

Thermal hydrodynamic transport between fluids and solids

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The equations of hydrodynamics are based on conservation principles and relatively simple constitutive equations. From a mathematical point of view the equations require boundary conditions in order to obtain a unique solution. These boundary conditions are formulated phenomenologically. It is possible to give a microscopic foundation to the hydrodynamic equations either from kinetic theory or from non-equilibrium statistical mechanics through the use of projection operators [1]. The latter approach is well-known since the sixties of last century. Only recently a microscopic basis for the boundary conditions themselves has been addressed, since the pioneering work of Bocquet and Barrat [2, 3]. Boundary conditions are an idealized way to deal with the interaction of the fluid with solid objects (or other fluids) surrounding the fluid of interest. Microscopically, the forces that the solid exerts on the fluid are confined to a thin region of molecular size. With recent interest in nanoscale and microscale devices, it is important to understand in more fine detail the interaction between solid walls and the fluid. At these nanoscales, the local fluid structure and molecular correlations become important issues that are usually disregarded in usual derivations of the hydrodynamics from microscopic first principles.

In this work, we present a first principles theory for thermal hydrodynamic transport that takes into account the microscopic interactions between fluid and solid. The fluid is described with the local conserved quantities of mass and energy density fields while the solid is described with the total energy. The interactions of the fluid with the solid appear directly in the equations of hydrodynamics governing the fluid variables, as “external forces” of reversible and irreversible nature.

Under a number of approximations (like a quadratic form for the entropy functional, that includes molecular correlations, and an equilibrium evaluation of non-local transport kernels) we can predict the evolution of a sudden increase of the temperature of the crystalline wall in contact with a fluid.

We also perform MD simulations of a system of one solid crystalline slab and a fluid with periodic boundary conditions in the three dimensions, see Figure 1. Once the system is equilibrated at a particular temperature, the slab is suddenly heated. This is modeled by re-sampling the velocities of the atoms of the crystal from a Maxwellian at a high temperature. The microscopic as well as coarse-grained evolution of the system is monitored. In the ongoing work, we aim at comparing the results of the simulation against the predictions of the previously developed theory.

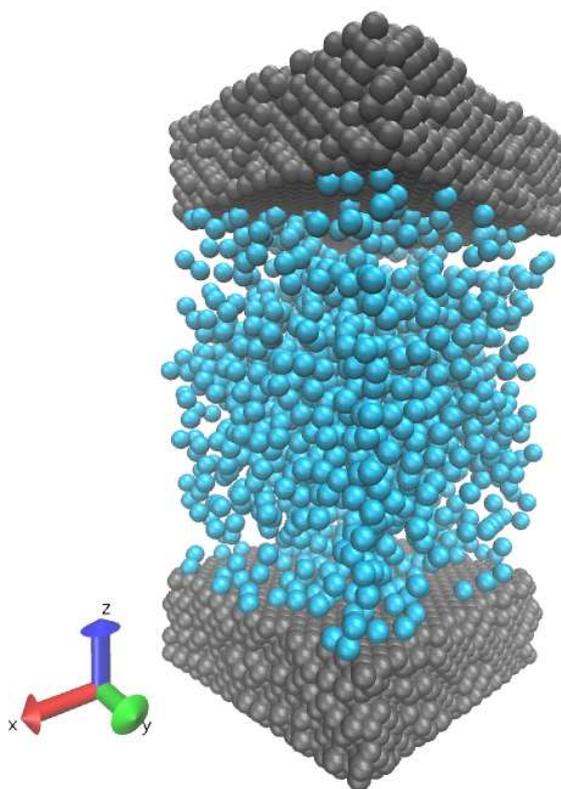


Figure 1: Two solid slabs separated by a fluid with periodic boundary conditions. Because of the periodic boundary conditions the two slabs can be considered as only one.

[2] L. Bocquet and J. Barrat, *Phys. Rev. Lett.* **70**, 2726, (1993).

[3] J. Barrat and F. Chiaruttini, *Molecular Physics*, 37 (2003).

[1] H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Mechanics* (Springer, 1982).