Hydrodynamic Transport Coefficients in Graphene Nanochannels

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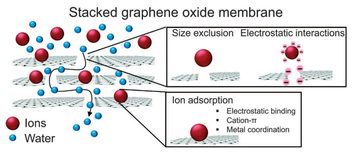
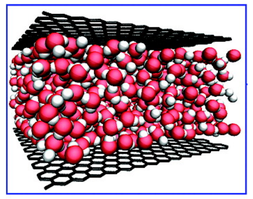
Graphene Nanochannels

1. Graphene possesses a high slip length due to dense network of covalent bonds, smooth surface, and weak interaction with liquid in confinement.





2. If understood, can be used to manufacture efficient microfluidic devices for nanofiltration. One particular important application is water desalination.

Boundary Conditions

1. The general boundary condition states that slip length is dependent on both slip velocity and strain rate in the direction of flow.

2. Slip velocity and strain rate are easily extrapolated from nonequilibrium simulation.

$$u_s = L_s \frac{u_x}{y}\bigg|_{y=y_w}$$

1. Alternative boundary condition connects viscosity of liquid and interfacial friction coefficient between wall and liquid.

2. Physical properties can be calculated from a variety of methods such as Green-Kubo relation.

$$L_s = \frac{\eta}{\lambda}$$

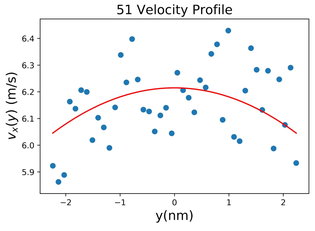
Nonequilibrium Simulation

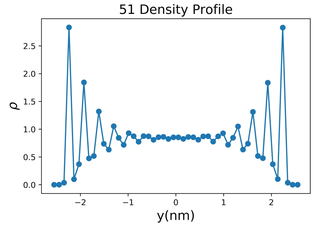
1. Liquid-liquid and liquid-carbon interactions were modeled by LJ potential. Graphene was modeled by 2nd generation REBO potential.

2. Langevin thermostat at 120k is applied to the graphene,

3. The center of mass of each wall or the center of mass of each carbon atoms is fixed to a spring where the equilibrium distance is starting position. Two layers of graphene were put on each boundary.

4. Liquid Particles are driven to resemble a Poiseuille flow.





Friction Coefficients

Hansen Method

1. Consider a slab of liquid near the wall.

$$\tilde{C}_{uF}(s) = -\tilde{\gamma}(s)\tilde{C}_{uu}(s) = \frac{-B}{s+D}\tilde{C}_{uu}(s)$$

$$\gamma(t) = Be^{-Dt} \quad \lambda = \frac{B}{DA}$$

2. Exponentially decaying friction kernel I is Inadequate.
   - No Galilean-invariance

$$\int_{-\infty}^{\infty}\gamma(t) = \int_0^{\infty} Be^{-Dt}dt = \frac{1}{D}$$

   - Response of liquid is instantaneous

$$\tilde{\gamma}(s\to\infty) = \lim_{s\to\infty}\int_0^{\infty} Be^{-(D+s)t}dt = 0$$

BB Method

1. A Green-Kubo relation. Consider all interactions between liquid and wall.

$$\lambda = \frac{1}{Ak_BT}\int_0^{\infty}\langle F_{wl}(t)F_{wl}(0)\rangle_0\, dt$$

2. Rigorous and physical assumption of the memory kernel.
   - Galilean-invariance

$$\tilde{\gamma}(s=0) = \int_{-\infty}^{\infty}\gamma(t)dt = 0$$

   - Response of liquid is not instantaneous

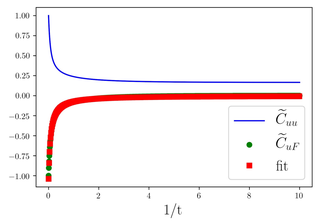
$$\tilde{\gamma}(s\to\infty) = 1$$

Equilibrium Simulation

Hansen Method

1. Cross correlation function is very noisy and requires extensive data.

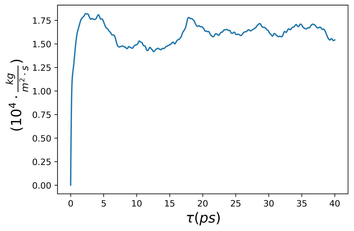
2. Parameters fitting in Laplace space requires a lot of effort at the lower end.



BB Method

1. Integrate correlation function is less noisy but convergence is difficult.

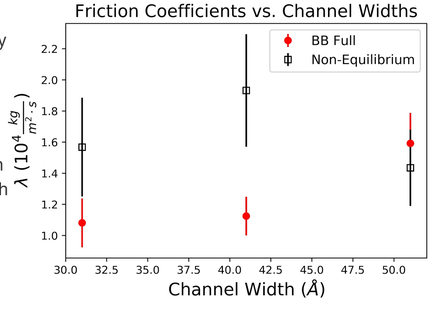
2. Simple and unambiguous computation.



Dependence on Aspect Ratios

1. Nonequilibrium results have high variance because bulk liquid gradually disappears as the channel width shrinks, obstructing the fitting of velocity profile.

2. Both EMD and NEMD suggest friction coefficient is relatively unchanged with respect to change in channel width.



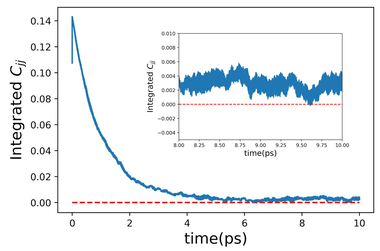
Heat Transfer Coefficient

Equilibrium Simulation

1. Heat current from liquid through wall is related to heat transfer coefficient via a Green-Kubo relation.

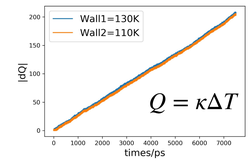
$$\kappa = \frac{1}{3Vk_BT^2}\int_0^{\infty}\langle J(0)\cdot J(t)\rangle_0\, dt$$

2. Extending damping time allows a slowly-decaying correlation to be observed.

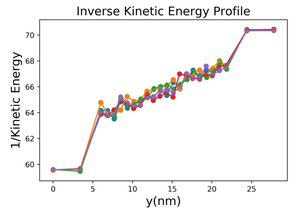


Nonequilibrium Simulation

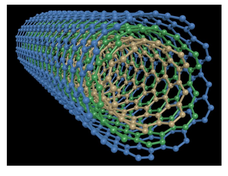
1. A temperature gradient is imposed on two sides.



2. Appropriate temperature gradient in linear response regime requires trials and errors. Can be checked by an inverse temperature profile plot.



Conclusion and Outlooks



1. Theories and practical implementations of two well-known methods to calculated friction coefficients in equilibrium was discussed. Reasons for the discrepancies and agreement with direct NEMD were proposed. Different geometries such as tubes should be studied as well.

2. Heat transfer coefficient between LJ particle and graphene studied via a Green-Kubo relation. The connection between fiction and heat transfer should be studied as a cross correlation should be studied theoretically and computationally.

$$\begin{bmatrix} \lambda & \int_0^{\infty}\langle F_{wl}(t)J(0)\rangle\, dt \\ \int_0^{\infty}\langle F_{wl}(0)J(t)\rangle\, dt & \kappa \end{bmatrix}$$

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