Molecular Dynamics versus Hydrodynamics in a Two-Dimensional Rayleigh-Bénard System

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We compare a microscopic simulation of a fluid made up of 5000 hard disks and maintained at a supercritical Rayleigh number to the corresponding macroscopic hydrodynamics. Very good quantitative agreement is demonstrated.

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Molecular dynamics (MD) provides an alternative "experimental" approach to the study of macroscopic and microscopic properties of simple fluids. Since the early development of MD methods, it has been noted that both equilibrium[1-3] and nonequilibrium[4,5] model systems display a variety of properties which can be understood on the basis of fluid mechanics. The validity of the fluctuating hydrodynamics formalism in far from equilibrium situations has been equally confirmed by simulation techniques.[6]

One of the latest complex problems simulated by the traditional MD methods was the flow past an obstacle[7,8] (previous works are reviewed in Ref. 9). The number of particles (argon atoms) involved was about 150000 and the computation required sophisticated parallel processing.[8] Phenomena like vortex shedding, Von Karman street, etc., have been observed, all in qualitative agreement with macroscopic hydrodynamics predictions. However, no quantitative comparison has yet been reported. Note that "cellular automata" models[10] represent an alternative approach to the handling of complex (high Reynolds number) flows, but again comparison with real experiments remains qualitative at best.

Another step in this direction was the MD simulation of a hydrodynamic instability.[11] By increasing the imposed temperature gradient in a horizontal fluid layer heated from below, the computer experiment shows the passage from the chaotic random behavior of the particles to an organized collective behavior, where convective rolls are observed (Rayleigh-Bénard instability[12]). The fascinating aspect of this simulation lies in the fact that the system was made up of 5000 particles (hard disks) only. Given the small number of particles and the very severe nonequilibrium constraints, it is legitimate to question the nature of the observed phenomenon. Is it still hydrodynamics or some other unknown microscopic effect? How can such a small number of particles ever give rise to a complex macroscopic ordering? A full answer to these questions is far from being simple, as it is likely to involve a reassessment of the basic ideas of nonequilibrium statistical mechanics. In this paper we shall address only a part of the problem, namely the applicability of classical hydrodynamics to such an extreme nonequilibrium situation.

In the original MD simulation of the Rayleigh-Bénard problem,[11] the aspect ratio was set equal to $2\sqrt{2}$. This implies the possibility of having an interplay between two or three convective rolls, which is precisely what has been observed. For the purpose of a precise comparison with a hydrodynamic approach, it is more suitable to choose an aspect ratio so that a unique convective pattern can hopefully settle down. We have therefore reconsidered the MD simulation of an assembly of 5000 hard disks enclosed in a rectangular box of aspect ratio 2 ($L_x = 2L_z$). The vertical sides ($X=0$ and $X=L_x$) are perfectly reflecting, meaning that the lateral boundaries are stress free and insulating in the macroscopic sense. The horizontal sides ($Z=0$ and $Z=L_z$) act only on the normal component of the incident particle velocity: Each time a particle hits a horizontal boundary, it is reinjected into the system, conserving its tangential velocity component V_x and having its normal velocity component V_z sampled from a Maxwellian distribution at the temperatures of the walls. The horizontal boundaries are therefore stress free with fixed temperatures. By an adequate choice of units, the disk diameter, the particle mass, the Boltzmann constant, and the equilibrium average temperature are set equal to unity. The global number density n ($=5000/L_xL_z$) is chosen in such a way that the values for the kinematic viscosity and the thermal diffusivity are as small as possible, which in turn maximizes the Rayleigh number. This gives $n=0.2$ with $L_z=111.8$ ($=L_x/2$). The temperatures of the walls are set equal to $T(Z=0)=1.61$ and $T(Z=L_z)=0.51$. The system is subjected to an external (gravitational) acceleration $\mathbf{g}=-0.011\hat{\mathbf{z}}$ leading to a Rayleigh number equal to 928, which is about 1.2 times the critical Rayleigh number. Note that the nonequilibrium constraints are extremely strong: setting the disk diameter to 3 Å, the average temperature to 300 K, and the mass to that of argon, one finds that the temperature gradient is 10^8 K/cm and the external acceleration field $g=10^{14}$ cm/sec^2.

A Fortran program has been written to integrate the particle positions and velocities in time and was run on an IBM model 4341. For the purpose of measurement,

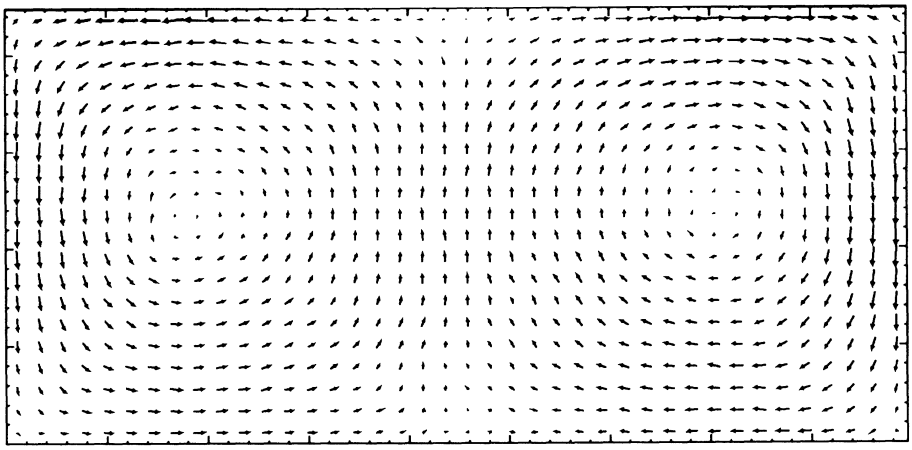

FIG. 1. Final velocity field of the MD simulations. The local velocities are averaged in time over the last 2×10^7 collisions.

the system was divided into 20×40 cells (about six particles per cell on the average) and local instantaneous macroscopic variables were defined as a space average for each cell. A time average was then taken over every 400 collisions per particle (CPP). After a short random period, the system shows strong coherent behavior exhibiting all kinds of convective patterns, switching from a single roll to two convective rolls and vice versa. After about 10000 CPP, the system finally ends up with two rolls which subsequently remain perfectly stable for the next 10000 CPP. The results we present here correspond to an average over the last 8000 CPP. Figure 1 represents the velocity field, Fig. 2 represents the horizontal component of the velocity for a slice located at the center of the first convective roll ($X=L_x/4$), and Fig. 3 represents the horizontal density profile at midheight position ($Z=L_z/2$). The error, estimated from successive statistics over 400 CPP, is of the order of 10% to 15%. Given the small number of particles per cell, this relatively large error had to be expected. Much better statistics is obtained for the vertical density and temperature profiles since for these variables a horizontal space averaging is also performed (around 240 particles per horizontal slice). Here, the estimated error does not exceed 5% (see Figs. 4 and 5).

Having obtained reasonably accurate data from our computer experiment, we next solve the macroscopic hydrodynamic equations. According to the basic assumption of classical hydrodynamics, we shall assume that both the form of the equation of state and the (state dependent) transport coefficients remain valid *locally* (local equilibrium assumption). In other words, we take the well known equilibrium form of the equation of state and of the transport coefficients of a hard-disk Enskog gas,[13] but we replace the density and temperature by their local values. With the boundary conditions defined above, the macroscopic problem is not complete.[14] Note

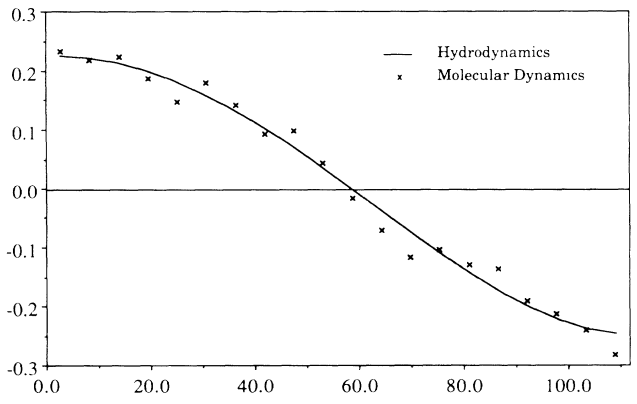

FIG. 2. Horizontal component of the velocity as a function of Z, for a vertical slice located at $X=L_x/4$. The curve refers to the hydrodynamical calculation whereas the crosses represent the MD data averaged over the last 2×10^7 collisions. Both axes are scaled in system units.

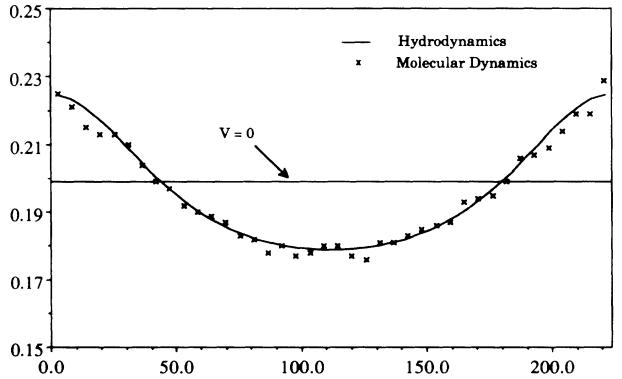

FIG. 3. Number density profile as a function of X, for a horizontal slice located at $Z=L_z/2$. See caption of Fig. 2 for details.

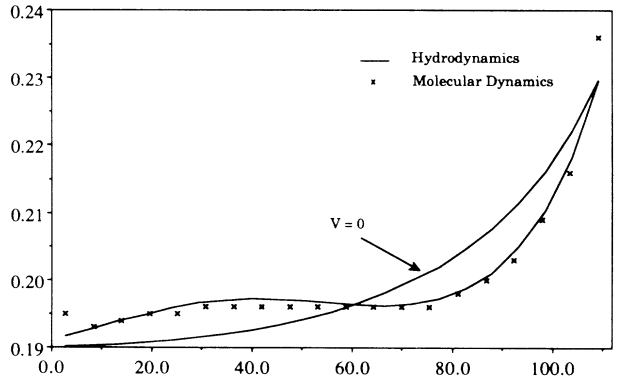

FIG. 4. Number density profile as a function of Z. The curve refers to the hydrodynamic calculation whereas the crosses represent the MD data averaged over the last 2×10^7 collisions. A space averaging over the horizontal shell is also performed. Both axes are scaled in system units. The static nonconvective density profile is also plotted ($V=0$).

that there is no adjustable parameter in the problem.

We first perform a linear stability analysis by assuming, for simplicity, constant transport coefficients throughout the system; this corresponds to a Prandtl number of 0.217 (see Ref. 15 for similar calculations). Figure 6 shows the marginal stability curve, i.e., the critical lower temperature as a function of the horizontal wave number. Since the system is finite, only discrete wave numbers are possible. Hence, for the wall temperatures taken in our computer experiment, either one or two convective rolls are possible. We therefore expect an interplay between both possibilities through natural fluctuations. This scenario is indeed observed in our computer experiment during a transient stage. For a longer period of time, however, only the double-roll pattern is established. In order to clarify this point, we solve numerically the complete hydrodynamic equations.

Besides the fact that the fluid is compressible and that the transport coefficients are state dependent, the main difficulty arises here from the boundary value problem since the small size of the system leads to finite-size effects which are expected to be as important as the dynamics itself. To overcome this difficulty, we used a finite difference scheme on a multigrid network so that the boundary conditions could be fulfilled as best as possible.[16] The system is divided into 22×43 "full-grid" and 21×42 "half-grid" points and an explicit integration scheme is used to follow the state of the system in time. After each time step, an appropriate interpolation scheme is performed in order to complete the state of all the grid points. A more detailed account of the algorithm we have used will be presented elsewhere (a similar algorithm for a one-dimensional system is described in Ref. 17). The code, written in Fortran, was first run on a Mac II. Two of the runs were tested against a system made up of 4 times more grid points which was run on a Cyber. No significant differences were detected so that in what follows we shall report the results obtained in our first grid network.

We have considered several runs with a variety of different initial conditions, including a random distribution of the velocities. The following common scenario has been observed for almost all the runs. After a short transient behavior, the system exhibits a single convective roll which lasts for a long period of time (corresponding to about 2000 CPP in the MD experiment). The center of the roll then starts to move slowly toward one of the vertical walls whereas another convective roll begins to emerge near the opposite wall. Finally, the system evolves very slowly to a symmetrical situation which then remains perfectly stable, even against strong ran-

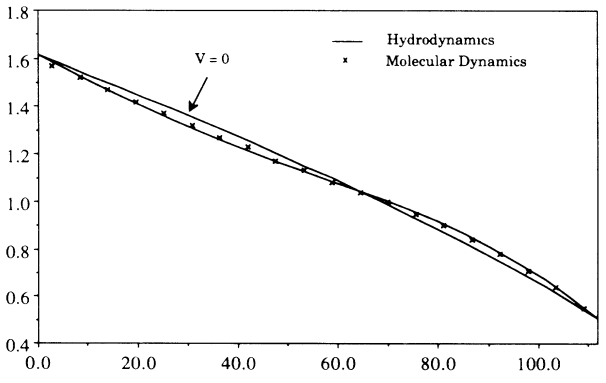

FIG. 5. Temperature profile as a function of Z. See caption of Fig. 3 for details.

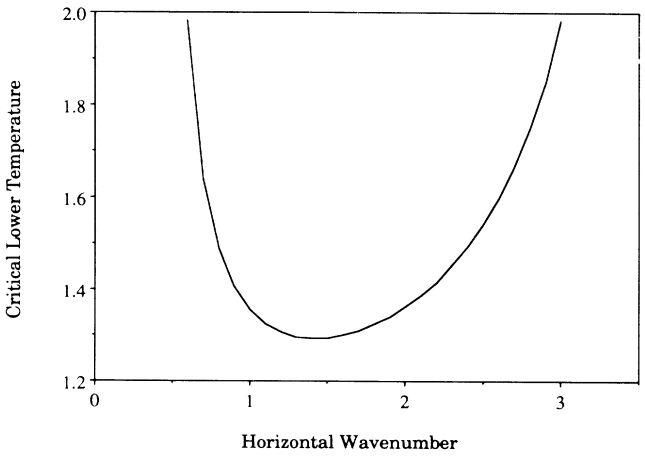

FIG. 6. Marginal stability curve. The vertical axis represents the critical lower temperature and the horizontal axis represents the wave number in the X direction. The values for the shear viscosity, bulk viscosity, and thermal conductivity expressed in system units are 0.340, 0.046, and 1.564, respectively.

dom perturbation of the velocity field. The final pattern resembles very much the one obtained in the MD simulation (see Fig. 1). A quantitative comparison is illustrated in Figs. 2 to 5 which clearly demonstrate a very good agreement.

To conclude, we note that besides their theoretical interest, our results have some potential practical implications. They show that with a few thousands of particles it is already possible to reproduce some of the complex behaviors in normal fluids. Todays supercomputers could easily handle 10^5 particles and very soon they would be able to handle much more. MD will therefore become a precious complementary tool both for the laboratory experiments and for the more traditional fluid dynamics numerical methods. For example, MD allows one to study the exact nature of boundary layers in some extreme situations, which then can be used as an input for the numerical integration of the Navier-Stokes equations. Work along this line has been recently reported in the literature.[18]

Since the completion of this work, Rapaport[19] has reported on similar numerical experiments where a 15000 hard-disk system shows a transition from a six-roll to a four-roll structure. Although the boundary conditions and the aspect ratio are different from ours, this transient behavior is similar to the transition from a one-roll to a two-roll structure described above and such transients can be expected for times smaller than the lateral diffusion time.

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