Water conformation at three-phases contact lines

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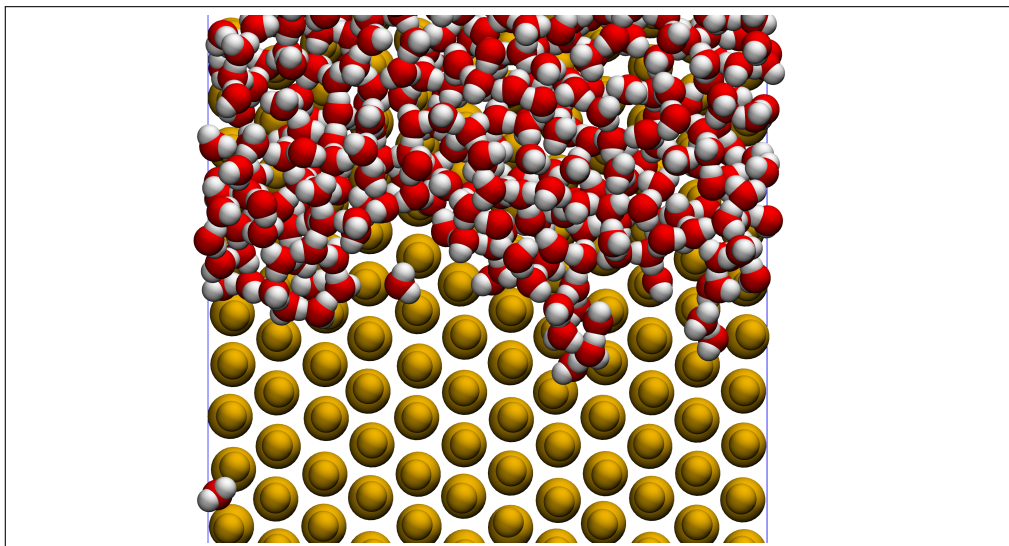

Figure 1: Top-down view of the control volume adopted to study molecular motion in the three-phase contact line region

1 Introduction

This dataset contains detailed trajectories obtained from molecular dynamics simulations performed using GROMACS [1]. The simulated system consists in a quasi-2-dimensional SPC/E water meniscus confined between solid substrates composed by silica quadrupoles. Details on the molecular model and the simulation technique can be found in [2]. The data collected in this dataset are utilized in a ongoing project aimed to demystify the motion of three-phases contact lines over hydrophilic surfaces.
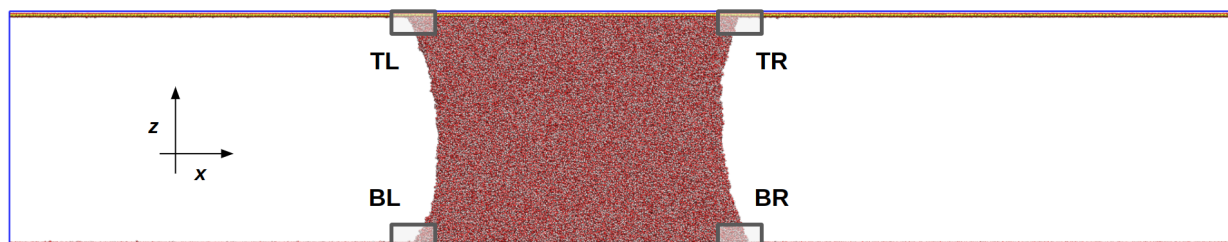

Figure 2: Location of the three control volumes used to extract molecular coordinates close to the three-phase contact lines.

The speed of a fluid-vapour interface moving on a flat solid surface can be related to the dynamic contact angle between the interface and the solid via a *contact line friction* model. This relation arises from assumptions on the mobility of liquid molecules in the contact line region ([3]). Recent molecular simulations ([4, 5]) have shown how the case of water moving on hydrophilic surfaces (e.g. silica) constitutes an interesting case to study: friction at advancing contact lines differs from friction at receding contact lines. This phenomenology can be captured by a angle-dependent contact line friction coefficient [6]. In order to validate this model we explore the conformation and the motion of water molecules in the contact line region, by focusing on control volumes spanning only a few nanometers in linear dimensions.

2 Structure of the dataset

Each `.zip` folder in the dataset contains a fully-detailed molecular simulations in `.xtc` format spanning 4ns and are samples every 1ps. The tar balls correspond to the frame snapshots of the water in the control volumes or the silica molecules in the solid substrate. The tags for the control volumes correspond to the ones in figure 2. The folder labels correspond to the equilibrium contact angle and to the wetting speed, in particular:

- 'Q3' $\rightarrow \theta_0 = 69°$
- 'Q4' $\rightarrow \theta_0 = 38°$
- 'Equil' $\rightarrow U_w = 0\text{nm/ns}$
- 'C0100' $\rightarrow U_w \simeq 3.30\text{nm/ns}$
- 'C0020' $\rightarrow U_w \simeq 0.66\text{nm/ns}$

Here is a sketch of the structure of the dataset:

```
📁 Water conformation at three-phases contact lines
    documentation.pdf
    📁 Q3-Equil
        automatic_selection.py
        control-volume.ndx
        droplet.gro
        selection_substrate.py
        selection.txt
        sub-select.ndx
        system.tpr
        trj.xtc
        trj-gro-bl.tar.gz
        trj-gro-br.tar.gz
        trj-gro-tl.tar.gz
        trj-gro-tr.tar.gz
        sub-bot.tar.gz
        sub-top.tar.gz
    📁 Q3-C0100
        ...
    📁 Q4-Equil
        ...
    📁 Q4-C0020
        ...
```

3 Obtaining molecular coordinates in a control volume

In this section we briefly explain how to select atoms in a given control volume using GROMACS. The procedure is divided in two steps: a selection step and a dumping step. Remind yourself that one can obtain brief instructions on how to run a given command by running: `gmx help <command-name>`.

1. **Selection**: given the fully-detailed trajectory it is possible to produce an *index file* enumerating the atoms within a given control volume for each time frame using the command `gmx select`. The syntax for atomic selections can be found in [7]. Here is one example of selection that can be parsed:

   ```
   same residue as resname SOL and x < 30 and x > 20 and z < 10
   ```

   which translates as "selects all atoms having residue name 'SOL', coordinate $x \in (20\text{nm}, 30\text{nm})$ and coordinate $z \in (0\text{nm}, 10\text{nm})$". It is recommended to write the selection to a text file and concatenate it to `gmx select`, in order to reduce the risk of typos:

   ```
   cat selection.txt | gmx select -f trj.xtc -s system.tpr -on control-volume.ndx
   ```

   this produces a index (`.ndx`) ready to be used to extract snapshots of the atomic coordinates.

2. **Dumping**: once the atoms in the control volume have been located, their coordinates need to be saved for further more advanced analysis. The command `gmx trjconv` allows to dump frames from a trajectory, given a index file. In order to dump the coordinates at frame `nframe` in a configuration file (`.gro`) one may run the following line:

   ```
   echo <nframe> | gmx trjconv -dump <nframe> -b <nframe-1> -f trj.xtc -s system.tpr
   ↳ -n control-volume.ndx -o cv<nframe>.gro
   ```

   the option `-b <nframe-1>` tells `gmx trjconv` to start reading the trajectory from frame `nframe-1`, thus saving time that would be spent reading useless frames. Running the above command outputs a *single* snapshot; if one is interested in studying the control volume over several frames, the commend must be executed for several values of `nframe`. We strongly advise against doing it manually: please have a look at the scripts named `automatic_selection.py` that can be found in each subfolder.

The selection procedure work both for water molecules ('SOL') and silica molecules ('SUB'); however, since the number of substrate molecules is far more contained compare to the one of liquid molecules, one may avoid creating a selection for a control volume and select all the sub state molecules in the box. Output configuration frames can be easily visualized using VMD [8].

Versioning

The version of this database `x.y.z` is updated as follow:

- `x`: +1 when a new batch of flow maps is added

- `y`: +1 when the example configurations or the reading script are updated

- `z`: +1 when the documentation is updated

Acknowledgments

References

[1] M. J. Abraham, T. Murtola, R. Schulz, S. Páll, J. C. Smith, B. Hess, and E. Lindahl, *GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers*, SoftwareX vol. 1-2, 19–25 (2015)

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[3] T. D. Blake and J. M. Haynes, *Kinetics of liquid-liquid displacement*, Journal of Colloid and Interface Science, vol. 30, 421–3 (1969)

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[5] M. Pellegrino and B. Hess, *Molecular Dynamics simulations of spreading droplets* [Data set v1.0.1]. Zenodo. `https://doi.org/10.5281/zenodo.6445485` (2022)

[6] P. Johansson and B. Hess, *Molecular origin of contact line friction in dynamic wetting*, Physical Review Fluids, 3, 074201 (2018)

[7] Gromacs documentation on selection syntax:
https://manual.gromacs.org/documentation/5.1/onlinehelp/selections.html

[8] Visual Molecular Dynamics: https://www.ks.uiuc.edu/Research/vmd/