Transient Time Correlation Function

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Overview

What I am going to talk about:

- Structure of the simulations;
- Some results from a simple case study;
- Transient Time Correlation Function method;
- Next steps.

Simulation method

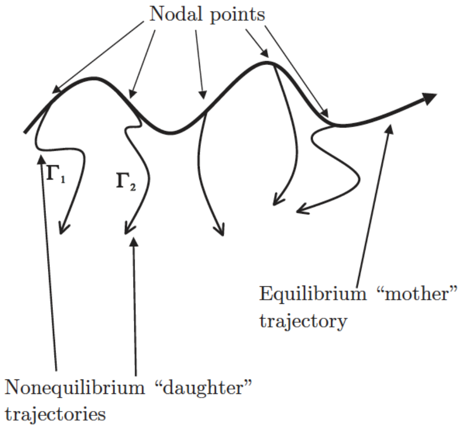


Figure: Schematic diagram of the simulation algorithm[1]

[1] Todd and Daivis, *Nonequilibrium molecular dynamics: theory, algorithms and applications*

Simulation method

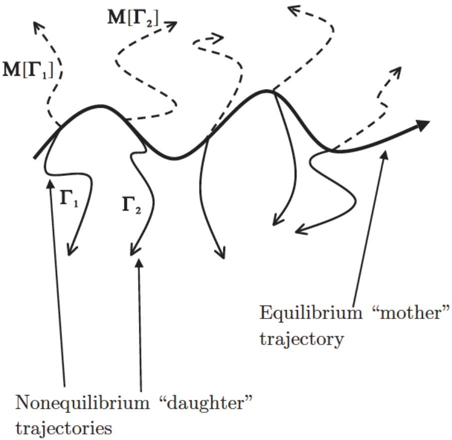


Figure: Schematic diagram of the simulation algorithm with mappings[2]

[2] Todd and Daivis, *Nonequilibrium molecular dynamics: theory, algorithms and applications*

Mappings

- $(x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi}) \longrightarrow (x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi})$
- $(x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi}) \longrightarrow (x_i, y_i, z_i, -p_{xi}, -p_{yi}, -p_{zi})$
- $(x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi}) \longrightarrow (-x_i, y_i, z_i, -p_{xi}, p_{yi}, p_{zi})$
- $(x_i, y_i, z_i, p_{xi}, p_{yi}, p_{zi}) \longrightarrow (-x_i, y_i, z_i, p_{xi}, -p_{yi}, -p_{zi})$

System

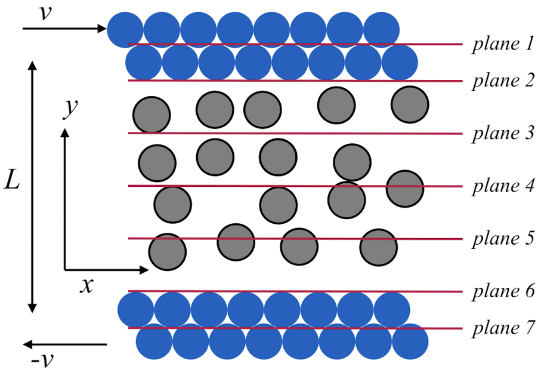


Figure: Schematic of the system[3]

[3] Maffioli et al., "Slip and stress from low shear rate nonequilibrium molecular dynamics: The transient-time correlation function technique"

System

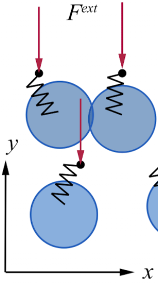


Figure: Schematic of the model for the wall atoms[4]

[4] Maffioli et al., "Slip and stress from low shear rate nonequilibrium molecular dynamics: The transient-time correlation function technique"

Results: shear pressure

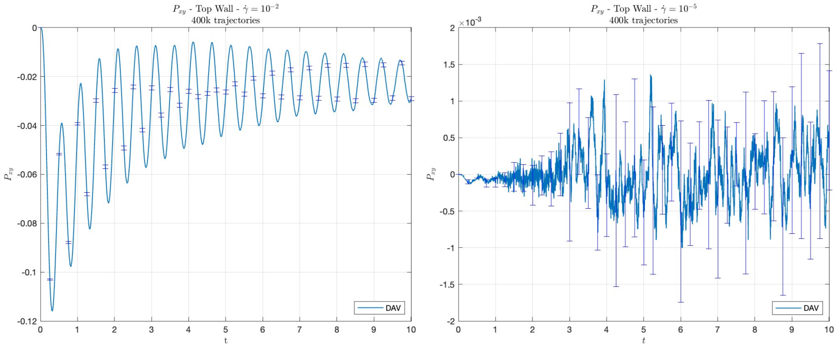
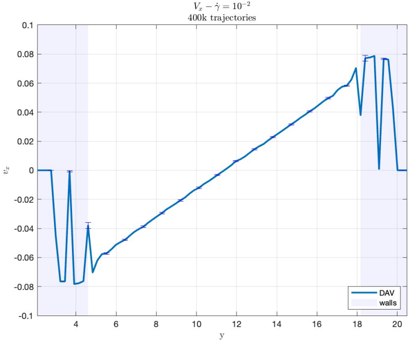
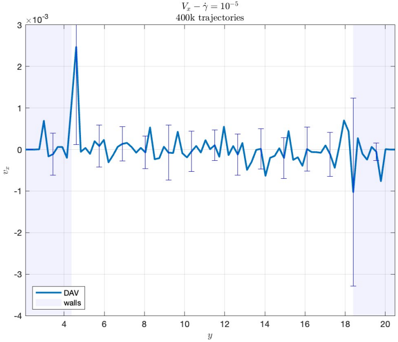


Figure: The shear pressure is computed at the interface between the wall and the fluid using the Method of Planes.

Results: velocity profile





Transient Time Correlation Function

For a generic phase variable B, the TTCF states the following

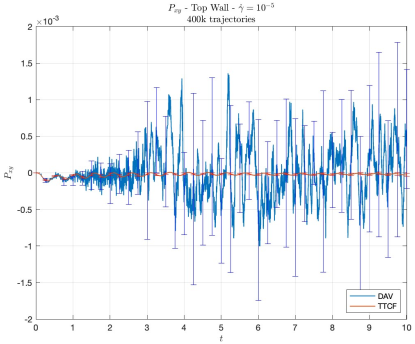
$$\langle B(t)\rangle = \langle B(0)\rangle + \int_0^t \langle \Omega(0)B(s)\rangle ds,$$

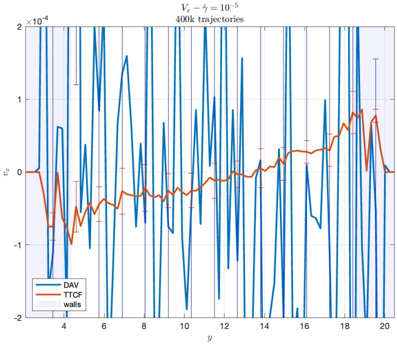
where $\Omega(0)$ is the dissipation function at $t = 0$ and for the considered system it is such that:

$$\Omega := -\beta \dot{U} = -\beta \sum_i^{Nl} k(r_{xi}^w - r_{xi}^l)v,$$

where v is the velocity of the walls, k is the harmonic constant for the springs and $r_{xi}^w - r_{xi}^l$ is the displacement between each wall atom and its lattice cite, along x direction.

Results: TTCF





Results: TTCF with different dissipation function

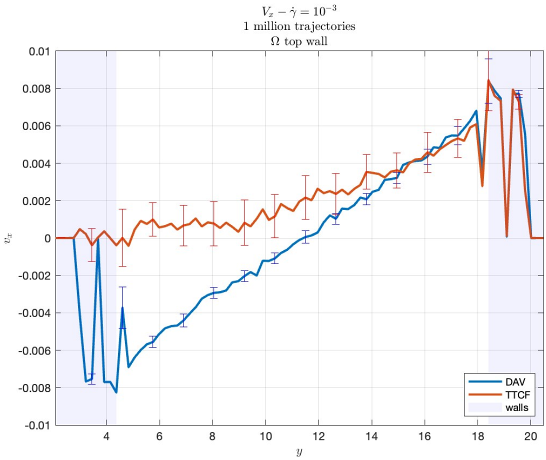


Figure: TTCF computed using Ω relative only to the top wall.

Results: TTCF with different dissipation function

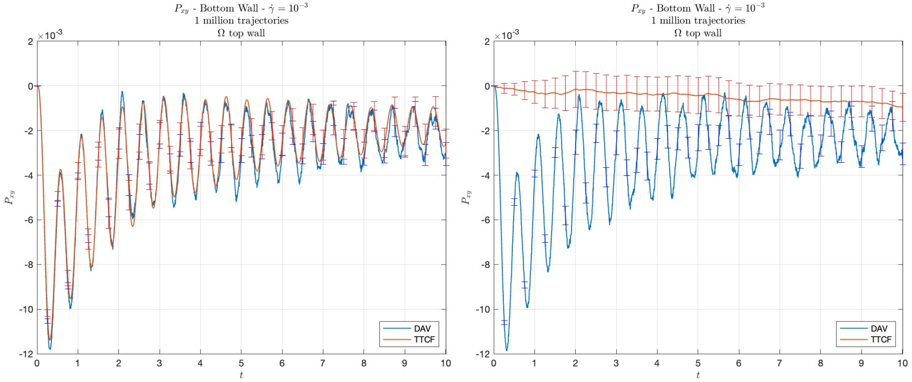
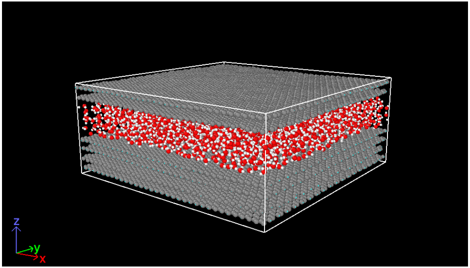


Figure: TTCF computed using Ω relative only to the top wall.

What's next?

The next step is to exploit the Transient Time Correlation Function to compute quantities of interest, such as the slip velocity or the slip length, for a system of water and graphene.



Bibliography

Todd, Billy D and Peter J Daivis. *Nonequilibrium molecular dynamics: theory, algorithms and applications*. Cambridge University Press, 2017.

Maffioli, Luca et al. “Slip and stress from low shear rate nonequilibrium molecular dynamics: The transient-time correlation function technique”. In: *The Journal of Chemical Physics* 156.18 (2022), p. 184111.

Slip Length

The slip length can be easily derived from $v_t = b\frac{\partial v}{\partial z}$