Time-dependent patterns in atomistically simulated convection

D. C. Rapaport
Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel
(Received 17 December 1990)

Periodically varying roll patterns have been produced in molecular-dynamics simulation of two-dimensional Rayleigh-Bénard convection using a hard-disk fluid in a square container with nonslip walls. In order to achieve the sufficiently high Rayleigh numbers required for clearly resolved time-dependent behavior the calculations involved systems containing almost 6×10^4 particles, an order of magnitude greater than the number needed to observe stationary convection patterns.

The past few years have witnessed the advent of the *ab initio* approach to computational hydrodynamics: Rather than attempting to describe flow phenomena in terms of conventional continuous fields—that ignore the atomistic nature of matter—the new method approaches the subject from the viewpoint of microscopic molecular dynamics (MD), in which the trajectories of the constituent particles are followed in full detail and the fields deduced by coarse-grained averaging over suitable space and time intervals. Although it is computationally intensive, MD simulation provides the opportunity to examine the collective motion underlying hydrodynamics in unprecedented detail, and avoids the empiricism inherent in the more traditional approach to fluid dynamics. Examples of flow problems which have been studied to date using MD—all in two dimensions—include eddy formation in flow past an obstacle,[1] the appearance of rolls in thermal convection,[2–4] and flow at moving two-fluid interfaces.[5]

In this Brief Report, an observation made in the course of a series of two-dimensional MD simulations of thermal convection in a Rayleigh-Bénard system[6] is described, namely the appearance of time-dependent flow structure. Previous MD studies of this problem[2–4] have described the appearance of transient roll patterns and stable and metastable patterns, as well as a quantitative comparison between the results of MD and the predictions of continuum theory for stationary flow patterns. The results presented here, obtained at higher Rayleigh numbers than previously, which in turn necessitated simulations based on significantly larger systems, show clear evidence of temporal periodicity. Periodic behavior in Rayleigh-Bénard systems is well known, and has been studied experimentally,[7] by theoretical stability analysis,[8] and computationally[9] (within the conventional continuum framework). Furthermore, confidence that the time-dependent MD results are a consequence of realistic hydrodynamic processes is justified by the fact that the actual values of the periods obtained from the MD and continuum calculations are in reasonable agreement.

The actual simulation that is the subject of this Brief Report involves a system of $N=57\,600$ hard-disk particles in a square container—the aspect ratio is $\Gamma=1$—at a mean number density of $\rho=0.4$. In the units used here the disks are of unit diameter; an indication of the microscopic size of the system follows from the fact that if the disk diameter is assigned a characteristic atomic value of 3 Å, then the container edges are of length 1140 Å. A hard-disk system has no intrinsic energy scale, so that if the disk mass and Boltzmann constant are both set to unity, a temperature $T=0.5$ corresponds to unit thermal velocity.

The container is bounded by nonslip walls; while there are various ways of prescribing wall-disk collision rules to achieve a nonslip effect, in this case each wall is divided into segments of length similar to the disk size and the collision rule alternates between specular reflection and velocity reversal for successive segments. The top and bottom thermal walls are maintained at temperatures $T_t=1$ and $T_b=16$, respectively, and the magnitude of the disk velocity following a collision with these walls is altered to correspond to T for that wall (the nonslip condition removes the need to compensate for bulk flow). No heat transfer occurs across the lateral walls, and a collision with either of these walls leaves the velocity magnitude unchanged; there is therefore no tendency for roll nucleation to occur at these walls. A gravitational field, $g=\Delta T/d$, acts to oppose the buoyancy produced by the thermal gradient, where d is the distance between the thermal walls and $\Delta T=T_b-T_t$; this choice of g equates the potential-energy change to the nominal kinetic-energy difference between the thermal walls. Initially the system is at uniform temperature gradient and density.

Macroscopic observables are extracted during the course of the simulation by means of spatial and temporal coarse graining. In this work these quantities include the flow velocity, temperature (adjusted to remove the effects of convective flow), and density fields. Typically a 50×50-cell grid is used for the spatial averaging, while time averaging employs intervals that are shorter than the time scales over which significant changes in the flow patterns occur. Other technical issues involved in carrying out hard-disk MD calculations in an efficient manner have been described elsewhere.[10]

Unlike continuum numerical fluid dynamics, which, in the Boussinesq approximation,[11] employs the Rayleigh number $\mathrm{Ra}=\alpha g d^3\Delta T/\nu\kappa$ and Prandtl number $\mathrm{Pr}=\nu/\kappa$—where α, ν, and κ denote the thermal-expansion coefficient, kinematic viscosity, and thermal diffusivity—as freely adjustable inputs that define the

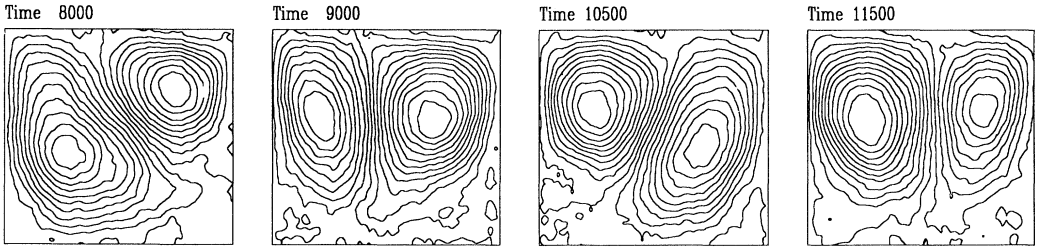

FIG. 1. Sequence of contour plots of the stream function at different stages in a single roll-oscillation cycle.

problem (together with the specification of the container walls), the MD approach is more akin to experiment, where, for given ΔT and d, the values of Ra and Pr are determined by the nature and state of the fluid. Following arguments used in the earlier quantitative comparisons,[4] the values of Ra and Pr applicable here are readily estimated; the calculation uses transport coefficients derived[12] from Enskog theory[13] together with an empirical hard-disk equation of state.[14]

Substituting the Enskog formulas for viscosity and thermal conductivity into the definitions of Ra and Pr leads to functional forms $\mathrm{Ra}=f_1(\bar{\rho})(\Delta T/\bar{T})^2 N/\Gamma$ and $\mathrm{Pr}=f_2(\bar{\rho})$, where f_1 and f_2 are known functions[4]; $\bar{T}$ and $\bar{\rho}$ are "average" values, and are taken to be $(T_b+T_t)/2$ and ρ, respectively. The resulting estimates are $\mathrm{Ra}=7.8\times10^4$ and $\mathrm{Pr}=0.45$; this value of Ra is approximately 20 times larger than in an earlier MD study[3] during which stable rolls developed (in that simulation, $\Gamma=4$, and a combination of slip and periodic boundaries were used). These estimates are subject to considerable uncertainty, not only due to the unreliability of the underlying theory[13] at moderately high ρ, but also as a consequence of such uncontrollable details as the extreme inhomogeneity of the system and the dependence of viscosity on density and shear rate; they nevertheless serve as rough guidelines to the kind of behavior that might be expected on the basis of the corresponding continuum analysis. (For reasons such as these, the utility of the dimensionless numbers of hydrodynamics, e.g., Ra, for classifying the behavior observed in MD simulation has yet to be established.)

A series of contour plots of the stream function showing typical states from the oscillatory phase appear in Fig. 1 (if density variations are ignored—see below—then the contour lines can be regarded as streamlines). Space constraints prevent us from presenting the full history here, which can be summarized thus: two counter-rotating rolls of almost equal size appear in the initial transient phase, eventually they fill the container, and then, throughout the remainder of the run, the boundary between the rolls oscillates in direction about the vertical. The line marking the boundary also undergoes translational oscillation, so that the rolls usually have different areas.

Figure 2 shows the time dependence of the angle between the extrema of the stream function—points lying close to the centers of the two smallest rings in the contour plots (this direction tends to be roughly perpendicular to the inter-roll boundary); the duration of the run covers two full cycles and the graph strongly suggests periodicity. The actual period can be estimated from the graph, and will be discussed below. In Fig. 3 the temperatures measured by four probes inserted into the system at symmetrically placed points a distance $d/3$ from the closer walls are shown; the same periodic behavior is again evident.

The possibility that the observed periodicity is merely a transient phenomenon cannot of course be excluded, and several more cycles of the roll oscillation would help strengthen the case for sustained oscillation. The problem is one of computational resources—the present simulations required some 300 h of IBM 3090E processor time (2×10^9 collisions at a rate of $\approx7\times10^6$ collisions per hour, by far the longest simulations of this kind carried out so far)—and the opportunities for conducting even longer runs, though desirable, are limited. For the same reason, at the time of writing, only a single realization (i.e., initial state) of a system of this size has been studied.

From the expression for Ra given above it is clear that there is an upper limit for a given N, irrespective of ΔT, with the clear implication that achieving larger Ra values requires even greater numbers of particles. The value of ΔT used here is essentially the limit beyond which little variation in behavior was noted during studies of smaller systems. In a system with $N\approx2\times10^4$ and $\Gamma=1$ (since ρ and Γ are unchanged, $\mathrm{Ra}\propto N$) only the barest hint of persistent time dependence could be detected, and prior to the present study it seemed reasonable to associate this

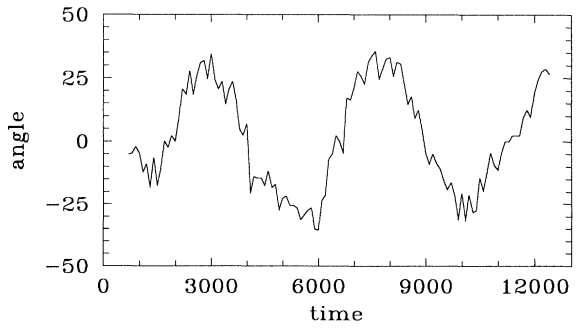

FIG. 2. The angle (in degrees) between the two extrema of the stream function (which occur at points close to the roll centers) as a function of time (MD units).

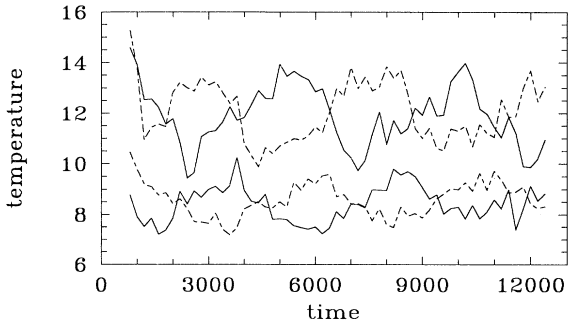

FIG. 3. Time dependence of the temperature (MD units) as measured by four probes (positioned as described in the text).

with random noise. In runs with even lower N (e.g., 10^4, with $\Gamma=1$), different initial states (the random initial velocities of the disks) led to distinct stationary single- or two-roll final states. Needless to say, further work on these systems is in progress (including a run with 10^5 disks that shows preliminary evidence of even more pronounced oscillatory behavior).

Additional information emerges from examination of the detailed temperature, velocity, and density distributions. For example, a large fraction of the overall temperature variation occurs in regions close to the thermal walls: Over a distance $0.06d$ from the bottom wall the horizontally averaged temperature drops to $T_b/2$, whereas over a similar distance from the top wall it grows to $2T_t$. The maximum convective flow velocity is measured to be $\approx 80\%$ of the thermal velocity corresponding to the cold-wall temperature (T_t). Density plots show the degree of compressibility of the system; there is a smooth $\approx \pm 5\%$ variation in density over most of the container when averaged across horizontal slices of thickness $0.02d$, but an abrupt density increase of $\approx 50\%$ occurs in a region of approximate width $0.04d$ abutting the cold wall.

As indicated earlier, periodic behavior is familiar from both experimental and (continuum) computational studies of Rayleigh-Bénard systems. The most appropriate comparison is with a two-dimensional numerical solution for $\Gamma=1$ carried out over a series of Ra and Pr values.[9] For values of these quantities not too distant from those estimated above for the MD simulation (viz., $\mathrm{Ra}=10^5$, $\mathrm{Pr}=0.71$), a strongly oscillating pair of rolls materialized—the boundary between the rolls actually oscillated around the horizontal rather than the vertical direction, but in view of the rich variety of flows exhibited by Rayleigh-Bénard systems in general,[6–8] it is the mere existence of time dependence rather than differences in the details of the flow patterns which should attract attention at this exploratory stage. Given the non-Boussinesq nature of the hard-disk fluid under the conditions of the simulation and the strong variation of the transport coefficients across the system (due to varying ρ, T, and flow shear rate) such deviations are tolerable.

A quantitative comparison between the oscillation periods of the MD and continuum systems can be made if both are expressed in terms of the characteristic thermal-diffusion time $\tau=d^2/\kappa$. The estimated periods are approximately 0.4τ and 0.2τ, respectively, a level of agreement that is reasonable in view of the reservations expressed earlier.

By way of conclusion, while it is impossible to predict what future studies of convection and other hydrodynamic problems based on the *ab initio* molecular-dynamics approach will reveal, the results obtained so far strongly suggest that this is an avenue worth pursuing. Expected improvements in computer performance and cost (in opposite directions) will, in due course, permit a detailed mapping of the parameter space of this rich and fascinating problem.

[1]D. C. Rapaport and E. Clementi, Phys. Rev. Lett. **57**, 695 (1986); E. Meiburg, Phys. Fluids **29**, 1360 (1986); D. C. Rapaport, Phys. Rev. A **36**, 3288 (1987).
[2]M. Mareschal and E. Kestemont, J. Stat. Phys. **48**, 1187 (1987).
[3]D. C. Rapaport, Phys. Rev. Lett. **60**, 2480 (1988).
[4]A. Puhl, M. Malek Mansour, and M. Mareschal, Phys. Rev. A **40**, 1999 (1989).
[5]J. Koplik, J. R. Banavar, and J. F. Willemsen, Phys. Fluids A **1**, 781 (1989).
[6]P. Bergé and M. Dubois, Contemp. Phys. **25**, 535 (1984); V. Croquette, *ibid.* **30**, 113 (1989); **30**, 153 (1989).
[7]J. P. Gollub and S. V. Benson, J. Fluid Mech. **100**, 449 (1980).
[8]E. W. Bolton, F. H. Busse, and R. M. Clever, J. Fluid Mech. **164**, 469 (1986).
[9]I. Goldhirsh, R. B. Pelz, and S. A. Orszag, J. Fluid Mech. **199**, 1 (1989).
[10]D. C. Rapaport, J. Comput. Phys. **34**, 184 (1980).
[11]D. J. Tritton, *Physical Fluid Dynamics,* 2nd ed. (Oxford University Press, Oxford, 1988).
[12]D. M. Gass, J. Chem. Phys. **54**, 1898 (1971).
[13]S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases,* 3rd ed. (Cambridge University Press, Cambridge, 1970).
[14]J. A. Barker and D. E. Henderson, Rev. Mod. Phys. **48**, 587 (1976).