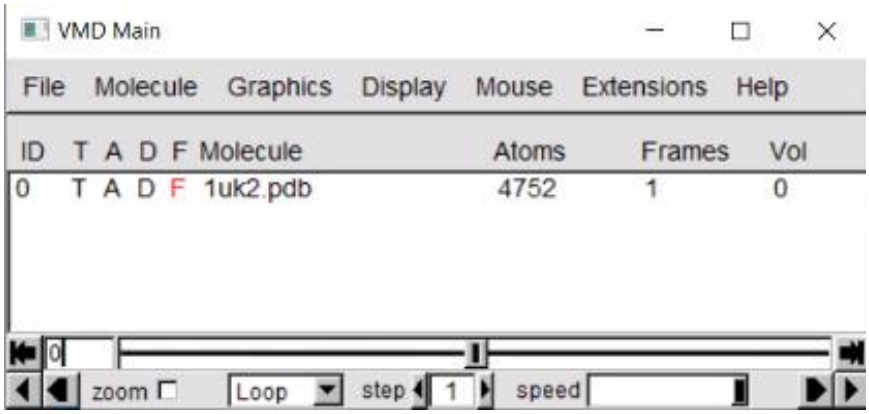
Assignment1

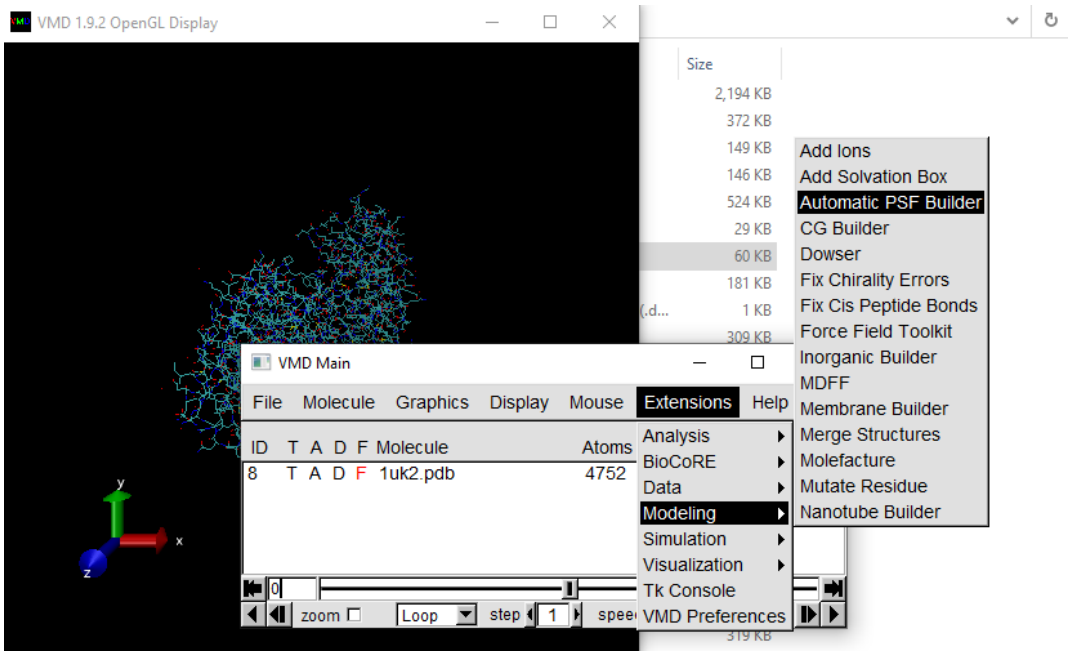
Task1 all steps

Step1: Generate Protein Structure File (PSF)

1.1 Load 1uk2 pdb file into VMD:



1.2 Build Protein Structure File:



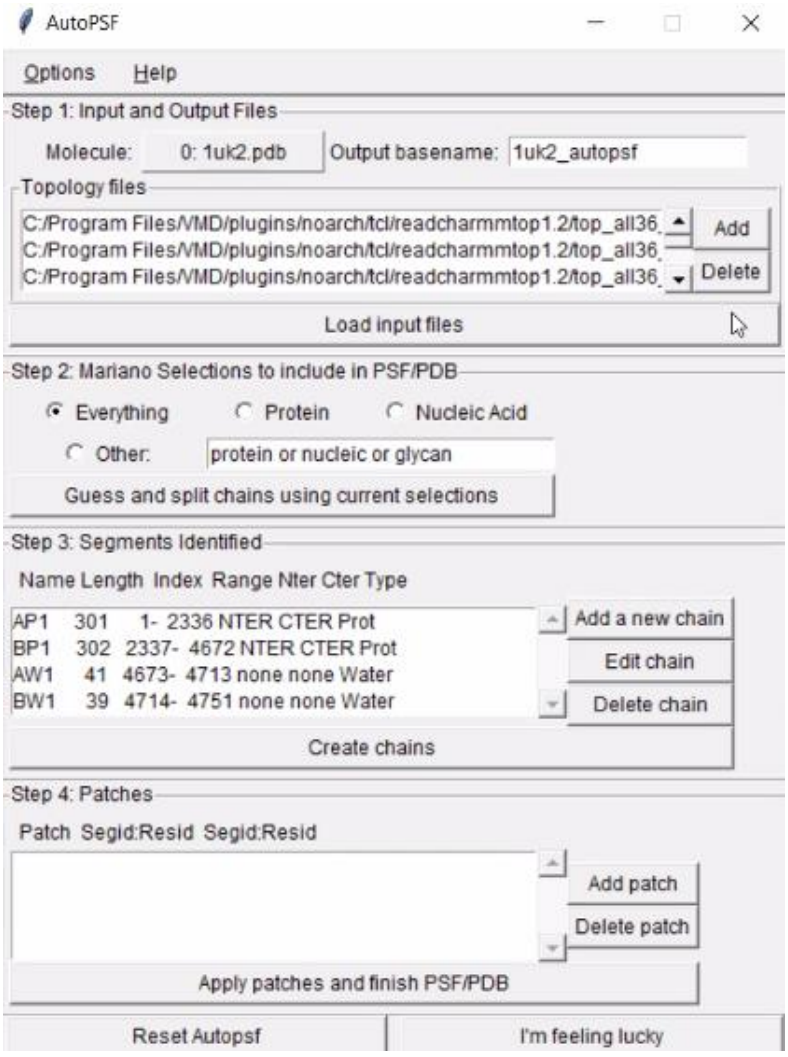
1.3 From the Automatic PSF Builder Window apply the following in order:

a. Load input files.

b. Guess and split chains using current selections.

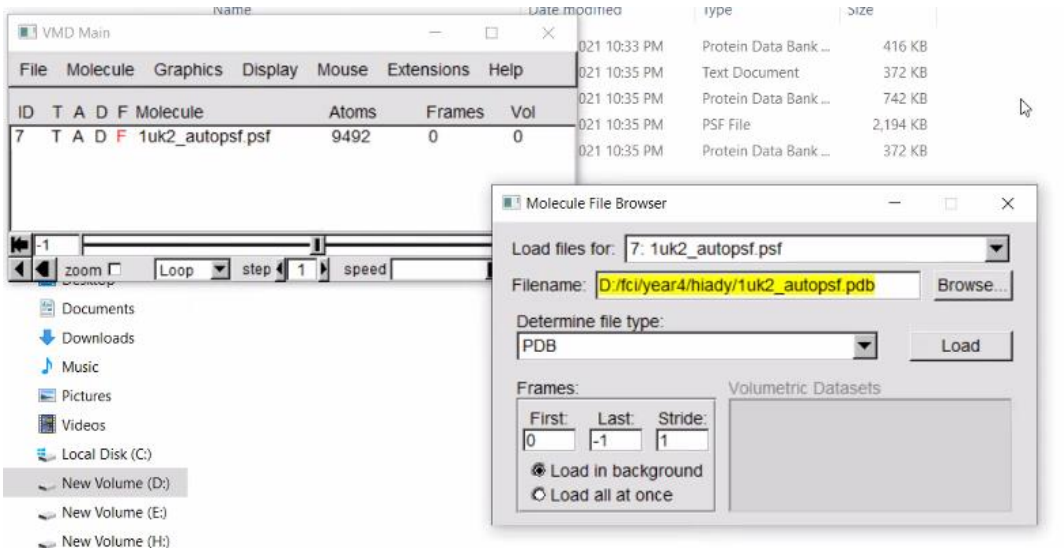
c. Create chains.

d. Apply patches and finish PSF/PDB.

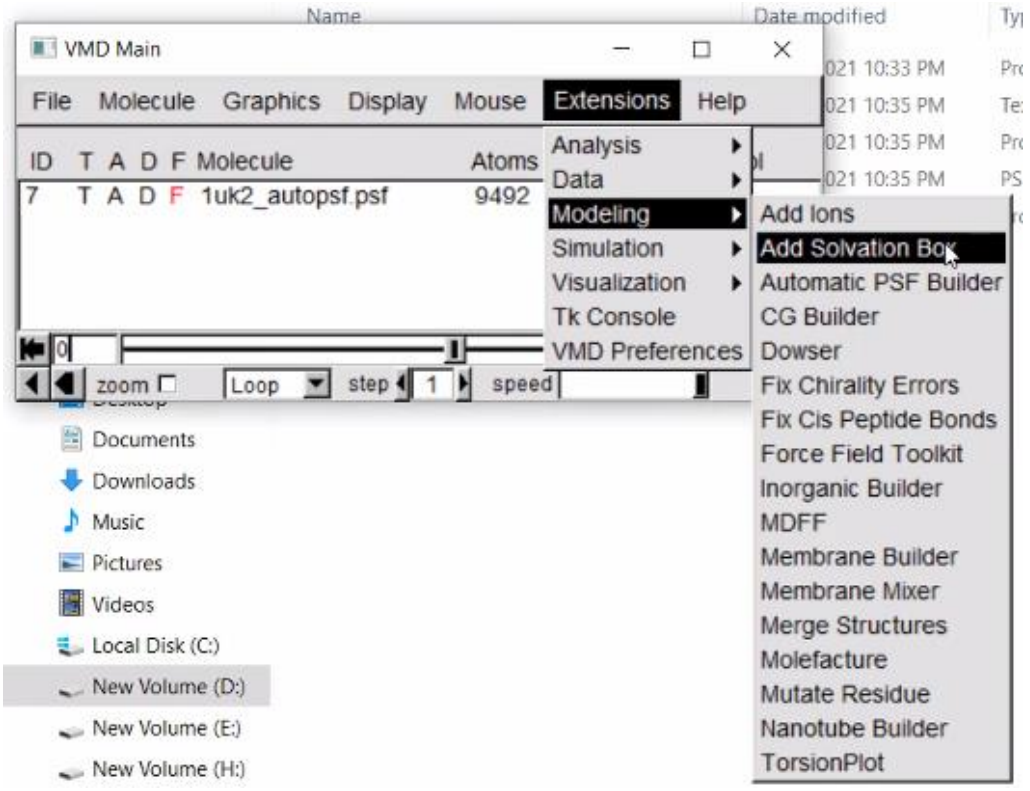


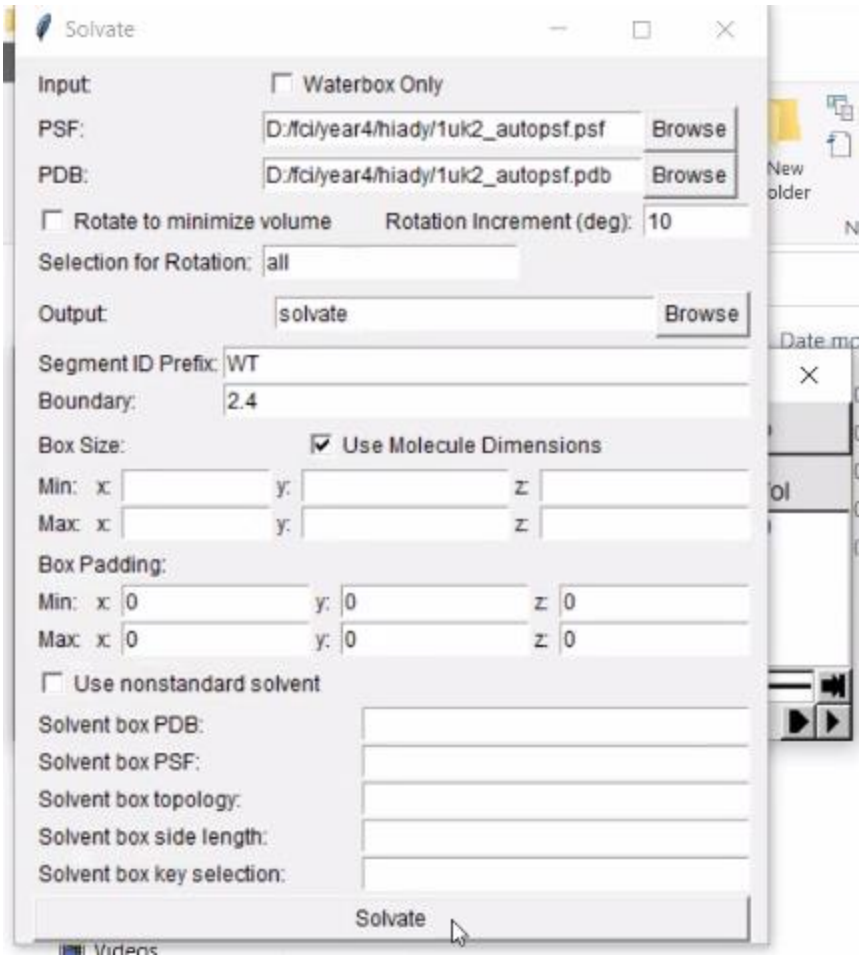
Step2: Solvating the Protein

2.1 Load the auto generated PSF file to the VMD main first, then load on top of it the new PDB:



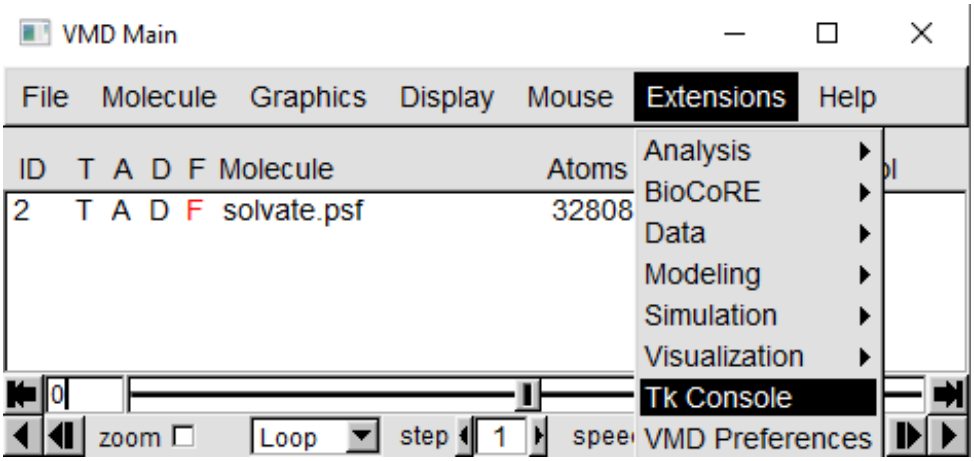
2.2 Create a Water Box around the molecule to simulate the cellular environment:





Step3: Configuration File Preparation

3.1 Load the solvated PSF file into the VMD main, then load on top of it the solvated PDB file, then open the VMD TK console.

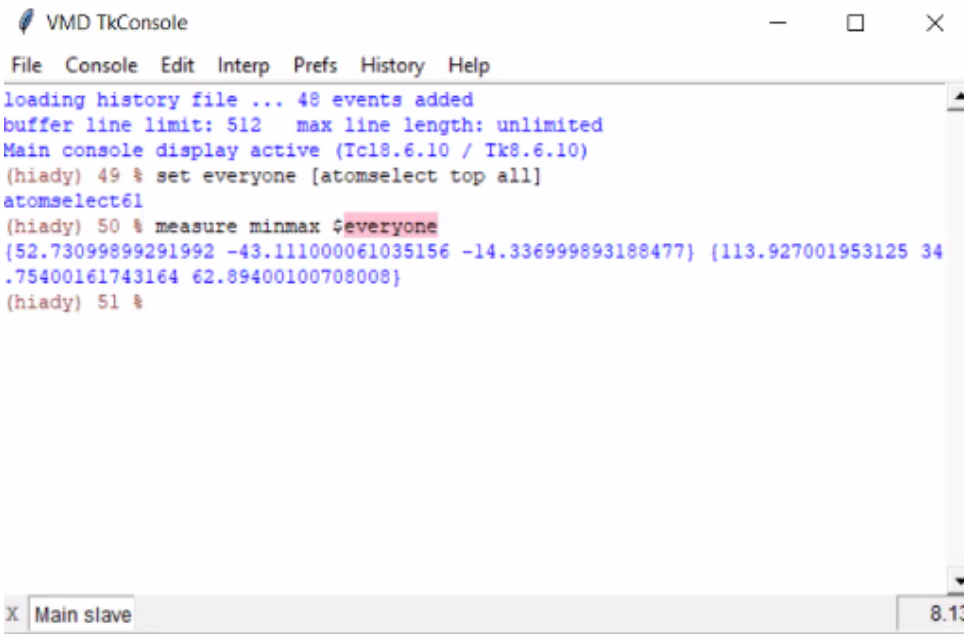


3.2 Run the following command to select all atoms of the molecule:

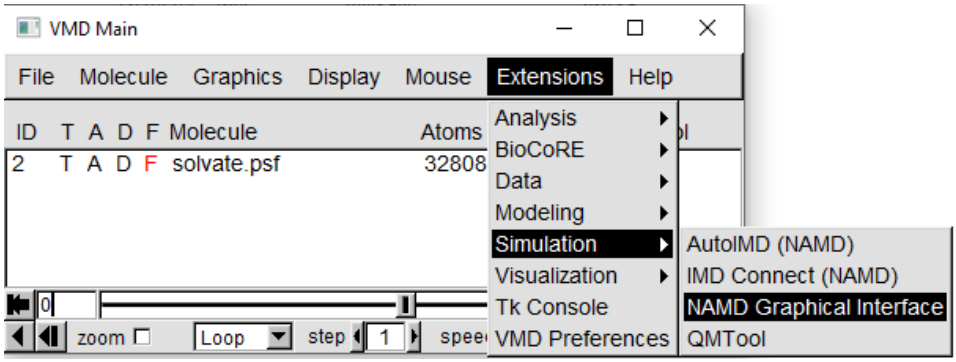
set everyone [atomselect top all]

3.3 Run the following command to extract the minimum and maximum coordinates of the water box:

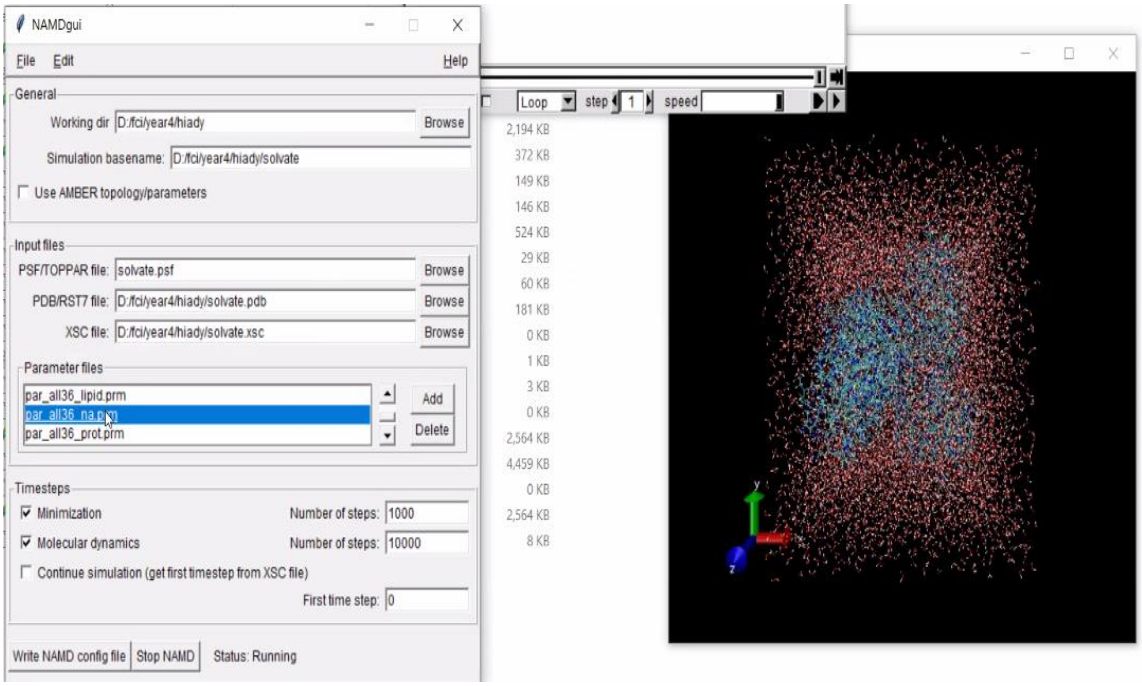
measure minmax $everyone



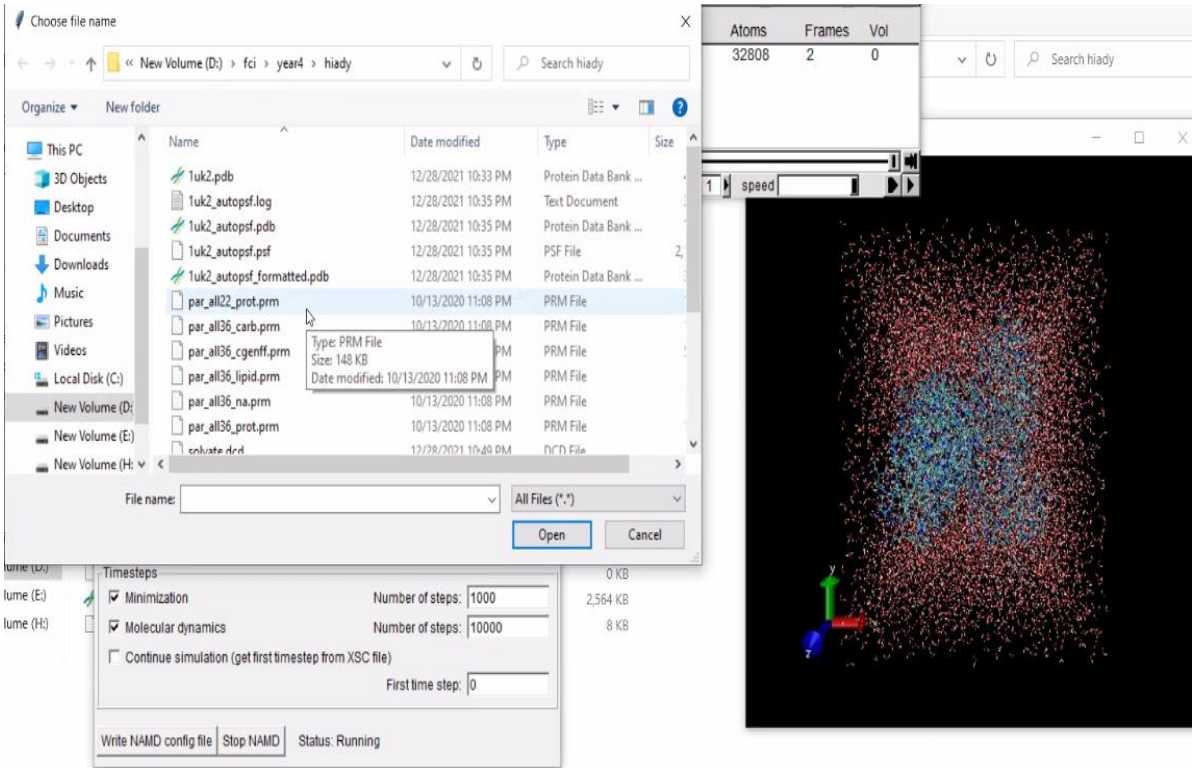
3.4 Open the NAMD graphical interface from the VMD main:



3.5 Select the (Minimization - Molecular dynamics) checkboxes from the timesteps section:



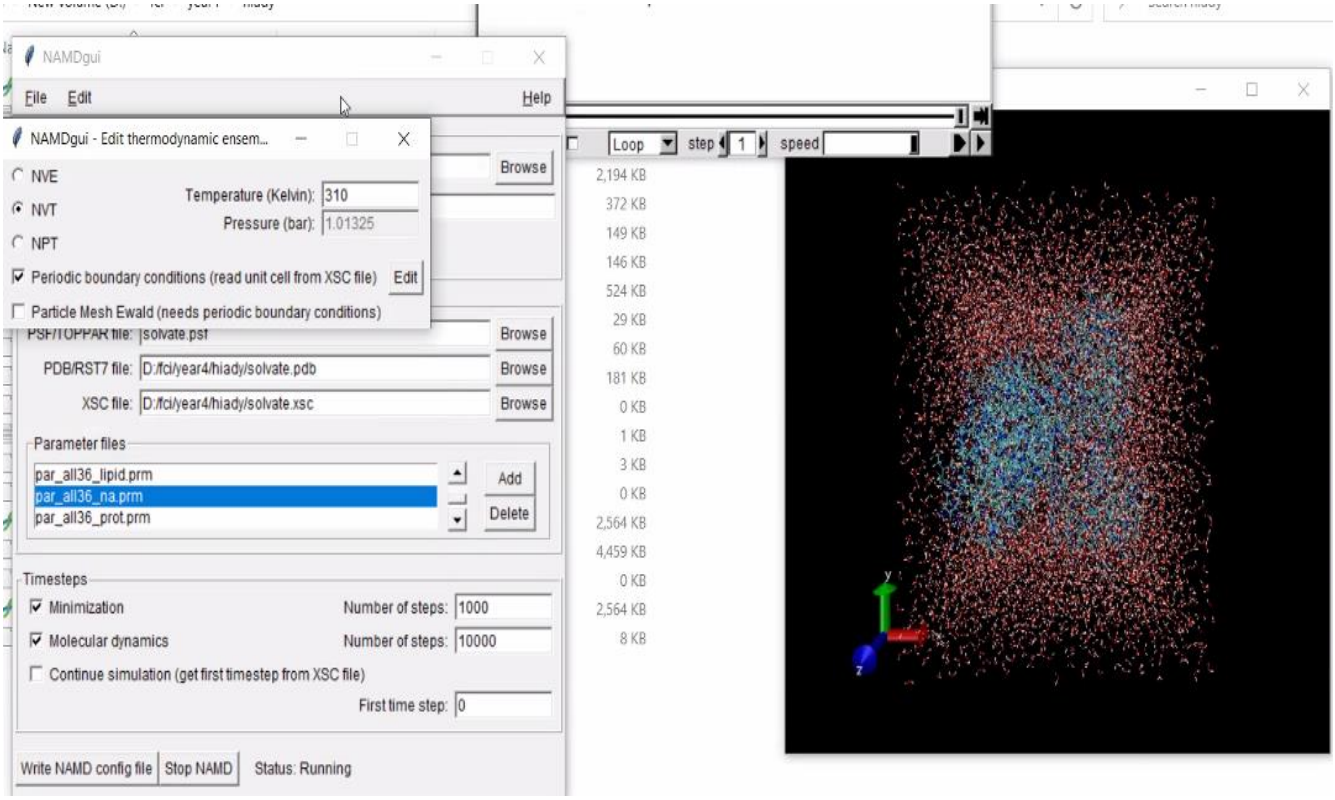
3.6 Select suitable parameter files for the loaded molecule:



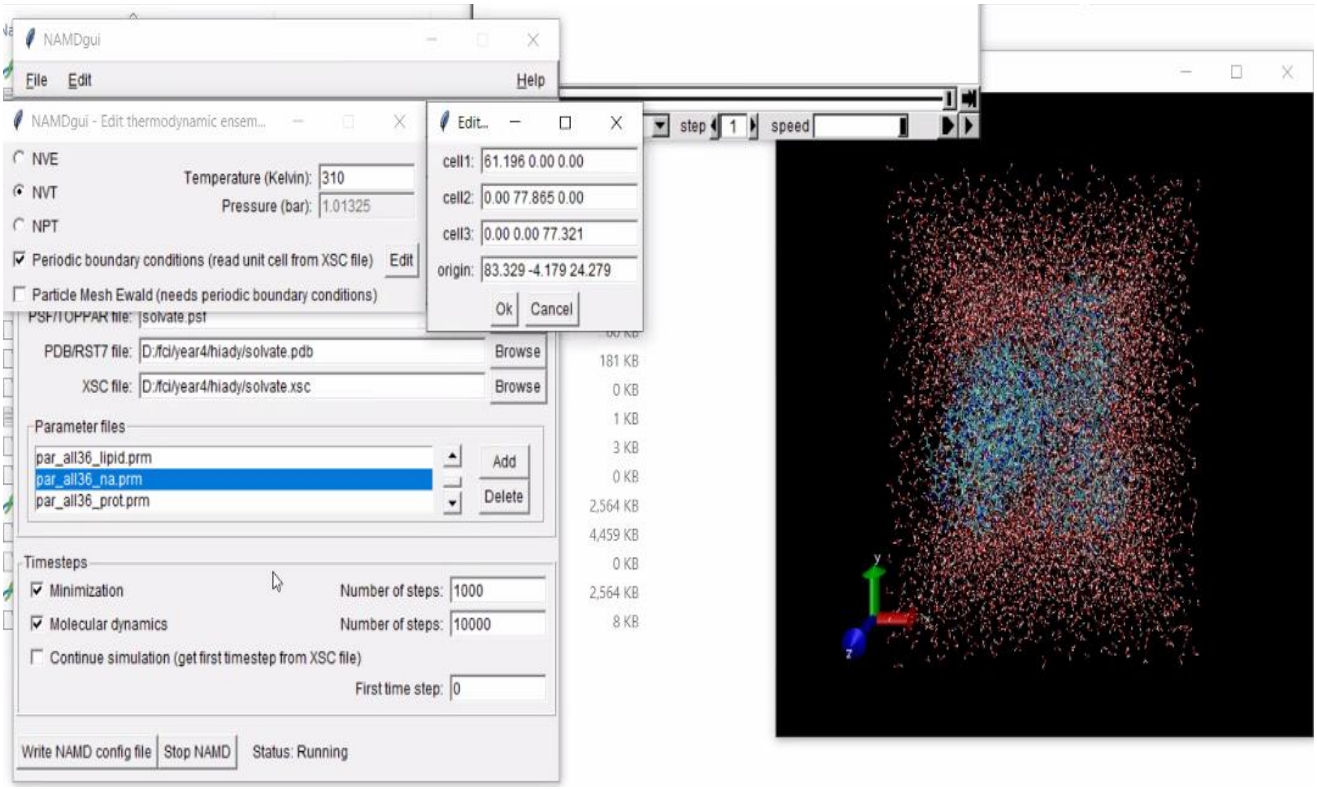
3.7 Modify the temperature in which the simulation will be carried out:

Set temperature to 310 K°

Select periodic boundary conditions checkbox



3.8 Edit the periodic boundary conditions with the calculated dimensions and origin that extracted in step 3.3

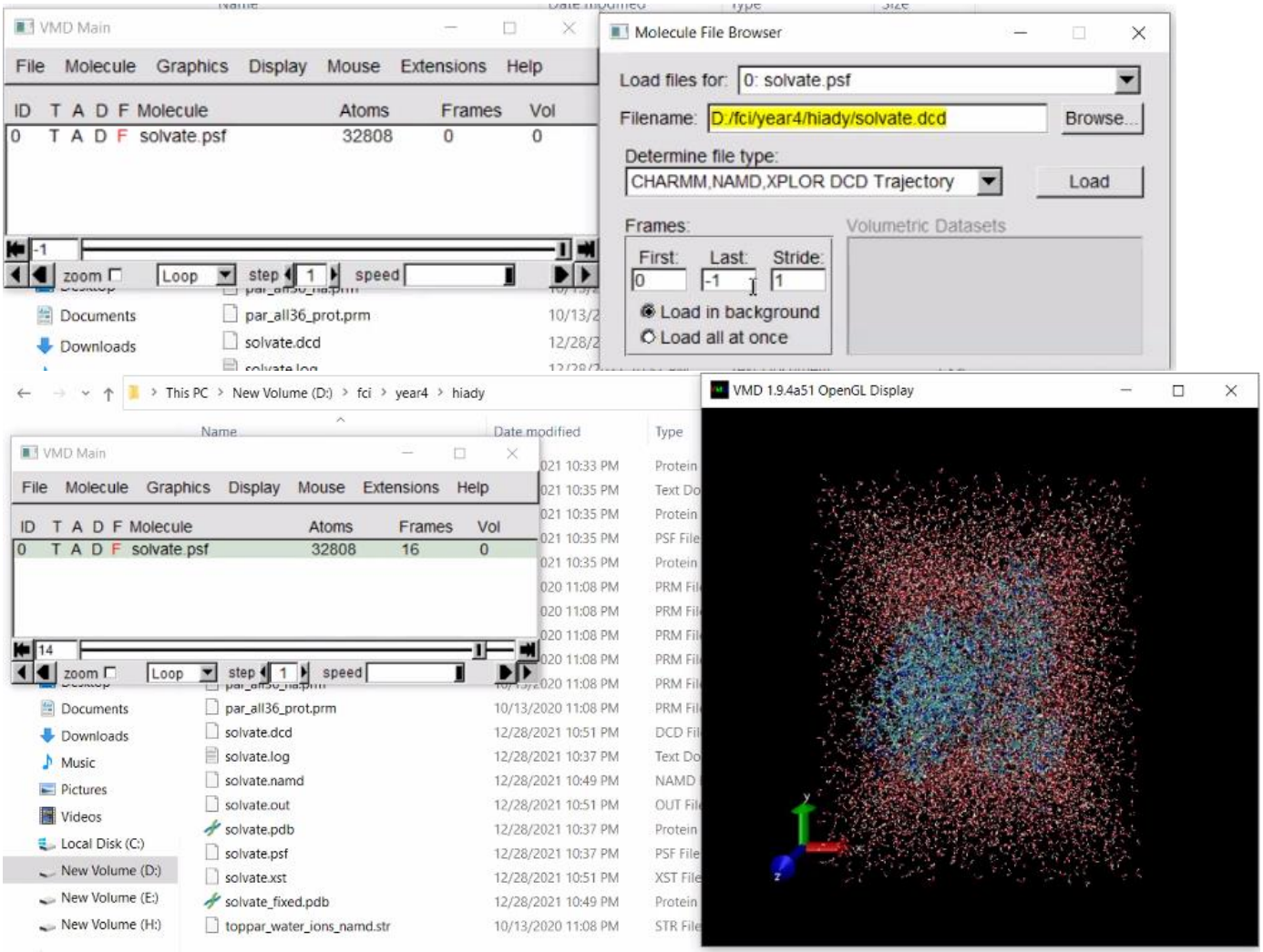


Step4: Run MD Simulation

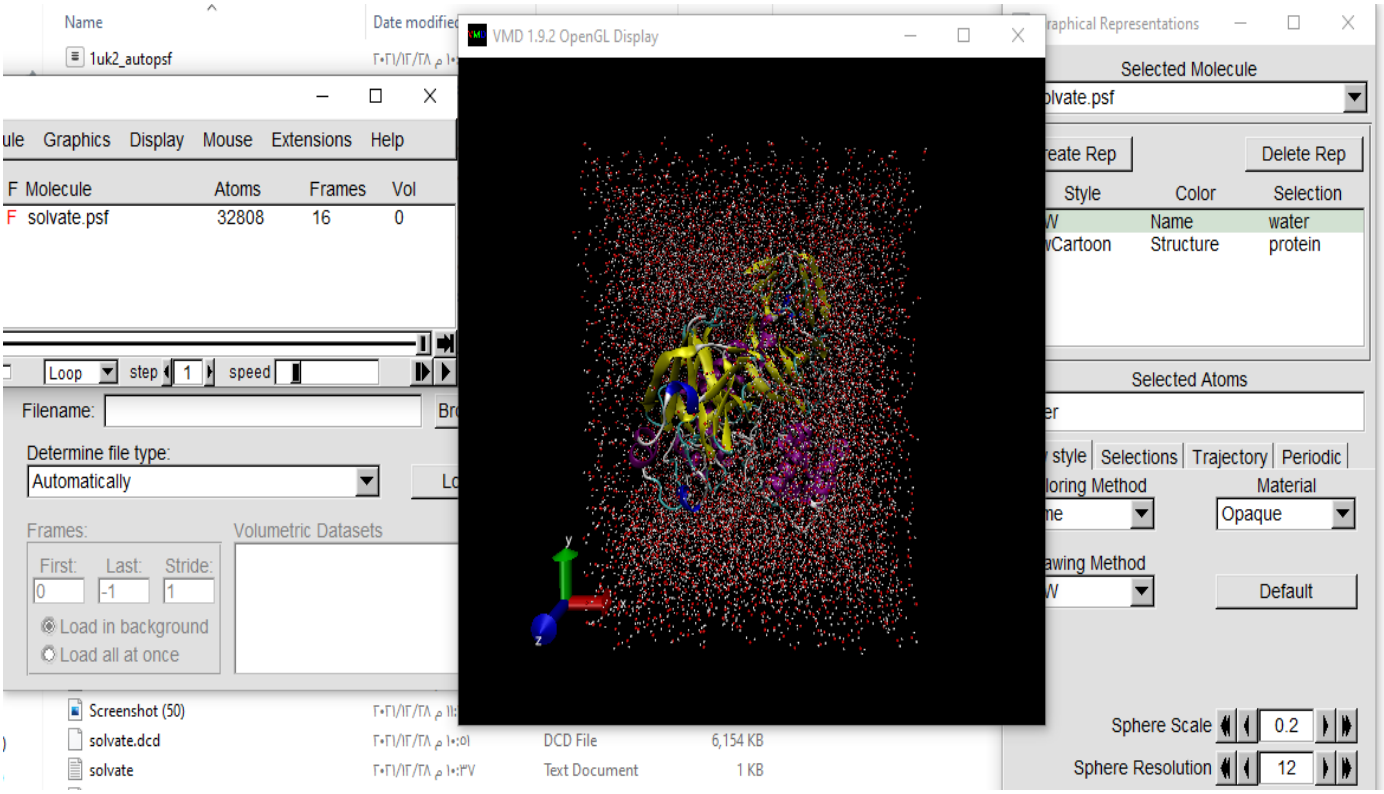
Now the configuration file is set up, and NAMD is ready to run the simulation.

Step5: Loading Trajectory File

5.1 Load the solvated protein PSF file, then load the DCD trajectory file on top of it:



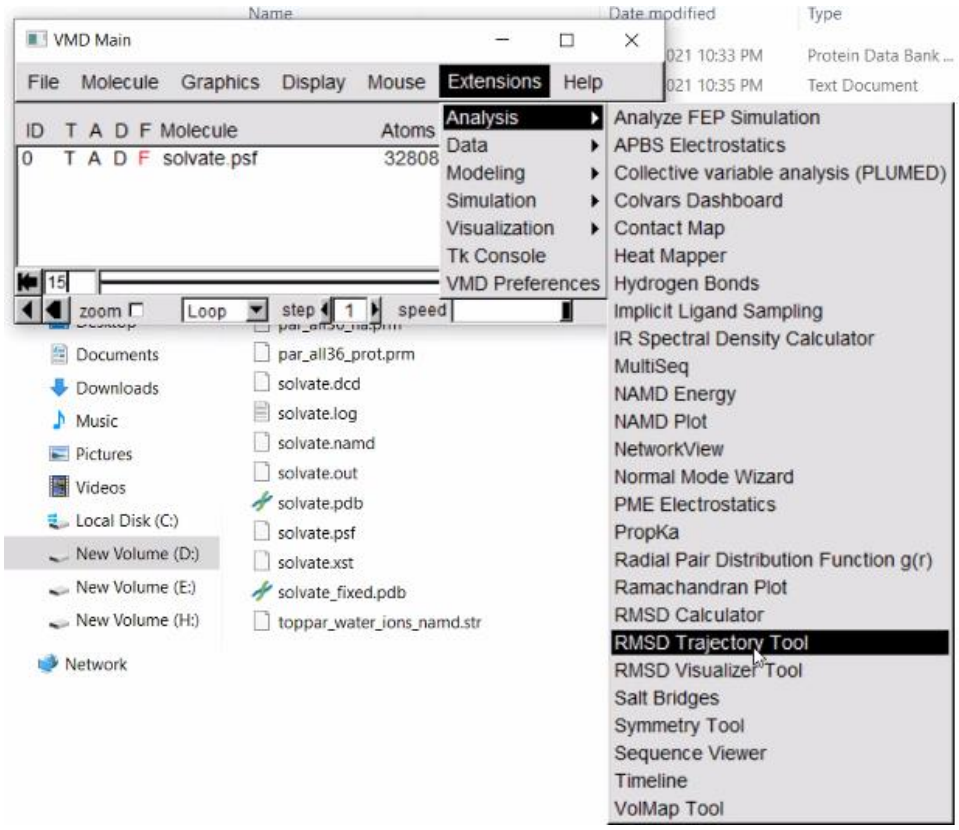
5.2 Display Molecule using Different Representations:



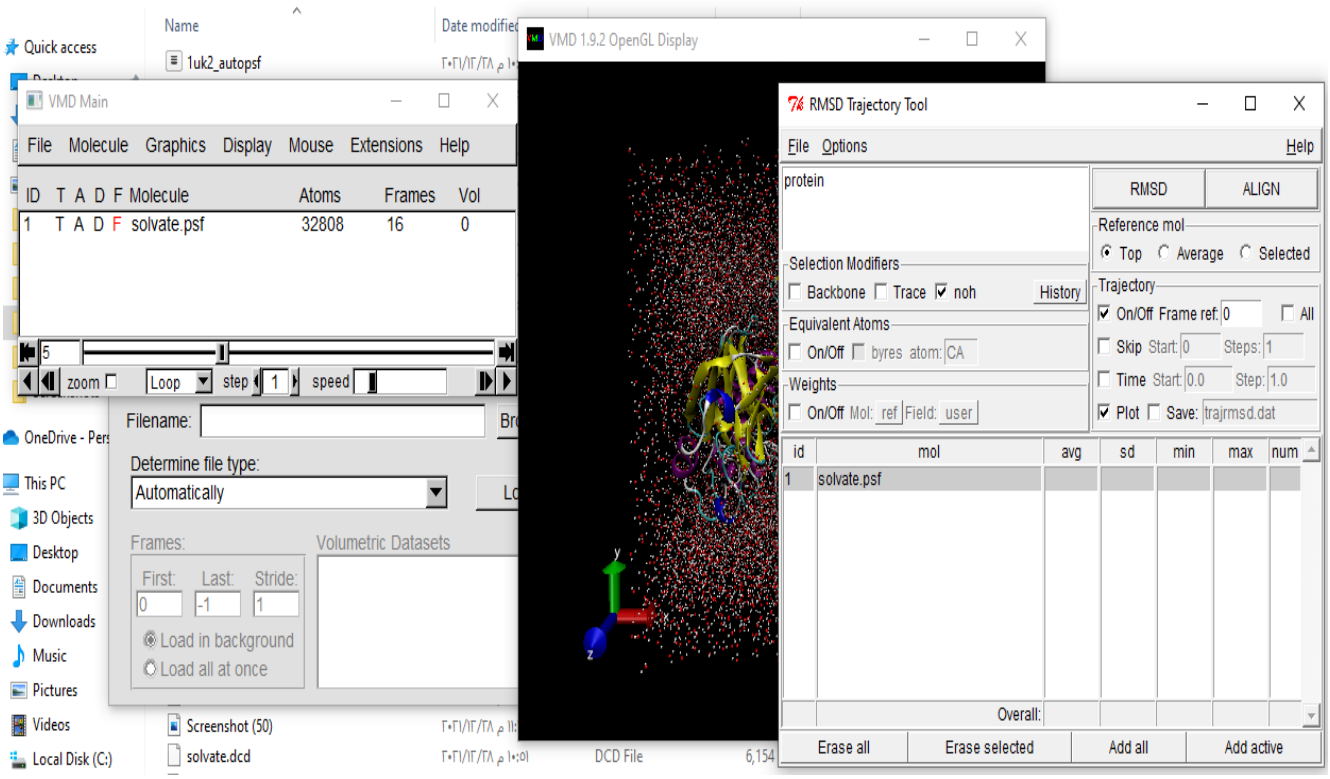
Step6: RMSD Analysis

Analyze the DCD trajectory file:

6.1 The active molecule should be the PSF File loaded in the main window of the VMD.



6.2 Click on ALIGN button, then RMSD button



6.3 The protein RMSD (in °Angstroms) vs. frame number is displayed in a plot.