Molecular-Dynamics Study of Rayleigh-Bénard Convection

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Fully developed convective rolls have been observed in microscopic simulations of a hard-disk fluid driven by opposed temperature and gravitational fields. Under certain conditions a relatively long-lived mode with higher wave number is found to occur instead of the familiar square–cross-section rolls; this mode eventually undergoes a transition to the preferred square-roll state.

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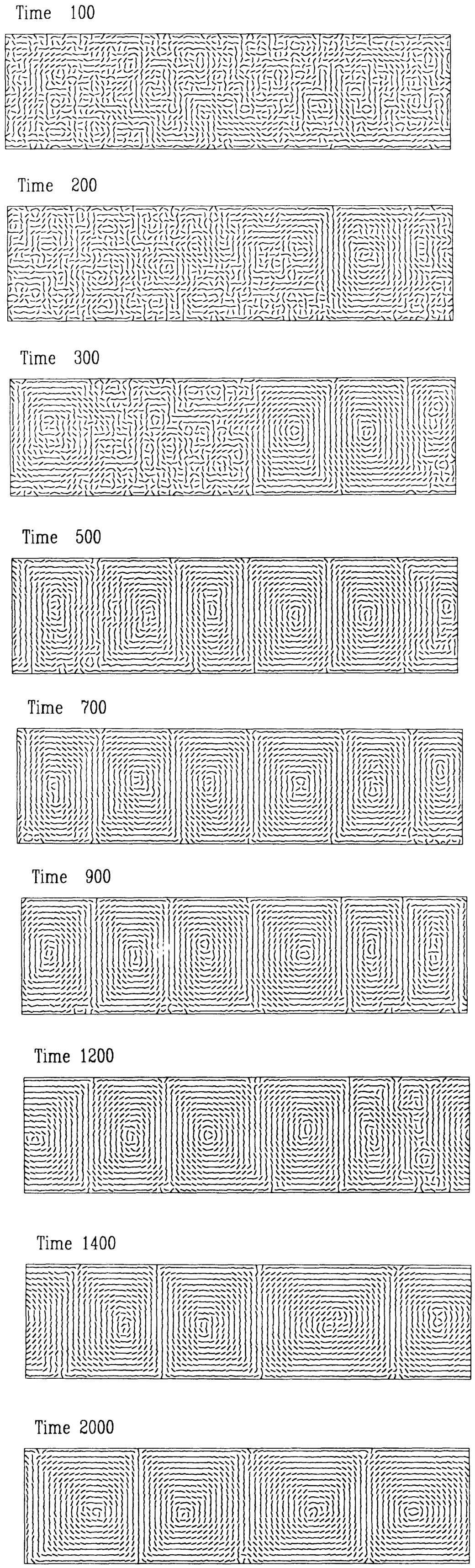
Spontaneous structure formation in dissipative systems—a problem with wide-ranging applications—has been the subject of extensive experimental and theoretical study. One of the most readily realized examples of this phenomenon is to be found in Rayleigh-Bénard convection[1,2]: A well-defined roll structure develops under certain conditions when heat is transported across a horizontal layer of fluid confined between horizontal plates, the lower plate being maintained at a higher temperature than the upper. While considerable progress has been made in an understanding of the experimental observations by means of stability analysis[3] and model calculations[4] that address simplified versions of the hydrodynamic equations governing the system, a full theoretical understanding of the symmetry-breaking and mode-selection mechanisms at work in this comparatively simple dynamical process has yet to be achieved.

Evidence has recently appeared that certain fluid-flow instabilities familiar on macroscopic scales are also observable at the microscopic level by means of molecular-dynamics (MD) simulation: (a) In studies of obstructed flow,[5] vortex shedding and wake instability at low Reynolds number have been observed, even though the diameter of the obstacle is a mere 250 Å. (b) Indications of convective rolls have been found in MD simulation of the Rayleigh-Bénard (RB) problem[6]; the roll patterns were, however, neither fully developed nor long lasting. Yet another example of the relevance of MD to hydrodynamics is a study of moving contact lines in channel flow.[7] Thus, despite the fact that the length and time scales that can be reached by the MD approach are orders of magnitude lower than those encountered experimentally, it appears that direct simulation will allow observation of the microscopic origins of flow instability.

In this Letter, I describe the results of a more extensive study of the RB problem using both a larger system and different imposed conditions. The observed behavior of the system not only resolves the question as to whether stable RB roll patterns can be reproduced in microscopic systems, but also suggests that new phenomena can be observed—in the present case, a convective mode that has not been detected in experiments to date.

The system under discussion is a two-dimensional fluid of 14160 hard elastic disks at a number density (disks divided by area) of 0.4 confined to a rectangular region of aspect ratio $L_x{:}L_y=4{:}1$; if the disk diameter is taken to be 3 Å, then $L_y=280$ Å. The upper and lower boundaries are maintained at constant temperatures T_0 and $T_0+\Delta T$, respectively; here $T_0=1$, while ΔT (>0) varies between runs. Disks colliding with these thermal boundaries are specularly reflected, and the departing velocities are scaled to match the specified boundary temperature; such boundaries, though rigid, are of the stress-free (slip) type. The lateral boundaries of the system are periodic in order to eliminate extraneous side-wall effects; organized large-scale motion will nevertheless be constrained by the value of L_x. A gravitational field acts in the $-y$ direction in opposition to the temperature gradient; the field strength is $g=k_B\Delta T/mL_y$ (in the units used here, both k_B and the particle mass m are unity) so that a disk that travels between hot and cold boundaries experiences a zero net energy change. In the initial state the disks are assigned random velocity directions, while the magnitudes vary gradually between hot and cold extremes; in equilibrium studies such details are actually of little consequence since their effect is rapidly erased, but in these simulations, the nature of the transient behavior and the eventual roll locations do depend on the initial state in an unpredictable manner. The computational techniques used to follow the evolution of the system have been described elsewhere[8]; on an IBM 4381 computer, the computation rate is close to 2×10^6 collisions/h.

A series of runs were carried out over a range of ΔT values, and certain runs were repeated with use of different initial states. For the smallest temperature gradient considered, $\Delta T=2$, no indication of convective flow was observed in a run extending over 90×10^6 disk collisions. At $\Delta T=3$, a convective roll began to appear after 36×10^6 collisions and a set of four square rolls had fully developed after 62×10^6 collisions. Similar behavior was observed for values of ΔT between 4 and 16, with the number of collisions needed for roll formation dropping to approximately 20×10^6. At $\Delta T=17$, however, instead of the system evolving directly into the expected four-roll pattern, a series of narrow rolls started to



emerge, and after 30×10^6 collisions a convection pattern consisting of six evenly spaced rolls appeared to have stabilized; see Fig. 1. This state persisted for a further 13×10^6 collisions, but then a merger of three adjacent rolls occurred; this was accompanied by a broadening of the remaining rolls, the eventual result after a total of 60×10^6 collisions being the appearance of the familiar four-roll pattern, which remained until the run terminated at 86×10^6 collisions.

Figure 1 shows a series of flow patterns at key stages during this particular run; each is a coarse-grained flow image produced by division of the region into an 80×20 grid and the averaging of the velocities of the disks in each grid cell over a period of 100 time units (there are approximately 43×10^3 collisions per unit time for this particular run—the collision rate is a function of temperature and density). Only the flow direction is shown here, but the flow rates are zero at the center of each roll and reach their maximum at the role periphery.

Observation of the comparatively long-lived six-roll state proved to be serendipitous; two further runs under the same conditions, but starting from a different choice of random initial velocity directions, resulted in only partial development of the narrower rolls; once a square roll emerges from the random initial state, the growth of narrow rolls is suppressed. Such irreproducibility is also observed experimentally when the stabilizing influence of lateral boundaries is removed; in cases where a thermal match between fluid and side wall exists, the pattern development is found to lack predictability.[9] In simulations carried out for larger ΔT (between 18 and 26) the four-roll patterns continued to appear but were generally preceded by a transient phase characterized by competing structures involving short-lived narrow rolls extending between hot and cold boundaries. It would appear that in addition to the critical ΔT (i.e., Rayleigh number) for the onset of convection, there exists a threshold ΔT (and hence a Rayleigh number) above which structural competition can be accommodated.

Fourier analysis of the velocity field allows quantification of the periodic features of the flow.[10] The development of the power spectrum of the coarse-grained vertical velocity field, restricted to cells within $\pm L_y/4$ of the midline between hot and cold boundaries, is shown in Fig. 2. From an initial state of zero convective flow, a peak at a wave number corresponding to wavelength $\lambda=L_x/3$ (the six-roll pattern) is seen to develop, and this subsequently shifts to $\lambda=L_x/2$ (four rolls). The sharpness of the peak is an indication of the complete development of the roll pattern at the preferred λ; there is a

FIG. 1. Series of coarse-grained flow plots showing the initial development of convective cells and the subsequent change in cell structure. (Note that the lateral boundaries are periodic.)

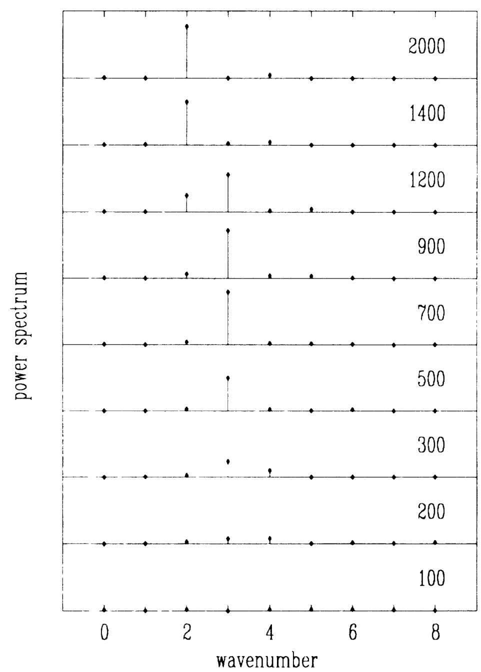


FIG. 2. Power spectra of the vertical component of the coarse-grained flow velocity at times corresponding to the flow plots of Fig. 1. When a single spectral peak predominates, the number of rolls is twice the peak wave number.

strong selection mechanism at work that suppresses the growth of other modes. Harmonic modes have been observed experimentally,[11] although a mode with roll aspect ratio corresponding to the six-roll structure has not been seen (one of the observed harmonics would, in fact, correspond to a twelve-roll pattern). The total exclusion of external noise from the simulated fluid may aid in the production of the sharp structure.

The principal differences between the conditions of the present simulation and that reported earlier[6] are the higher density (0.4 vs 0.2), the increased system size (almost 3 times as many particles), and a region whose aspect ratio is commensurate with the roll shape. Under the conditions of Ref. 6, no rolls appeared when periodic boundaries were used, and when rigid lateral walls were introduced the strongest roll development occurred adjacent to one of the walls. In the present work there are no lateral walls available to promote or otherwise influence the roll development. A run carried out with use of a region with aspect ratio 3:1 ($\Delta T = 15$) produced a pair of elongated rolls that failed to develop completely; the flow pattern refused to stabilize even after 70×10^6 collisions. This indicates that the higher density (and, hence, larger system) is an essential ingredient for the obtaining of complete roll development.

The similarity between the collective modes obtained in the simulations and those observed experimentally suggests that the MD approach should prove useful in the study of the mechanisms responsible for the onset of the instability and for mode selection; this is due to the fact that microscopic correlation functions are open to exploration at the MD level that are inaccessible to experimental probes. On the other hand, there are conspicuous quantitative differences between the simulated and real fluids. Two instances of such differences are as follows: (a) In the MD system, the maximum convective flow speed amounts to approximately $\frac{1}{3}$ of the rms particle velocity, whereas experimentally the ratio is typically 10^{-7}; (b) in experiments on fluids near room temperature, $\Delta T/T_0 \simeq 10^{-2}$, while for the MD fluid this ratio may exceed 20, implying a temperature gradient of 10^{11} K m^{-1} (if we assume that $T_0 \simeq 300$ K, in which case the duration of the run is of the order of 2 nsec). While these extreme conditions still lead to flows that resemble those of real fluids (a similar situation holds for obstructed flow[5]), the estimation of the dimensionless quantities that characterize the state of the system—the Rayleigh and Prandtl numbers—is made difficult by the fact that the transport coefficients on which they are based, the thermal conductivity and viscosity,[12] are strongly dependent on the local conditions and, in two dimensions, the system size as well; in view of the inhomogeneity of the flows that develop, and the variations in temperature and shear rate (two of the quantities on which viscosity depends) across the system, I have not attempted to determine these numbers.

In addition to the possibility of the extension of the present line of exploration with a series of detailed measurements on the freely developing convective structures, it should also be possible to exert some degree of control over the pattern formation by, for example, the introduction of local temperature perturbations into the system. Further study is needed to assess the potential value of the MD approach in the study of the microscopic origins of large-scale fluid instability, but the fact that organized structures involving thousands of particles are capable of developing in the course of the simulations suggests that the prognosis is favorable.

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