

Nanoscale hydrodynamics in periodic and confined planar geometries

Diego Duque-Zumajo, J. A. de la Torre, and Pep Español
Universidad Nacional de Educación a Distancia, Madrid, Spain

The behavior of a fluid at large scales is governed by the well-known Navier-Stokes equations of hydrodynamics. At the nanoscale these equations are no longer appropriate because the fluid starts to behave in a non-local way in both space and time, leading to Generalized Hydrodynamics [1, 2, 3, 4]. Correlation functions of hydrodynamic variables are defined in reciprocal space and measured in molecular dynamics (MD) simulations, thus providing a wealth of information about the behavior of fluids at small scales [5, 6, 7].

In this work, we address the problem of hydrodynamics at small scales of a fluid in periodic and confined planar geometries. While Generalized Hydrodynamics usually assumes rotational and translational invariance, in confined systems these symmetries are lost. For this reason, we work in real space and define the hydrodynamic variables in terms of slabs [8, 9]. We choose as relevant variable the transverse momentum after checking through MD simulations that the coupling between this component and the rest of hydrodynamic variables (density, rest of momentum components and energy) is negligible.

Mori projector technique is used to construct an exact linear equation for the correlation function of the transverse momentum, which contains a memory kernel. A clear separation of time scales is invoked in such a way that an approximate Markovian differential equation is obtained. The distinctive feature of the Markovian approximation in Mori

theory is to predict a (matrix) exponential decay of the correlation. We show that this prediction is satisfied in our simulations *after* a time of molecular size has elapsed. We also show that after this time, a local approximation seems to be sufficient for describing the decay of the momentum correlation.

This methodology is followed in both unconfined and confined fluids, allowing us to discuss the effects of solid walls on the fluid.

-
- [1] R. D. Mountain, *Adv. Mol. Relax. Process.* **9**, 225 (1975).
 - [2] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (McGraw-Hill, New York, 1980).
 - [3] J. P. Hansen and I. McDonald, *Theory of Simple Liquids* (Academic Press, London, 1986).
 - [4] W. E. Alley and B. J. Alder, *Phys. Rev. A* **27**, 3158 (1982).
 - [5] C. H. Chung and S. Yip, *Phys. Rev.* **182**, 323 (1969).
 - [6] I. de Schepper, E. Cohen, C. Bruin, J. van Rijs, W. Montfrooij, and L. de Graaf, *Phys. Rev. A* **38**, 271 (1988).
 - [7] R. E. Khayat and B. C. Eu, *Phys. Rev. A* **39**, 728 (1989).
 - [8] P. Español and I. Zuñiga, *J. Chem. Phys.* **131**, 164106 (2009).
 - [9] J. A. de la Torre and P. Español, *J. Chem. Phys.* **135**, 114103 (2011).