Nanoscale hydrodynamics near solids

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June 2019

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Agenda

1. Introduction
2. Nanoscalehydrodynamics theory for liquids near solids
3. Nanoscale hydrodynamics for planar geometries
4. Nanoscale hydrodynamics for unconfined fluids
5. NonMarkovian behaviour
6. Conclusions and future directions
7. Relevant references

Introduction

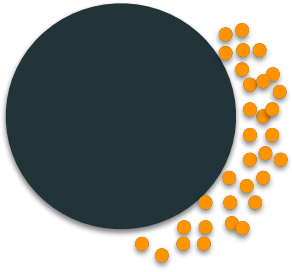
Roadmap

BEHAVIOUR
OF A FLUID IN CONTACT
WITH A SOLID IN THE
NANOSCALE

KAWASAKI-GUNTON
PROJECTION OPERATOR

+

MARKOVIAN
APPROXIMATION



$$\partial_t \rho(\mathbf{r}) = -\boldsymbol{\nabla}\cdot\mathbf{g}(\mathbf{r})$$

$$\partial_t \mathbf{g}(\mathbf{r}) = -\boldsymbol{\nabla}\cdot(\mathbf{g}(\mathbf{r})\mathbf{v}(\mathbf{r})) - \rho(\mathbf{r})\boldsymbol{\nabla}\frac{\delta\mathcal{F}}{\delta\rho(\mathbf{r})}[\rho,\mathbf{R}] + \boldsymbol{\nabla}\cdot\boldsymbol{\Sigma}(\mathbf{r}) + \boldsymbol{\mathcal{S}}(\mathbf{r})$$

$$\dot{\mathbf{R}} = \frac{\mathbf{P}}{M}$$

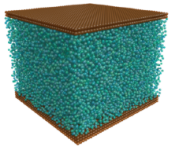
$$\dot{\mathbf{P}} = -\frac{\partial\mathcal{F}}{\partial\mathbf{R}} - \int d\mathbf{r}\boldsymbol{\mathcal{S}}(\mathbf{r})$$

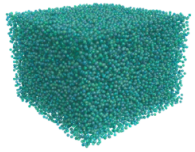
MORI THEORY

$$C(t) = \exp\{-\Lambda^* t\}\cdot C(0)$$

MD SIMULATIONS

SLIP BOUNDARY
CONDITION





Roadmap

1. The study of the behaviour of a fluid in contact with a solid in the nanoscale.
2. Theory of Coarse-Graining in order to obtain the equations of motion of a fluid in contact with a huge solid sphere.
3. To address the plateau problem.
4. MD simulations.
5. Mori theory

Derivation of the slip boundary condition from NESM

- Through the measurement of the correlation of the transverse momentum and comparison with the predictions of continuum (local) hydrodynamics [**Bocquet1993**, **Chen2015**].
- Through linear response theory relating the force on the walls with the velocity of the fluid [**Bocquet1993**, **Petravic2007**].
- By formulating linear, in general non-Markovian, conections between friction forces and velocities [**Hansen2011**], where the meaning of this quantities is often understood implicitly.

The Theory of Coarse-Graining

CG variables

The entropy

The dynamics

The Kawasaki-Gunton projection operator

Mori's Generalized Langevin equation

Nanoscalehydrodynamics theory for liquids near solids

Overview

The system and the CG variables

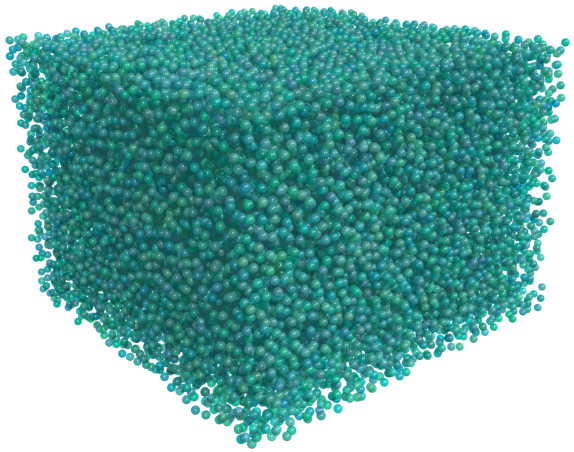
Nanoscale hydrodynamics for planar geometries

Simpler theory

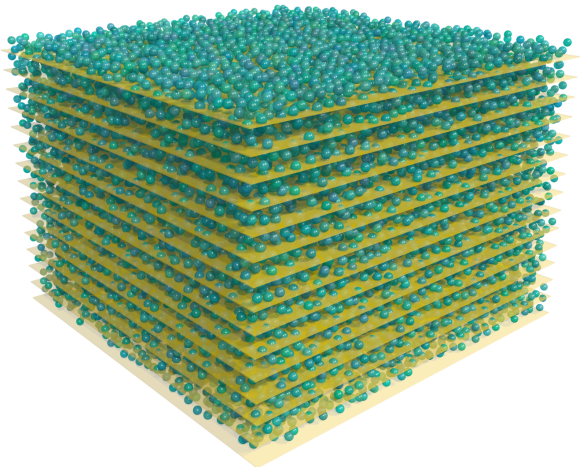
Simple theory

Nanoscale hydrodynamics for unconfined fluids

The system



The system

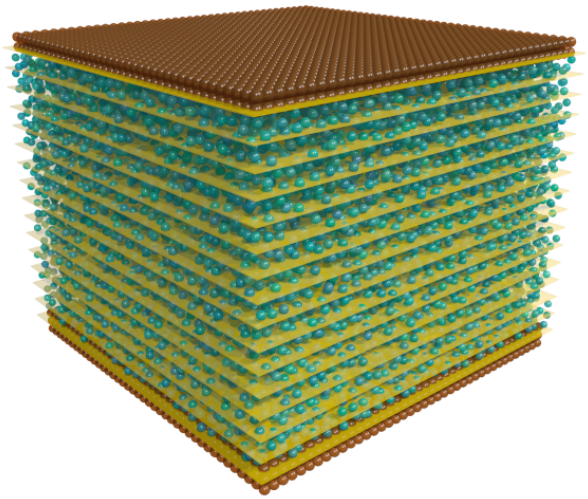


NonMarkovian behaviour

Nonmarkovian

Texto

The system



Conclusions and future directions

Conclusions

Future directions

Relevant references

References

Muchas gracias