Unpredictable convection in a small box: Molecular-dynamics experiments

D. C. Rapaport

Physics Department, Bar-Ilan University, Ramat-Gan 52900, Israel

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The Rayleigh-Bénard problem has been studied using discrete-particle simulation of a two-dimensional fluid in a square box. The presence of temporal periodicity in the convective roll structure was observed, but, more significantly, different simulation runs under identical conditions but with initial states that differed in ways that are seemingly irrelevant at the macroscopic level exhibited very different forms of pattern evolution. The final state always consisted of a horizontally adjacent pair of rolls, but not all initial states evolved to produce well-established periodic behavior, despite the fact that very long runs were undertaken. Results for both hard- and soft-disk fluids are described; the simulations included systems with over $10^5$ particles.

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I. INTRODUCTION

For over 30 years the technique of molecular dynamics (MD) has been used to study equilibrium and transport properties of matter in its various states, and a vast body of information, unobtainable by other means, has been amassed [1–3]. This has resulted in an improved understanding of the microscopic behavior of liquids in particular, and a clearer appreciation of the general relation between motion and structure on the atomistic scale and experimental observation conducted at the macroscopic level.

In keeping with accepted practice in experimental science, reproducibility is a vital requirement for any MD simulation, and indeed the kinds of applications in which MD has been used to date have not resulted in any properly conducted study failing this test. In particular, the results extracted from any single simulation, assuming inherent fluctuations to be smoothed out by averaging, are free of the effects of the somewhat arbitrarily chosen initial state of the system. This is indeed a prerequisite for invoking the ergodic hypothesis in order to equate trajectory averages with ensemble averages.

The growing awareness of the role of chaos [4] has led to the investigation of a variety of systems—both theoretical and experimental—in which the detailed behavior is unpredictable, in that it is extremely sensitive to the initial (and, where relevant, boundary) conditions imposed on the system. Well-known theoretical instances of this total absence of predictability include the three-mode reduced version of the convection problem [5], in which the effects are observed in the numerical solutions of coupled differential equations, and the one-dimensional logistic map [6]. There are numerous experimental studies in which such behavior is also observed, including mechanical, electrical, chemical, biological, and fluid systems; despite the apparent extreme simplicity of many of the systems, the presence of nonlinearity allows extremely complex behavior to occur [4]. One experimental system that is particularly relevant to the present paper is a study of thermal convection in a container where the stabilizing effects of the lateral walls are eliminated by careful thermal matching, with consequent irreproducibility in the details of the resulting spatial roll patterns [7].

In each of these problems there are regions of parameter space in which the detailed behavior is totally unpredictable. But unlike, for example, the molecular trajectories of a fluid [8], which are not only unpredictable even over relatively short time scales (of the order of just a few mean collision times), but are also irrelevant since a self-averaging process operates to yield reproducible bulk averages that depend only on the macroscopic parameters of the system, in this class of problem it is the “macroscopic” observable(s) themselves that cannot be determined in advance. Turbulence is, of course, the extreme instance of unpredictability (although, fortunately, certain reproducible average quantities exist), but here, unlike some of the other cases cited, there is no illusion of smooth spatial and/or temporal behavior on the length and time scales at which observations are made.

The increasing power of the computer has reached the stage where it is now possible to simulate structured flow phenomena at the atomistic level using the MD approach, including the two-dimensional version of the well-known [9–15] Rayleigh-Bénard convection problem. While the onset of convective roll patterns can be observed without excessive effort—both in terms of the number of particles that constitute the simulated fluid and the time period covered by the simulation—examples of the potential richness of the system only become manifest in simulations carried out on a substantially larger scale, both spatial and temporal. In the only study that has attempted to examine the behavior that does arise given a sufficiently large system [16]—a square container holding 57 600 hard elastic disks—a pair of counter-rotating rolls was observed; the boundary between the rolls was not stationary, however, but oscillated about the vertical in an apparently regular periodic fashion.

The purpose of this paper is to describe, to a large extent at the qualitative and visual levels, the results of
a series of MD simulations of the Rayleigh–Bénard problem aimed at exploring the time-dependent behavior that can appear in large systems. In the course of the work it became apparent that reproducibility (or lack thereof) is also an issue in these simulations, and that the system does not necessarily evolve into a regular oscillating state. Indeed, the entire course of development is determined in some uncontrollable way by the initial state, and both the short-term transients and the long-term behavior show a surprising richness of form. The consequences of these observations have been investigated at some length. Because of the large amount of computation demanded by simulations of this kind, the work addresses only the two-dimensional problem; this is not a totally academic exercise because, while it does not appear possible to construct an experimental realization of such a system (except in the context of the Hele–Shaw cell), the analogous continuum problem can be solved numerically [17] and is found to exhibit both periodic and chaotic behavior.

II. BACKGROUND

A. Thermal convection

The Rayleigh–Bénard problem deals with a horizontal layer of fluid confined between two rigid plates. If the lower plate is only slightly hotter than the upper plate, heat is transported across the layer by conduction, but once the temperature difference (or, more precisely, the Rayleigh number) exceeds some critical value, convection begins to offer a more efficient means of heat transfer, and various kinds of structured flow patterns start to appear. Studies of this phenomenon have concentrated on many different aspects of the problem, including the threshold of convective instability, the structure of the roll patterns (the most familiar being cylindrical rolls and hexagonal cell arrays), subsequent instabilities and time-dependent behavior, and the onset of turbulence. A considerable body of experimental, theoretical, and numerical information has been assembled over the years [9–15].

Analytical and numerical treatment of the problem is based on the standard equations for fluid mass, momentum, and energy conservation, with the added assumption—the Boussinesq approximation [10]—that the only allowed variation in density is a (negative) linear dependence on the temperature change. The standard additional assumptions that the material properties of the fluid, such as viscosity, are constant, leads to a considerably simplified set of equations in which all reference to the fluid properties and the driving forces is absorbed into two dimensionless quantities. These are the Rayleigh and Prandtl numbers, defined as

$$Ra = \frac{\alpha g L_y^3}{\kappa},$$

$$Pr = \frac{\nu}{\kappa},$$

respectively, where \(\nu, \kappa,\) and \(\alpha\) are the kinematic viscosity, thermal diffusivity, and thermal expansion coefficient, \(L_y\) is the layer height, \(g\) the gravitational acceleration, and \(\Delta T\) the temperature difference between the plates. The simplified fluid dynamical equations, supplemented by appropriate boundary conditions, form the basis of most studies of the convection problem. Even these equations remain highly complex, and further simplifying assumptions are sometimes made before embarking on numerical studies [18].

Linear stability analysis [9] can be used to predict the critical value \(Ra_c\) at which convection initially appears (the result turns out to be independent of \(Pr\)). If physically realistic nonslip boundaries are used in the analysis, then for a layer of infinite horizontal extent, \(Ra_c = 1708\). The same analysis predicts the preferred wavelength of the ensuing convective roll pattern—the width of each roll is very close to the layer height and thus the rolls have an almost circular (or square) cross section. For convection to persist the total effect of the buoyancy force arising from the temperature gradient must be adequate to overcome the viscous drag present in the organized flow. The shape of the rolls represents a compromise between wide rolls which would reduce both the diffusive heat transfer between the ascending hot fluid and the descending cold fluid as well as the viscous losses from adjacent oppositely directed flows, and narrow rolls which would reduce shear losses close to the thermal (horizontal) walls.

The effect of the lateral (vertical) wall is to introduce further shear into the system, thereby increasing the value of \(Ra_c\) as well as restricting the wavelength of the roll pattern if the overall flow structure is to be commensurate with the container size. While the effect on \(Ra_c\) is relatively minor provided the aspect ratio \(\Gamma\)—the ratio of the larger horizontal dimension of the container to the height—exceeds 2, below this value \(Ra_c\) grows rapidly, and for \(\Gamma = 1\) is in the vicinity of 5000 [11, 14].

Depending on the value of \(Pr\), a quantity dependent only on the material properties of the fluid, the initial roll-formation instability is followed by a variety of other kinds of instability that can lead to highly intricate flow patterns. The initial roll formation is primarily a two-dimensional effect, but subsequent bifurcations involve flow patterns that are inherently three dimensional, and even time dependent. Once the flow pattern is nonstationary a whole gamut of possible kinds of behavior can be observed [12, 15, 19]; one particularly interesting sequence of events that can occur in certain experiments as \(Ra\) is increased is a set of subharmonic bifurcations leading to temporal chaos [20, 21]. Some indication of the complexity of the general convection problem can be deduced from the three-dimensional graph (with axes formed by \(Ra, Pr\), and the wave number of the roll pattern) showing the regions of stable convection and the kinds of instability that arise upon leaving the region along different paths in parameter space [12]. But even the linear and nonlinear stability analyses that produce such a figure do not necessarily capture the full richness of the system.

The Rayleigh-Bénard problem is clearly a complex one, even in the highly simplified Boussinesq approximation. The fluids studied by MD simulation are unable to sat-
isfy the Boussinesq condition fully because, in order to force the system into a convective state, the driving forces (temperature difference and gravity) and the response of the system (e.g., density variation, shear rate) are much larger than those prevailing under normal experimental conditions—by at least several orders of magnitude. Thus the quantitative predictions of the simplified theory need not be adhered to particularly closely. Nevertheless, theory can provide useful guidelines as to the kinds of simulation to conduct and the properties to examine.

One further distinction between experiment and simulation is that while the former is nearly always three dimensional, the latter, because of prevailing computational limitations, is restricted to just two dimensions. While the initial roll-formation instability is basically two dimensional, subsequent behavior is undeniably three dimensional with the clear presence of a vertical component in the vorticity. Thus the results of MD simulation will, for the present, have to be compared with numerical solutions of the continuum fluid equations in two dimensions. But even these are sufficiently rich—displaying both periodic time dependence and temporal chaos—that this limitation leaves adequate scope for exploring the capabilities of the MD approach. (The Hele-Shaw cell [22] provides for two dimensional experimentation, but because the configuration corresponds to infinite Pr the relevance is questionable.)

**B. Molecular-dynamics simulation**

MD simulation embraces a class of numerical techniques for solving classical atomistic N-body problems. It is an ab initio approach since all that is required is a description of the structure of the individual atoms or molecules and the functional form of the interatomic potentials. The coupled Newtonian equations of motion of the particles in the system are solved numerically, and various averages and correlation functions computed that correspond to macroscopic observables—typically thermodynamic quantities, measures of spatial structure and order, and transport coefficients. The MD approach has proved surprisingly effective at yielding insight into a variety of different problems in condensed-matter science, in most cases with the expenditure of only modest amounts of computational effort. Descriptions of methodology and applications are readily available [1–3].

Until recently, MD applications tended to focus on simulations of systems in thermodynamic equilibrium and on steady-state transport processes. The ability to study larger systems for longer time periods has resulted in several exploratory studies of nonequilibrium fluid phenomena, one of these being the thermal convection problem (the others are flow past an obstacle [23] and the motion of an interface between immiscible fluids flowing through a channel [24]). The overall goal of MD simulations of fluid flow and instability phenomena should not be regarded as an attempt to compete with the well-established techniques of computational fluid dynamics that are in routine engineering use, but rather an effort to try to bridge the gap between the atomistic and continuum pictures in order to learn how the microscopic details lead to the observed macroscopic behavior.

**C. MD studies of convection**

In previous MD studies of thermal convection—all involving hard-disk fluids—the evidence tended to suggest that provided the number of particles exceeded some fairly small threshold (typically 5000), the most interesting behavior that could be expected was a time-invariant roll structure, the details of which were determined by the aspect ratio Γ and the external conditions. It should be stressed that rolls appear spontaneously in the MD simulations; no extraneous initiating mechanism is involved.

The earliest work [25] involved a system of N = 5040 particles, with Γ = 2√2, density ρ = 0.2, thermal walls with partial slip, and smooth lateral walls. Roll nucleation occurred at the lateral wall and three rolls eventually developed, but this structure then faded away to be replaced by a similar structure with reversed flows. Total run length was 35 × 10⁶ collisions (the degree of computational effort required for hard-disk studies is measured in terms of collision count).

Subsequently, results obtained with an N = 14 160 system at ρ = 0.4 showed that larger systems admitted other kinds of behavior [26]. For a container with Γ = 4, slip (i.e., stress-free) thermal walls and periodic lateral boundaries, apparently stable four-roll patterns were obtained for several values of the temperature difference ΔT. In one case, a well-formed set of six rolls appeared as a relatively long-lived metastable state which eventually transformed into a four-roll pattern; the four-roll pattern fills the container with rolls of square cross section, a shape close to that predicted by stability analysis and also observed experimentally. These runs also produced evidence of sensitivity to the initial conditions: runs that only differed in their initial velocity distributions went through very different transient phases (such as partial development of some of the rolls expected in a six-roll pattern), but all eventually produced the same final four-roll state. The maximum run length in these simulations was 86 × 10⁶ collisions.

The next reported work [27, 28] considered 5000 disks at ρ = 0.2, with Γ = 2, and thermal walls that conserved tangential velocity but thermalized the normal component (i.e., a certain amount of thermal "slip" was allowed). A stable two-roll pattern emerged in a run whose length was 50 × 10⁶ collisions. Pressure, density, temperature, and velocity were all found to agree quite closely with numerical solutions of the compressible hydrodynamical equations. The possibility of generating a single roll in a Γ = 1, N = 1500 system was also demonstrated.

Evidence for an oscillatory roll pattern emerged [16] only when the system size was increased substantially—to N = 57 600. In the original run on a system of this size in a square container (Γ = 1) with nonslip thermal and lateral walls, a pair of rolls developed, and the boundary separating them was observed to oscillate in a regular fashion about the direction perpendicular to the thermal
walls. Two complete periods were followed in the course of a simulation extending over $2 \times 10^9$ collisions. The oscillation period—scaled by the vertical thermal diffusion time ($L_d^2/\kappa$)—was reasonably close to the value obtained by numerical solution of the continuum equations [17].

A further run involving an even larger system, with double the number of particles, again revealed periodic behavior, but with a larger oscillation amplitude. The ratio of the periods in the two cases was consistent with thermal diffusion being the mechanism governing the rate of oscillation (i.e., the period was proportional to the linear size squared). Further runs on systems with the smaller $N$ showed evidence of unpredictable transient and long-term behavior, as well as revealing that the periodic behavior could be accompanied by considerable noise, even to the extent of completely swamping the regular oscillations. These results form the basis of this paper.

It must be stressed that all the conclusions are based on runs whose lengths are severely limited. While runs exceeding $10^9$ collisions (the longest was slightly over $10^{10}$) and systems with $N > 10^6$ represent the most extensive (both the longest and the largest) hard-disk simulations ever to have been carried out, the data presently available can only hint at the true behavior of these systems, and even more extensive computations will be required to produce a complete picture (e.g., a phase diagram). Furthermore, in comparing the simulation results with the theory and experiment, it must be remembered that the simulated fluid does not fully obey the Boussinesq approximation, and that the gradients are such that the transport coefficients cannot be assumed constant throughout the fluid.

III. METHODOLOGY

A. Hard-disk MD

MD simulation of a hard-disk fluid [29] is based on event-driven simulation [30]. The computational process advances the state of the system in a long series of discrete time steps corresponding to the intervals between successive two-particle collisions; in contrast to the more familiar fixed time-step methods used for integrating the equations of motion of a system based on differentiable potential functions, the time steps in the event-driven approach are determined by the particles themselves. Between collisions the particles follow linear trajectories if no external force is applied; in the convection simulations the particles follow parabolic trajectories corresponding to free fall in a uniform gravitational field. The collisions themselves are elastic, with the outcome being determined by basic energy and momentum conservation considerations.

The principal problem with this approach is the need to ensure the constant availability of a list of future collisions of each particle. Assuming that such a list is constructed at the start of the simulation, it must somehow be updated each time a collision occurs to ensure that it reflects the current situation; the key point is that the necessary changes can only be allowed an amount of computational work which is either independent of, or at worst, only very weakly dependent on, the total particle number $N$. Given that the simulations will involve upwards of $10^4$ particles and $10^9$ collisions it is obvious that any substantial $N$ dependence would be prohibitive. An efficient scheme that does deliver a satisfactory level of performance and which depends only logarithmically on $N$ is available; it is based on dividing the region occupied by the fluid into a grid of cells to minimize the number of candidate particles which must be examined as potential future collision particles, as well as on the use of a binary tree to organize the information concerning future collision events [30].

B. Soft-disk MD

The techniques used for MD simulation of soft-disk fluids are well known and require little discussion here [2, 3]. The particles interact by a shifted and truncated version of the Lennard-Jones potential that contains only a short-range repulsive term

$$V(r) = \begin{cases} 
4(r^{-12} - r^{-6}) + 1, & r \leq r_c = 2^{1/6} \\
0, & r > r_c 
\end{cases}$$

in conventional MD units. The amount of work required to compute the interactions experienced by each particle can be reduced to a constant that is independent of $N$ by using a neighbor list that records all pairs lying within or just outside the interaction cutoff range $r_c$. This list remains valid for several time steps on average, and is updated whenever the possibility arises that additional particle pairs may have come within interaction range. Updating the neighbor list makes use of a cell subdivision of the simulation region to ensure that the processing required per particle is once again $N$ independent. While the fact that the fluid exhibits convective flow means that neighbor-list updates are more frequent than in an equilibrium simulation (once every 3–4 steps on average, as opposed to one update every 10–20 steps), the saving in computational effort still makes the technique worthwhile. Integration of the equations of motion uses the standard leapfrog scheme; the gravitational field contribution is simply added to the vertical component of the acceleration.

C. Boundary and initial conditions

All the simulations described here employ containers whose walls are roughened to provide the nonslip boundary conditions that apply to real fluids, even though this is not an essential requirement for MD modeling. Unlike some of the earlier MD simulations of convection which used periodic boundary conditions for the lateral edges [26], the present work uses rigid walls; these both help to confine the roll patterns and facilitate the use of wall roughness to impede fluid rotation (as occurs in real fluids). Rough walls discourage the formation of just a single roll, which appears to be a favored state in a square
container with smooth walls. To produce the stationary boundary layer that is the signature of a rough wall, slightly different techniques were used for the hard- and soft-disk computations.

For the hard-disk fluid, collisions with the walls are energy conserving (the heat transfer that occurs at the thermal walls will be addressed subsequently). Each wall is regarded as consisting of a series of strips in which the outcome of a wall collision alternates between specular reflection and velocity reversal. The width of the strips is approximately the particle radius. The net effect of this scheme is essentially identical to the use of corrugated walls constructed out of immobile disks that are suitably spaced along the periphery. The lateral walls are insulating, implying that the local wall temperature matches the adjacent fluid element; if this were not the case the walls themselves would encourage roll development because of the consequent horizontal temperature gradient.

Heat is introduced and removed from the system by the top and bottom thermal walls which are maintained at constant temperature—these walls have an effectively infinite thermal conductivity. At the microscopic level heat exchange is accomplished by simply rescaling the velocity magnitude of a particle colliding with a thermal wall to ensure the departure velocity corresponds to the wall temperature (velocity components both parallel and perpendicular to the wall are affected). Since the mean flow velocity is zero within the boundary layer there is no need to correct the enforced temperature to account for any local streaming flow. Note also that there is no randomness associated with the wall collision mechanism. There is an element of arbitrariness to the scheme as a whole, as there is indeed with any conceivable alternative, but there is neither reason nor evidence to suggest that the observed behavior is in any way adversely affected by the method adopted.

The soft-disk simulations employ corrugated walls constructed from immobile disks identical to those of the bulk fluid. To enhance the effective wall roughness, the boundary disks are arranged in a zigzag formation that tends to further impede motion parallel to the wall in the boundary layer. Heat transfer to and from the fluid at the thermal walls is again accomplished in a rather arbitrary fashion, in this case by periodically rescaling the velocities of all fluid particles within interaction range of the wall particles so that the mean-square velocity in the boundary layer corresponds to the adjacent wall temperature; this is done sufficiently frequently (typically every 20 time steps) to ensure adequate thermal coupling between fluid and wall.

The initial states for all simulation runs are identical, except for one minor, but—in retrospect—important, detail. All particles are placed on the sites of a lattice, evenly spaced as prescribed by the mean density, and assigned velocity magnitudes that correspond to an initially linear temperature gradient between hot and cold walls. The directions of the velocities are assigned randomly, and the only element that varies between runs for each system size is the initial seed value used for the random number generator. At the “macroscopic” level this detail should of course be irrelevant, although the results prove otherwise.

D. Performance issues

Simulations of both soft- and hard-disk fluids are rarely combined in the same study, and the present work provides an opportunity to discuss the relative merits and shortcomings of the two approaches.

From the computational point of view, soft disks have the advantage of a very simple algorithm (even when neighbor lists are included), whereas hard disks necessitate a comparatively complex event-driven approach. Although not of concern here, soft-disk MD is also readily amenable to vector and distributed processing with near-maximal efficiency. The present series of calculations used scalar processors only, namely an IBM 3090E mainframe computer and an IBM RISC/6000 model 320 workstation; the performance of the latter was between 50% and 70% of the former (with hardware costs differing by almost two orders of magnitude). In attempting to compare the computational efficiencies of the hard- and soft-disk approaches, probably the most relevant measure is the amount of time required to generate a single roll oscillation when the systems are at similar state points, although not enough is known about the effective Rayleigh and Prandtl numbers of the model fluids for too precise a comparison; the estimate is that the soft disks require about 3–4 times as much computational effort as the hard disks. This comparison is only meaningful for a given kind of processor architecture—the availability of vector and/or distributed processing could favor the soft-disk approach [31].

For the thermal convection problem, hard disks do have one particular advantage, which helps account for the better performance. Soft-disk MD uses a fixed time step $\Delta t$ which applies to all particles in the system; the magnitude of $\Delta t$ is dictated by the velocities in the hot region of the fluid, and must be chosen to ensure the required degree of accuracy in the numerical integration. Since the velocities of the hot particles are typically several times those of the cold particles there is clearly a considerable amount of computational effort wasted given that the cold region could easily tolerate a larger value of $\Delta t$; the possibility of using a multiple time-step method in which $\Delta t$ is a (step) function of the vertical coordinate has not been investigated, although it would lead to improved performance. Hard-disk MD on the other hand has no inherent time-step, and the collision rates adjust automatically according to the local temperature and density.

E. Analysis methods

A MD simulation run generates a complete set of trajectory histories. The wealth of detail potentially available is enormous, but it is clearly impossible to record all this information; thus, prior to a MD run, it must be decided what analysis will be carried out in the course of the run, and what data will be retained for subsequent
analysis.

The principal quantities of interest in the flow simulations are those that correspond to the vector and scalar fields addressed by continuum hydrodynamics, namely flow velocity, temperature, and density. This information is extracted from the simulation by means of coarse-grained spatial averaging over a grid subdivision of the system; the measurements are also averaged over fixed intervals of time. The data items actually recorded for each grid cell are the mean flow velocity vector for the particles occupying each cell at the instant of measurement, together with the mean-square speed and the occupancy count; from this data it is possible to reconstruct flow patterns, temperature (after elimination of the bulk flow contribution), and density fields. Details of grid size and sampling period are dictated by the length and time scales of the phenomena to be observed, as well as by the inherent fluctuations in the data and the constraints set by available storage resources.

The flow patterns can be represented in various ways: flow velocities can be displayed as vector plots, but the most informative way of visualizing the kinds of flow observed in this work is by use of contour plots of the particle flux

$$\psi = \int \rho \mathbf{u} \cdot dl,$$

in which $\psi$ denotes a line integral of the coarse-grained fluid momentum $\rho \mathbf{u}$ from an arbitrary origin to the grid cell in question; for an incompressible fluid the contour lines are in fact the flow streamlines [10]—a good approximation in the present case except, possibly, very close to the walls. Each such streamline plot provides only a static image that captures a moment in the flow history; a fuller appreciation of the flow behavior is best achieved by observing an animated sequence of such plots, either generated on the fly from previously stored data using a sufficiently fast graphics display facility, or else recorded on video a frame at a time. (Color-coded regions can be used as an alternative to contour lines; better video images are obtained in this way.) These techniques have been employed in the present work but, regrettably, the printed medium only permits a very small sampling of the images obtained.

**IV. RESULTS**

**A. Description of runs**

Most of the results described in this paper were obtained from the hard-disk simulations; this is a consequence of the relative performance of the two approaches (discussed in the preceding section). Though earlier work involved a range of systems sizes and container shapes, the results presented here are based on systems with $N = 57600$ and $N = 115600$, in a square box ($L = 1$), and at a number density $\rho = 0.4$. The actual size of the larger system, assuming the disk diameter to be that of a typical atom such as argon, would correspond to a container of edge 1500 Å. Other runs have been carried out with different values of $\Gamma$, $N$, and $\rho$, but the work to be described here is limited to the above values, where most of the computational effort has been concentrated. Even so, because of the surprisingly rich behavior, the picture is far from complete.

The temperatures of the thermal walls are $T_{\text{cold}} = 1$ and $T_{\text{hot}} = 16$; work on smaller systems indicated little change in behavior for $\Delta T = T_{\text{hot}} - T_{\text{cold}}$ larger than about 15—except, of course, for a uniformly more rapid development of the flow patterns. Note the use of reduced units in which the particle mass and diameter, as well as the Boltzmann constant, are unity. The unit of time for a hard-disk system is completely arbitrary since no intrinsic energy scale exists; the arbitrariness is removed by the prescription that a particle with unit velocity has a kinetic temperature $T = 0.5$. The strength of the gravitational field is

$$g = \frac{\Delta T}{L^2},$$

a choice that equates the thermal-energy change experienced by a particle traversing the system vertically to the potential-energy difference. All walls are rough, an effect achieved using the methods described above. The time step for the soft-disk simulations, in reduced MD units, is $\Delta T = 0.004$, equivalent to approximately $10^{-14}$ s. The run lengths ranged from $2 \times 10^9$ to $10^{10}$ collisions for the hard disks, and to over $5 \times 10^8$ time steps for the soft disks; in terms of real time these values amount to several ns. Total computation times for several of the runs exceeded 1000 h.

The grid size used for the analysis is $50 \times 50$; the time interval used for averaging is 100 or 200 time units (for $N = 57600$ and $N = 115600$, respectively), an interval during which changes in the flow patterns are comparatively minor. In the case of $N = 115600$ the typical grid cell contains approximately 50 disks; if the flow characteristics change significantly over a single cell then the details will not be resolvable—such a situation arises in the boundary layers where the coarse graining is on a scale comparable to the layer thickness (a variable grid size could be used to probe the boundary layers in greater detail).

Estimates of the nominal $Ra$ and $Pr$ values for the present simulations can be obtained [28] from a combination of Enskog theory [32] and an empirical hard-disk equation of state [33]. The key ingredients are the density expansions for the transport coefficients [34]

$$\nu = \frac{\sqrt{T}}{\rho} \mu'(\rho),$$

$$\kappa = \frac{\sqrt{T}}{\rho c_p} \lambda'(\rho),$$

where $c_p$ is the constant-pressure specific heat, the density-dependent parts of the viscosity and thermal conductivity are

$$\mu'(\rho) = 0.2555\sqrt{\frac{2}{\pi \chi}} + \rho + 0.4365\pi \chi \rho^2 + \cdots.$$
\( \lambda'(\rho) = 1.029\sqrt{\pi} \left[ \frac{2}{\pi \chi} + 1.5\rho + 0.4359\pi \chi \rho^2 + \cdots \right] \), (9)

and the pair correlation \( \chi \) is given by

\[ \chi = \frac{1 - 7\pi \rho / 64}{(1 - \pi \rho / 4)^2} \] (10)

together with the equation of state

\( P = T \rho H(\rho) \), (11)

where

\[ H(\rho) = \frac{1 + \pi^2 \rho^2 / 128}{(1 - \pi \rho / 4)^2} \]. (12)

The thermal expansion coefficient can be written

\[ \alpha = -\frac{\alpha'(\rho)}{T} \], (13)

where the density-dependent part is

\[ \alpha'(\rho) = \left[ \rho \frac{d}{d\rho} \ln(\rho H) \right]^{-1} \]. (14)

The resulting expressions for \( \text{Ra} \)—using \( g \) from Eq. (5)—and \( \text{Pr} \) are

\[ \text{Ra} = \left( \frac{\rho^2 c_p \alpha'}{\mu' \lambda'} \right) L_y^2 \left( \frac{\Delta T}{T} \right)^2 \], (15)

\[ \text{Pr} = \frac{c_p \mu' \lambda'}{\lambda'} \], (16)

where the \( \rho \) dependence of the material properties is implicit, and it is assumed that they are evaluated at the mean density of the fluid; \( T \) is the mean temperature.

The value of \( \Delta T/T \) is 1.76 (the limiting value is 2 as \( T_{\text{hot}}/T_{\text{cold}} \to \infty \)); thus for the present series of simulations (\( \Gamma = 1 \), \( \rho = 0.4 \)) the values are \( \text{Ra} = 1.05N \) and \( \text{Pr} = 0.45 \). For \( N = 57600 \) the value is \( \text{Ra} = 6.0 \times 10^4 \), whereas for \( N = 115600 \) the value is doubled. The maximum of \( \text{Ra} \) occurs near \( \rho = 0.2 \) and is about 50% higher [28]; earlier simulations suggested, however, that the higher density is preferable for studying roll formation [26]. These estimates cannot be regarded as particularly reliable since the truncated \( \mu' \) and \( \lambda' \) expansions are of questionable validity at \( \rho = 0.4 \), and the transport coefficients cannot be regarded as constant because the local values of \( T \), \( \rho \), and the flow shear rate vary significantly across the system. Indeed, if the "local" values of \( \text{Ra} \) and \( \text{Pr} \) vary substantially their utility is questionable; at best, these estimates serve as rough guides as to the kind of macroscopic system with which the simulation results should be compared. Experimentally [35], deviations from the Boussinesq approximation are known to result in behavior of even greater complexity than that expected within the framework of the approximation.

**B. Roll development**

The behavior observed in the various simulation runs is best summarized by several sequences of snapshots that show the key stages in the evolution of the flow patterns and which stress both the unpredictableability of the transient state and the nonstationary—sometimes fully periodic—two-roll state eventually reached. This will be done using contour plots of the particle flux \( \psi \), which, as pointed earlier, are essentially plots of the streamlines. The flux values at which contour lines are drawn are constant for each sequence of frames shown, and are uniformly spaced over the measured range of values; thus individual plots may show slight variations in the numbers of contour levels, depending on the spread of \( \psi \) values.

Figures 1, 2, and 3 show the flow patterns at various times during the early stages of three \( N = 57600 \) simulations (not including the run reported previously). There is very little similarity between the histories of the different runs, which differ only in the initial random assignments of disk velocity directions. The observed histories include the near-symmetric growth of a pair of rolls (Fig. 1), the growth of a large irregular pattern that develops into a roll occupying nearly the entire container before a small corner roll begins to compete (Fig. 2), and a short-lived initial three-roll pattern (Fig. 3). In each case (a total of five runs with this value of \( N \) were carried out) the final state consisted of two rolls, similar in average size, and separated by a boundary whose direction (and position) varied with time. The degree to which this variation is periodic will be discussed below.

Figures 4 and 5 show results for two \( N = 115600 \) systems; the two sequences of snapshots are shown at identical times. In one case the transient phase includes four rolls (Fig. 4), in the other (Fig. 5) two rolls appear.

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**Fig. 1.** Streamline plots of the early evolution of an \( N = 57600 \) hard-disk system. The streamlines are evenly spaced with respect to mass flux. Each frame shows the average over 100 time units, and is based on coarse-grained spatial averaging over a \( 50 \times 50 \) grid.
FIG. 2. Same as Fig. 1, but for a system with a different initial velocity distribution (see text).

FIG. 3. Another example of the early flow patterns (as in Figs. 1 and 2).

FIG. 4. Streamlines during the transient phase of an $N = 115,600$ hard-disk system. Each frame is averaged over 200 time units, and spatially as in Fig. 1.
almost immediately. Both runs eventually lead to an almost noise-free oscillatory state (see below).

Figure 6 shows the flow at several instances during a single oscillation of one of the $N = 115600$ systems. The interval covered by each frame is only a fifth of the interval between frames. Three such cycles were followed for both systems, and once in the oscillatory phase there is no indication that any further change is likely to occur; further analysis of these flow patterns appears below.

C. Periodicity measurements

One of the advantages of MD is that it allows a far more detailed examination of the system than is possible experimentally: for example, to measure the time dependence of the flow, "probes" of various kinds are readily inserted in the fluid. In the initial study of time-dependent flow [16] the locations of the extrema of the stream function were identified, and the quantity monitored was the angle of the perpendicular to the line between these two points. An essentially equivalent measure, but one that is slightly less prone to noise, is the mean flow direction through the central region of the box (more precisely, a $10 \times 10$ cell region); the time dependence of this quantity is analyzed here. The estimates are derived from time-averaged snapshots of the type shown in Fig. 6, each of duration 100 or 200 time units.

Figure 7 shows the results for all five simulations carried out on the $N = 57600$ systems; the graphs only begin when roll development is practically complete and they exclude the transient stages. The topmost graph is the same run described previously [16], but now analyzed using the mean flow direction. Figure 8 shows the

FIG. 6. Streamlines during a segment of the oscillatory phase of the same $N = 115600$ system shown in Fig. 5.
corresponding results for the two $N = 115\,600$ systems; in this case the behavior is sufficiently similar that the graphs can be superimposed. The bigger systems exhibit larger oscillations, and the period is close to double the value for the smaller systems, as is expected given that the natural time scale in the Boussinesq approximation is the vertical thermal diffusion time $\tau = L_y^2/\kappa$; in terms of the numerical values for the transport coefficients introduced above, $\tau = 0.085 L_y^2$ which amounts to $1.2 \times 10^4$ and $2.4 \times 10^4$ for the two values of $N$. The observed period is close to $0.4 \tau$ for the smaller systems in those cases where oscillations are clearly discernible, as well as in both instances of the larger system; this result compares favorably with the value $0.2 \tau$ obtained from a numerical solution of the continuum equations [17] in a square container with $Ra = 10^5$ and $Pr = 0.7$. The periods can be obtained by direct measurement from the graphs, and the estimates are supported by Fourier analysis, which, for four of the five graphs in Fig. 7, and both graphs in Fig. 8, results in a peak close to the expected frequency, with a width that reflects the apparent “quality” of the periodicity.

Another useful probe—one corresponding to a method often used experimentally—is the thermometer. Figure 9 shows the temperature measurements obtained during the shorter $N = 115\,600$ run; the four temperature probes are symmetrically placed in the box, each located a distance $L/3$ (where $L_x = L_y = L$) from a pair of adjacent edges. To further emphasize the periodic nature of the flow, Fig. 10 shows a temperature-temperature plot of the same data (a phase-space trajectory) based on a hot and cold probe (corresponding to the solid curves of Fig. 9); three full cycles are shown and, after making allowance for the noise, the cyclic nature of the plot is clearly visible.

The considerably larger computational effort needed for the soft-disk studies limited the results obtained for
FIG. 10. Temperature-temperature phase-space plot based on the solid curves of Fig. 9; three full roll oscillation cycles are shown.

this class of system to one extensive simulation having \( N = 57 \, 600 \), with the other parameters identical to the hard-disk systems. A run of over \( 5 \times 10^8 \) time steps resulted in less than two complete roll oscillations. The estimated period is approximately \( 10^4 \) MD time units, a value double that of the corresponding soft-disk systems. Given that a soft-disk fluid is inherently more compressible than a hard-disk fluid, deviations from Boussinesq behavior may be even greater, and thus the absence of better agreement may be acceptable.

D. Flow velocity, temperature, and density

Several other aspects of the behavior are described here. For definiteness, all are based on the shorter \( N = 115 \, 600 \) simulation, but the results shown are typical of all the runs.

Details that are not apparent from the flow contour plots can be seen in arrow plots showing the spatial variation of the magnitude and direction of the velocity field. Figure 11 is one such plot based on the same data used for the final frame of Fig. 5. The flow direction in the middle of the system is upward, as is the case in each of the runs; there is a clear advantage (in terms of thermal transfer efficiency) to keeping the upward flow away from the lateral walls in the early stages of roll development, and once this feature of the flow becomes established there is little reason for it to disappear. The strong flow associated with the rolls should be contrasted with the near-zero flow in the vicinity of the walls; if slip boundaries had been used, strong flows would occur right up to the walls—a clearly unphysical effect. There is little convective heat transport adjacent to the thermal walls, where the principal transport mechanism is conduction;

the temperature plots (below) will show that much of the vertical temperature variation occurs close to these walls in order to enhance the conduction mechanism.

The two graphs in Fig. 12 plot the velocity components parallel to each of the four walls; each graph shows the velocities in the layers of coarse-grained cells adjacent to both walls in the \( x \) or \( y \) direction, and, by way of contrast,
FIG. 13. Temperature contour plot for the state shown in Fig. 11; the contour levels are uniformly spaced.

the velocities in a parallel strip of cells through the center of the box. The values are averaged over ten frames straddling the state shown in Fig. 11 in order to smooth the data; no significant change to the flow pattern occurs over this interval. The fact that the coarse-grained cell velocities are not identically zero at the boundaries can be understood if it is recalled that the cells used for spatial averaging each hold an average of approximately 50 particles; when the boundary layer is strongly sheared (cf. Fig. 11, where the rolls can be seen to almost touch the walls at several points) the coarse-grained cell averages will differ from zero. Smaller cells are necessary to resolve details of the boundary-layer flow.

A contour plot of the temperature field corresponding to the flow state of Fig. 11 is shown in Fig. 13. The tendency for the temperature variation to concentrate near the thermal walls is apparent, as is the correlation of the contour pattern with the known roll structure and flow direction, namely a hot jet of fluid rising through the center of the system and bearing to the left.

Figure 14 complements this contour plot by showing the temperature variation along three equally spaced vertical cell strips. In order to smooth the data, the results have again been averaged over ten frames centered on the state shown in Fig. 13. The prominent features of this graph are the deviation from the linearity of a purely conductive state, and the abrupt temperature variations that occur in the thermal boundary layers—recall that \( T_{\text{hot}} = 16, T_{\text{cold}} = 1 \). The temporal development of the mean (horizontally averaged) temperature profile during the early stages of the simulation is shown in Fig. 15; the gradual changeover from the initial linear profile (already distorted near the hot wall in the first time-averaged set of data) to the S-shaped curve signifying enhanced temperature variation at the walls can be seen.

The density variation throughout the system is shown in Fig. 16, for the same flow state as before. The actual change in density is quite small except very close to the cold upper boundary. Quantitative details of this variation appear in Fig. 17, which shows the local density in three vertical strips. With the exception of the immediate neighborhood of the cold thermal wall, density variations amount to no more than about 10% of the mean.

FIG. 15. Evolution of the vertical temperature profile based on the mean temperature of a set of horizontal strips that span the container.

FIG. 16. Density contour plot corresponding to Figs. 11 and 13; the contours are evenly spaced over a range from 0.8 to 1.5 times the mean.

FIG. 14. Temperature cross sections along three evenly spaced vertical strips.
E. Heat transport

Experimentally, the heat flux is an important probe for monitoring time-dependent convective flow. A numerical study of the corresponding continuum problem [17] resulted in either periodic or chaotic time dependence of the heat flux, depending on the values of $Ra$ and $Pr$. The periodic state was produced by a pair of rolls whose boundary oscillated about a horizontal axis; this entails a significantly larger degree of flow pattern rearrangement than appears in the present series of MD simulations, with the vertical component of the flow velocity through the central region of the box alternating in direction (in the MD results it is always upward). This rearrangement has a strong effect on the heat flux, but analogous behavior is absent from the MD results (the difference could either be due to the system being at a different state point, or because of deviations from Boussinesq conditions).

An alternative use for the heat-flux measurements is to study the nature of the bifurcation which occurs at the onset of convection. This bifurcation between the purely conductive and convective states at $Ra_c$ corresponds to a symmetry breaking in the flow velocity field (which is identically zero for $Ra<Ra_c$), a phenomenon reminiscent of a second-order phase transition. The Rayleigh-Bénard problem has indeed been analyzed from this point of view [13]. A simple mean-field theory can be formulated in which the characteristic convective flow velocity, or the deviation from the linear temperature profile of the conducting state, plays the role of the order parameter. Furthermore, the response of the system to a temperature perturbation can be described by analogy with the critical slowing down that occurs near a second-order transition.

If $\varphi_{\text{cond}}$ is the conductive heat flux in the absence of convection ($\varphi_{\text{cond}} \propto \Delta T$ by Fourier's law), and $\varphi_{\text{conv}}$ the additional flux arising from convective flow above $Ra_c$, then the Nusselt number $Nu$ is defined as

$$Nu = 1 + \frac{\varphi_{\text{conv}}}{\varphi_{\text{cond}}}. \quad (17)$$

The mean-field analysis predicts a singularity at $Ra=Ra_c$; the characteristic flow velocity just above the transition is

$$v \propto (Ra - Ra_c)^{1/2}, \quad (18)$$

and the variation of $Nu$ is given by

$$Nu = 1 + \text{const} \times (Ra - Ra_c). \quad (19)$$

Experiment provides support for these predictions [13, 14].

To study the convection transition, the total heat flux $\varphi = \varphi_{\text{cond}} + \varphi_{\text{conv}}$ and the maximum coarse-grained cell speed $v_{\text{max}}$—an estimator for $v$ in Eq. (18)—were measured as functions of time for an $N = 10000$ system as $T_{\text{bot}}$ gradually increased; initially $\Delta T = 1$, and the value was raised by 0.5 every 1000 time units ($g$ is also adjusted to maintain the potential and thermal energy balance). This is a considerably smaller system than those discussed earlier in this paper because the purpose of this very preliminary study was simply to examine whether any indication of a reasonably abrupt transition to the convective state could be detected.

The two graphs in Fig. 18 show the measured values of $\varphi/\Delta T$—a quantity proportional to $Nu$—and $v_{\text{max}}$ (measurements were made every 100 time units); the stepped values of $\Delta T$ are also indicated. Roll development was complete close to time 6500, just where $v_{\text{max}}$ changes gradient; the final state for this run consisted of just a single convective roll. The results are subject to considerable noise, but are not inconsistent with the predicted gradient discontinuity [note that from Eq. (15), $Ra-Ra_c \propto \Delta T - \Delta T_c$ when $Ra=Ra_c$, where $\Delta T_c$ is the value of $\Delta T$ at $Ra_c$]. A more extensive investigation of

![FIG. 17. Density cross sections along three evenly spaced vertical strips.](image)

![FIG. 18. (a) Total heat transfer rate $\varphi$ divided by $\Delta T$ vs time for an $N = 10000$ hard-disk system; the dashed lines show $\Delta T$. (b) Maximum flow velocity $v_{\text{max}}$ vs time for the same run.](image)
the convection threshold is in progress, aimed at characterizing the behavior near the bifurcation.

V. SUMMARY

The modern notions of chaos and unpredictability have laid to rest the Laplacian vision of predicting detailed large-scale behavior given sufficient information about initial and boundary conditions at the individual particle level. The present simulations demonstrate this admirably, but also reveal that if there is no competition between different modes of behavior—in other words, there is only a single basin of attraction in phase space—then most of the detail contained in the initial conditions is irrelevant to the long-term collective motion, with the exception of the absolute phase (or time origin). On the other hand, if there is some degree of mode competition, or if the focus is on the nature of the transient patterns as the system approaches its terminal state (or state cycle), then the minutest details of the initial state are seen to be all important.

The amount of information presently available for these systems is still very limited because of the large amount of computation required to follow just a single system at a single state point. Although calculations of this magnitude would have been utterly unfeasible until only recently (and if technically feasible, then unaffordable), the appearance of comparatively inexpensive workstations in the past two years, that are sufficiently powerful to begin to address the problem, has permitted a certain amount of exploratory work to be carried out. However, present levels of computer performance still mean that a single calculation can require several weeks, or more, of computation. With further improvements in both performance and cost, as well as the increasing availability of distributed processing, one can look forward to being able to handle even larger problems, with whatever surprises they may have in store. But it must be realized that the rate of growth of the system size which can be accommodated will only increase sublinearly with total processing power because there are intrinsic processes at work—such as thermal diffusion—which impose their own time scales on the system, and that these scales are themselves also size dependent.