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Part 1 – Trp-Cage case study

```
f) Copy my README.bash script from the Scripts directory to this Gromacs
directory as the script run_setup.sbatch. Compare my script to the other
one, do you see what the differences are?
```

Answer:

a. In README's heading, it uses '#! /bin/csh' to use C-shell instead of bash shell

b. In csh, add 'set' before definition like 'set A = B' instead of 'A = B' in bash

c. Both in csh and bash, we use '$(var)' to get the value of variable 'var'. However, when a calculated value, e.g., the value of 'A-B', is being assigned to variable 'var2', bash would use 'var2 = $($(A)-$(B))' while csh would use '@' as '@ var2 = $(A) - $(B)'

d. For the 'while' sentences, csh goes like

```
while ()
        XXX
end
```

, and bash goes like

```
while []
do
        XXX
done
```

e. For the 'if else' sentences, csh goes like

```
if () then
XXX
else
XXX
endif
```

, and bash goes like

```
If []; then
        XXX
else
```

XXX

Fi

f. When comparing two integers, in csh, we use '==', '<=', etc. While in bash, we use 'A -eq B' to mean 'A == B'. Similarly, '-lt' (less than) for '<', '-gt' (greater than) for '>', 'ne' (not equal to) for '!=', 'le' for '<=', 'ge' for '>='.

As a result, to conduct 10 times of step_5, the provided bash script should be modified to 'while [${cnt} -le ${cntmax}]' so as to match 'while (${cnt} <= ${cntmax})' in the original README file

g. In the original README file, it does not use MPI command to run the gromacs, so in bash, we replace 'gmx grompp' with 'mpirun -np 1 gmx_mpi grompp' and replace 'gmx mdrun' or 'gmx_d mdrun' with 'mpirun gmx_mpi mdrun'. 'gmx_d' in the README means double precision.

Part 2 – Water&Ions case study

```
d) Modify the step5_production.mdp to write out snapshots, velocities, and
forces every 10 ps (which option is this)
```

Answer:

a. For snapshots, change 'nstxout' to 5000 steps (nstxout*dt=5000*0.002=10 ps). 'nstxout' controls number of steps between outputs of coordinates into .trr file (the trajectory file)

b. For velocities, change 'nstvout' to 5000 steps. 'nstvout' controls the elapse of velocity outputs into .trr file.

c. For forces, change 'nstfout' to 5000 steps. 'nstfout' controls the elapse of energy outputs into .trr file.

d. For later reference, https://manual.gromacs.org/documentation/current/user-guide/mdp-options.html

```
f) Concatenate the trajectories and this time, unwrap using the ' trjconv
-pbc nojump ' option of gromacs. If you open in VMD, you will see the
molecules seem to spread out!
```

Answer:

a. Notes for opening vmd

module load vmd/1.9.3

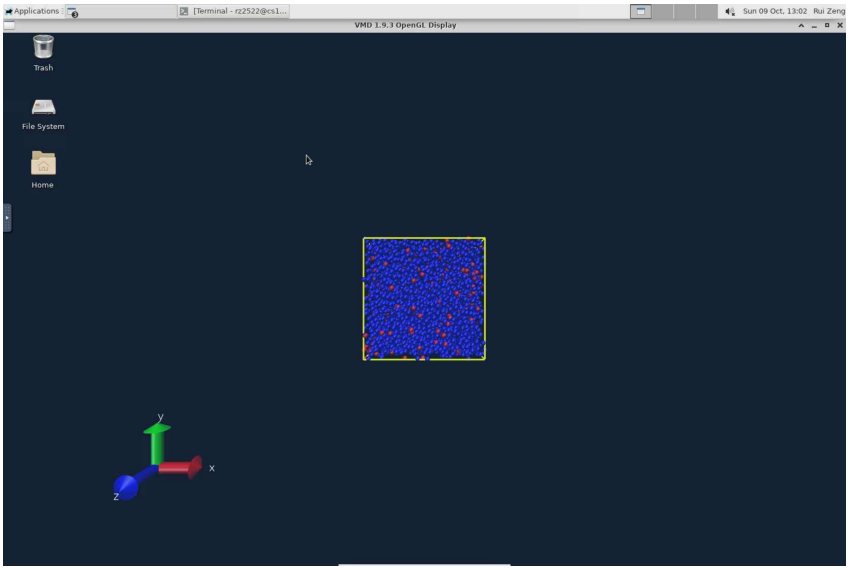
vmd

for pbc box

pbc box -color yellow

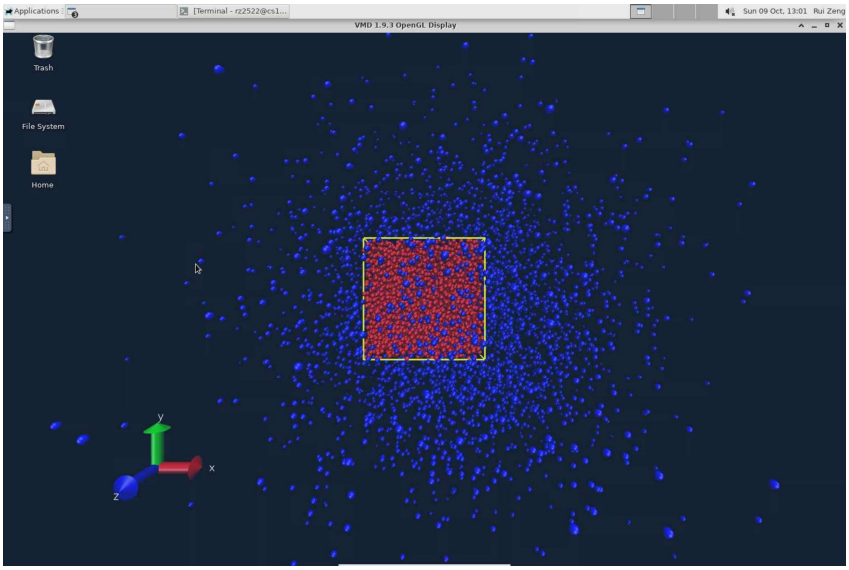
b. The status of molecules at **time = 0 ns** (red for wrapped system, blue for unwrapped system; representation-bead; period boundary conditions (pbc) box is shown in yellow)

Both are confined in the pbc box



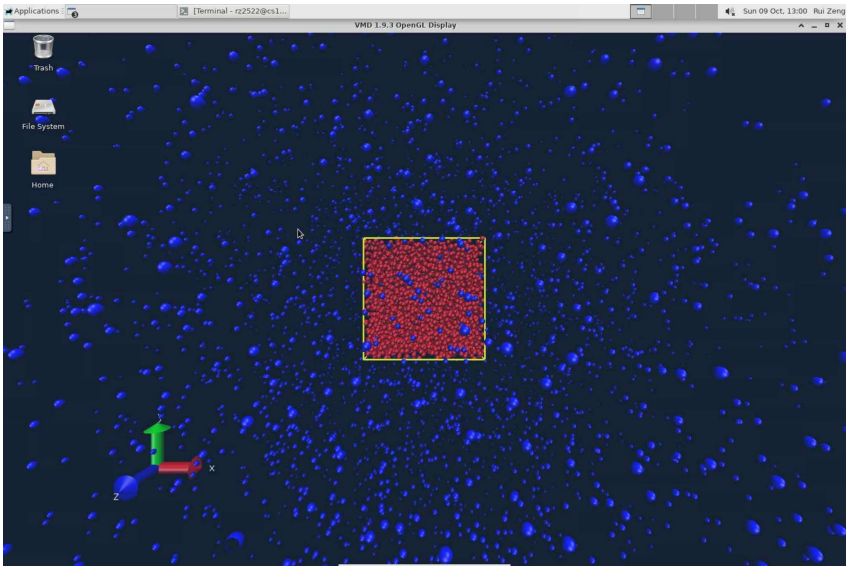
c. The status at **time = 1 ns**

unwrapped molecules start to spread out and diffuse out of pbc box



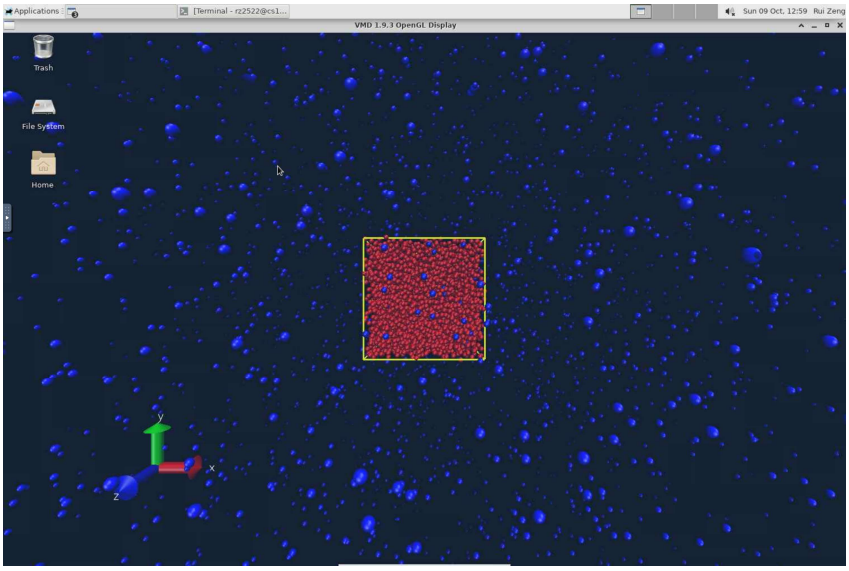
d. The status at **time = 5 ns**

unwrapped molecules spread out more



e. The status at **time = 10 ns**

unwrapped molecules are dispersed everywhere, and in the display window, they look much less concentrated



f. Therefore, if use 'trjconv -s [topology file] -pbc mol', the center of mass of molecules would be confined in the center of pbc box, so it looks like wrapped in the box. (To provide structure and mass information, a topology file is need for '-s' option)

If use 'trjconv -pbc nojump', the jump (when an atom goes out of the box, make it enter from the opposite side) will not happen, and a continuous trajectory will be got, which also leads to diffusion out of the pbc box. (topology is not needed if the output is just xtc)

g. For future reference: VMD pbc command https://www.ks.uiuc.edu/Research/vmd/plugins/pbctools/