Workflow: Membrane Viscosity via Green-Kubo Relation

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1 Introduction

I've made changes to these files since the last time I ran a system myself, so there *may* be typos... Parts of this I transferred over from Stampede2 and haven't run on Bridges2, and some of it I wasn't using 'best High Performance Computing practices'...

I'm including some files that I'm keeping on my github page: https://github.com/sheamusfitz/g-k-viscosity. The first of these to show up, I think, is `eq.batch`. If there are files in there that I don't mention in this document, then you don't need them, and they're either development versions just for me, or else they're some analysis code I've written and we ended up not using.

As a brief rundown of the procedure: in 2 we use CHARMM-GUI to set up the system, and 3 use the default minimization/equilibration procedure that the GUI generates. Then, 4 we need to make a custom index file, `grompp` the NPT simulation, and 5 run it.

The purpose of running this NPT simulation before the main (NVT) simulation is so that we can find the ideal simulation box size for each replica of the system, and then initialize the NVT simulation with the frame from the NPT simulation closest to the 'best' size.

2 CHARMM-GUI

From the web browser on whatever local machine you're currently looking at, charmm-gui.org

step 1 "Membrane Only System"

step 2
- water thickness: 40Å
- length of X & Y: 100Å
- pick lipid ratios you want for the lipid you want
- view system info
- go to next page
- *takes ∼1 min*

step 3
- click view structure *(i've never personally seen anything wrong here, but it's good to look)*
- replacement method: uncheck "include ions" (unless the lipid you're looking at has a net charge)
- *takes ∼1m*

step 4.1
- view structure
- continue
- *takes ∼1m*

step 4.2
- view structure, again
- go, again

– *takes ∼1m*

step 5
– view structure
– CHARMM36 (not CHARMM36m)
– Gromacs
– generate grid info for PME FFT autocmatically
– NPT ensemble
– Temperature:
  * check the phase transition temperature of the lipid here: https://avantilipids.com/tech-support/physical-properties/phase-transition-temps (or just google "avanti phase transition temperatures") If it's not on their list, uh, find it somewhere else.
  * use $10\,^{\circ}$C above the transition temperature, or just $10\,^{\circ}$C—whichever is higher.
– *∼3 min*

step6
– download the `.tgz` file
– immediately rename that from `download.tgz` to `POPC.tgz` before you forget. *I'm going to always use 'POPC' as the example lipid here, but obviously name the file whatever you want*
– move the file wherever you want it to be (probably `scp` onto whatever remote machine you're going to run the simulations on.)

– to unzip it, use `tar -xvzf POPC.tgz`

from the machine you're going to run the simulations from

3 Minimization and Equilibration

In the file `POPC/gromacs/README`:

- (using vim or nano or whatever text editor you want), replace all occurrences of `gmx_d` and `gmx` with `gmx_mpi`. If you're using `vim`, that's `:%s/gmx\(_d\)\?$/gmx_mpi/g` because *for some reason* you need to escape parentheses and question marks, *but not* underscores or dollar signs. idk.
- delete or comment-out the last ~ 15 lines of code: everything after '`# Production`'

From inside the folder `/wherever-the-folder-is/POPC/` on the remote machine, just from the terminal

```
for r in {1..5}; do
   mkdir r$r
   cp -r gromacs/* r$r
done
```

This creates the folders `r1, r2, r3, r4, r5`, and then copies the `gromacs` folder as each of those. Now there are 5 identical folders. (Don't worry: one of the equilibration steps that we are about to run will make the replicas different, it has to generate the velocities randomly)

Then, from the same location:

```
$ sbatch eq.batch
```

This puts a job in the SLURM queue on the computer you're using (if you're using a SLURM machine), and when it runs it will minimize and equilibrate all of the systems, using the default files generated by CHARMM-GUI.

This puts one job in the SLURM queue, but once it launches it will actually become 5 separate jobs. I'm

not entirely sure if the 7 hours allocated to it is enough, I just changed how I'm launching it soooo we'll see.

4 Preparing NPT and NVT files

NPT refers to constant number of particles, simulation pressure, and simulation temperature

4.1 Step 7 & 8 MDP files

In both `step7_boxsize.mdp` and `step8_nvt.mdp`, change `ref_t` to the same temperature you used in system generation (for both times the temperature is listed).

4.2 make index files and grompp

Again, in the command line of the remote machine

in the `/blah/POPC/` folder

```
~$ sbatch makeindex.batch
```

This does two (quick) things: it makes a new index file for the systems, which are called `MEMB` and `SOL_ION`. I did this because I don't want to go through all of the `.mdp` files that I copy between systems and change all the instances of, say `DMPC` to `POPC` (i.e. the last lipid I simulated to the next one I'm about to simulate).

After that it '`grompp`'s the simulation stuff for the next step, so step 7 is ready to launch.

5 Run the NPT Simulation

At this point, you're ready to run the NPT ('boxsize') simulation. Literally all you need to do is:

(from the terminal on the remote machine, of course)

```
~$ sbatch boxsize.batch
```

6 Get the box sizes

again again, from the remote machine, run:

```
~$ sbatch get-boxsize-arr.batch
```

This outputs a file `box.xvg` (human readable, it's basically a `.csv` file) in each of the run folders. The only thing in it will be the box size of the system at every frame, from the `step7_boxsize` simulation.

7 Find best starting frame

remote machine command line

```
~$ interact
```

(wait ∼1 minute)

```
~$ python3 find-best-frame.py
```

`interact` (at least on Bridges2) lets you run commands straight from the command line rather than waiting in the queue. Okay yes technically the `interact` environment has to wait super briefly in the queue, but whatever.

This python script finds the average box size for each replica over the 'boxsize' simulation. Rather than just saving those into a file, it creates a text

file `grompp.txt` which includes all of the `grompp` commands for the replicas for the NVT simulations, starting from the 'best' frame in the NPT simulations.

8 NVT Simulation

8.1 grompp

```
~$ sbatch step8-grompp.batch
```

The setup of this `batch` file was a little complicated for me. I'm *mostly* certain it will work... Famous last words.

8.2 launch

```
~$ sbatch step8-launch.batch
```

I'm also not certain that this is enough nodes. I think it is? 2 nodes gave ~ 160 ns, so 3 nodes ought to be able to do 200 ns. If not, you'll have to compromise between slightly shorter simulations or more nodes.