

Modeling α -helical
pore-forming-protein nanopores
in Martini

Supplemental Information

October 16, 2019

1 Scripts

All the scripts that were used to run, analyze and plot the simulations can be found in:

`/coarse/lorenzo/projects/nanopores/report/scripts/`

Here is a list of those script with the respective function in the pipeline:

- `ELNEDIN_to_domELNEDIN_itp_martinize2.tcl`: based on `domELNEDIN`, modified to work on `martinize2` topologies
- `mdscript.sh`: Prepare the system and run it. Small tweaks were needed to change from `martini 2` to `martini 3`
- `analyze_all.sh`: wraps all the other analysis scripts and creates and navigates subdirectories. Also runs some of the analysis code that did not warrant a separate script.
- `runfluxer.sh`: wrapper that prepares the simulations and then runs `fluxer.py`
- `fluxer_fix.py`: original `fluxer.py`, with a small change to fix a bug
- `plot_flux_water.py`: creates the flux plots shown in this report
- `poreplot.py`: calculates the pore size using `MAnalysis` and `HOLE-traj`, then plots it
- `plot_membrane_height.py`: creates the plots showing the difference in membrane height relative to the protein

Additionally, these scripts were used as part of the preliminary test of mutant generation and computational electrophysiology:

- `makeMutants.sh`: preliminary script that generates a mutant using `stitch.py` by dr. Tsjerk, prepares and runs a simulation
- `run_mutants.py`: new improved take on the previous script implemented in python
- `plot_flux_ions.py`: was used to inspect the results of the computational electrophysiology experiment

2 Simulation files

All the simulation files (raw data, mdps, analysis, plots) can be found in:

```
/coarse/lorenzo/projects/nanopores/wildtypes/frac/refined/
```

Each subdirectory contains one simulation in triplicate, a **AA** and a **CG** directory – used for pre-production. Each **RUN** contains all the files needed for minimization, equilibration and production. **analysis** contains all the products of the analysis scripts.

3 WDV files for MDAnalysis and HOLE

The files for martini 2 and martini 3 can be found in:

```
/coarse/lorenzo/projects/MDAnalysis/
```

References