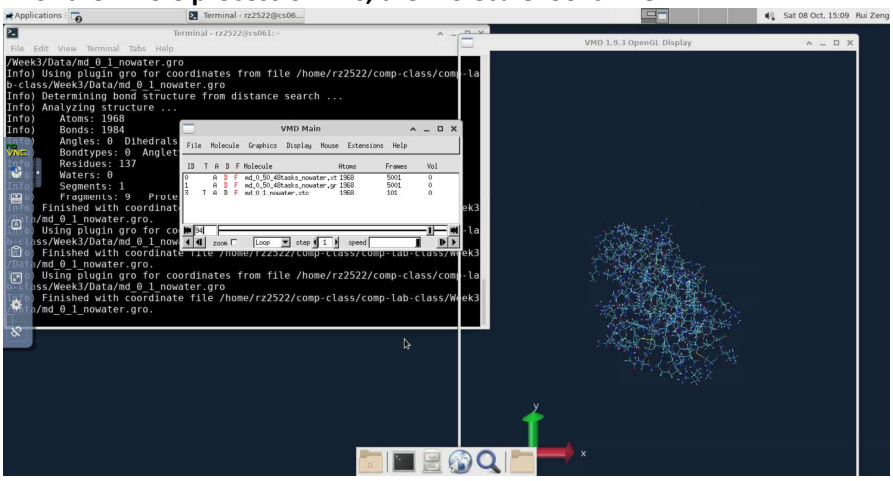
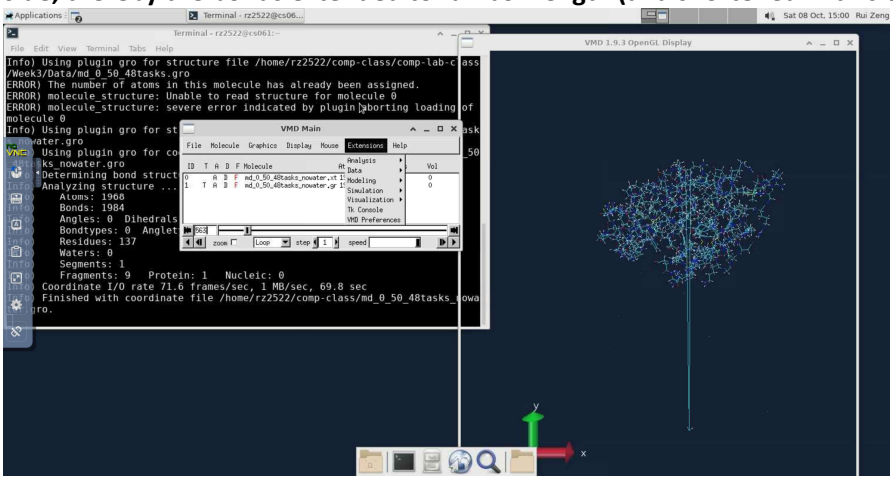
Part 1 – commands to open VMD
open desktop in greene—open terminal
module load vmd/1.9.3
vmd
load file

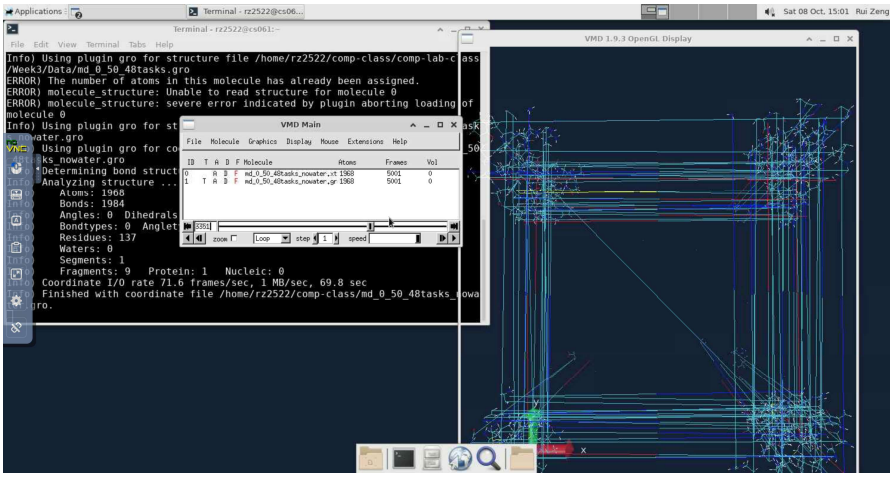
 # Part 2 – VMD results for 1 ns and 50 ns (no water)
 # for the whole process of 1 ns, the molecule looks fine



 # after ~5 ns, some atoms in the molecule cross the boundaries, and jump back from another side, thereby the bonds extended to full box length (and shortened with closer distance).

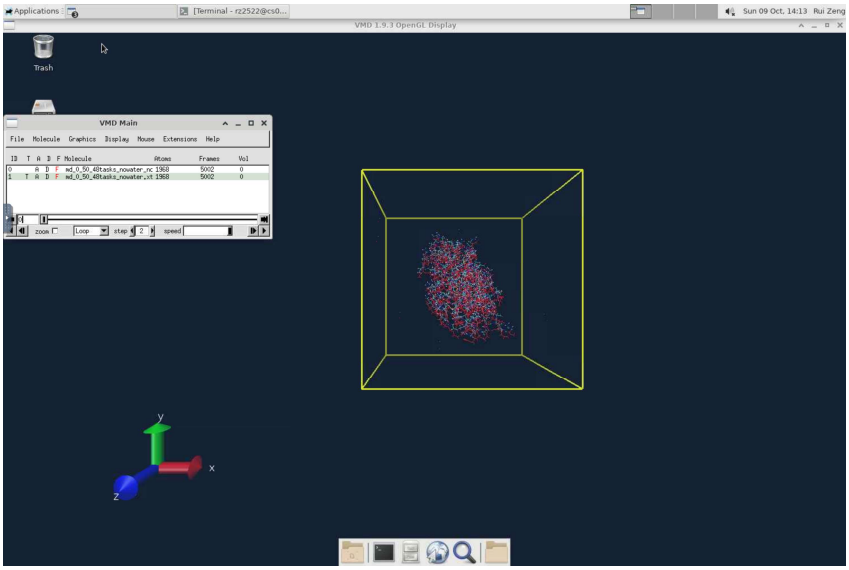


 # from ~5 ns to 50 ns, the whole simulation becomes much disordered



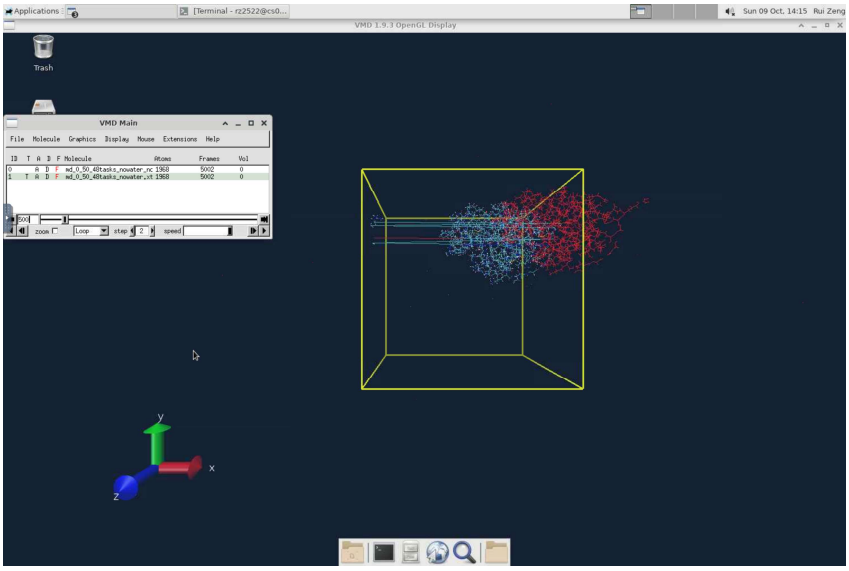
 # try to fix with pbc treatment '-nojump'

 # time = 0 ns (red molecules are fixed with nojump, yellow box is PBC box)



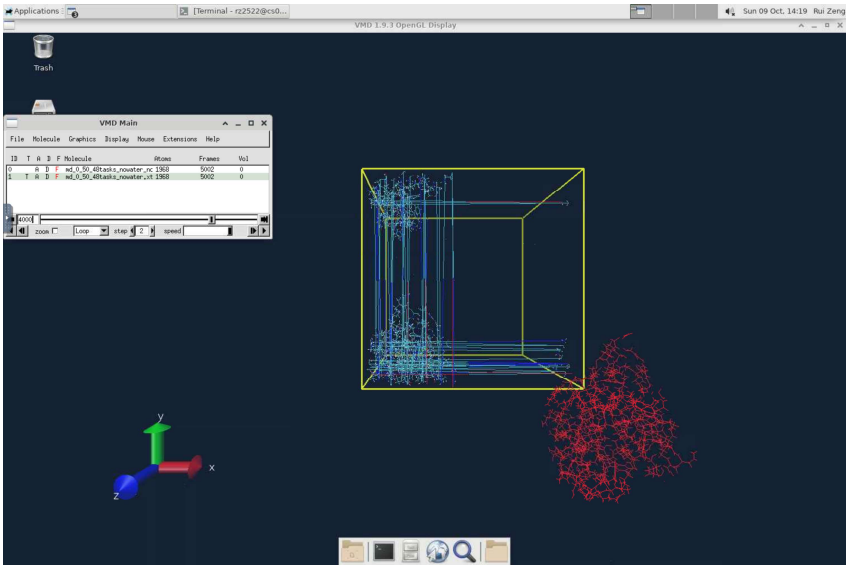
 # time = 5 ns

some molecules in the wrapped system jump, leading to extended bond length; meanwhile the molecules in the unwrapped system move partly out of the box



 # time = 40 ns

This is why in wrapped system it looks so disordered. With continuous trajectory, the molecules would almost move out of the box



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); thereby this gro file only works to provide topology information and won't cover the coordinates and velocities of all the time range.**

command

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

here, -f is the input trajectory file; -s option provides topology information (structure and mass of the system, because to output .gro file, besides the trajectory information, we also need topology information
If the '.xxx' in -f option is '.gro' or '.cpt', the output gro file would only contain 1 frame, because the input gro/cpt only contains one frame
Large_file_error: If the '.xxx' in -f option is '.xtc', then the output gro file would contain 5001 frames (because the input xtc file contains 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. Because when use 'traj=mdtraj.load (XXX.xtc, top=XXX.gro)', the 'traj' would combine both the trajectory information from .xtc and the topology information from .gro, and this process works like 'gmx trjconv' using xtc file with 5001 frames as input.