Smog_AA run setup

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1 Introduction

This is a guide to re-run the original simulations in another server. I explain how to run it directly from the directories

2 Gromacs-SBM

The Gromacs-SBM version used for these runs can be downloaded from the SMOG server.
`http://smog-server.org/extension/gromacs-4.5.4_sbm1.0.tar.gz`
In any case, I have included it as a tarball in the directory where the run setup is located. You will have to install this version of Gromacs; please make sure you specify that its commands have the underscore "`_sbm`" so that you differentiate it from the usual gromacs. For example, the command that is used to run the simulations is "`mdrun_sbm`".

3 Run "as-is"

- I have uploaded two directories, one for R15 and the other for R16. The pre-determined temperatures are the ones that I have found to be closest to the equilibrium temperatures.
- The `run.slurm` and `rst.slurm` files are obviously configured for NOTS, with a time limit of 24 hours. These runs take about 80 hours on a single node. You would have to modify this according to the resource management system installed there.

- As mentioned in the "Introduction to the LWO model" file that I sent you together with this one, the way for me to obtain more folding and unfolding events with the time constraints given by NOTS is to run 6 simultaneous trajectories starting from a different frame.

- If possible (and manageable), it would be nice to run a single or maybe 2 or 3 trajectories for longer than 50 ns or 10^8 frames, so as to completely avoid any correlation between the runs.

- If you make such modifications to the `nvt.mdp` file, remember to recompile the .trp file by executing:
`grompp_sbm -f nvt.mdp -c smog.gro -p smog.top -o topol_4.5.tpr`

- The command to run the simulation is:
`mdrun_sbm -s topol_4.5.tpr -nt 1`

- I specify 1 thread in -nt. If you would like to continue a job that stopped before its completion you can use:
`mdrun_sbm -s topol_4.5.tpr -cpi state.cpt -nt 1`

4 Modify temperature/Ionic strength

- If you would like to change the temperature at which the run is performed, then you would have to change two files:

- The first one is `nvt.mdp`, where you would have to modify the temperature in the two places where it is stated.

- The second one would be to generate a different table.xvg. For that purpose, I created a little python script that does this for you called `create_table.py`. You just have to open this python file and modify the temperature variable at the beginning, and then execute the file. You can also modify the ionic strength.

- Once these two are modified, you have to generate the new .tpr file by executing as usual:
`grompp_sbm -f nvt.mdp -c smog.gro -p smog.top -o topol_4.5.tpr`

5 Calculate Q per frame

- Once the runs are completed, you can use the following command included in the package to calculate Q per frame:
  `g_kuh_sbm -s smog.gro -f traj.xtc -n smog_long.ndx -o Q -noshortcut -noabscut -cut 0.3`

- This will yield a Q per frame file (Q.out). If you look at, for example, the `contacts_12.slurm` file you will find the command to calculate the Q per frame for a specific interface between the three helical segments of the protein (in this case, the first and second)