HYDRODYNAMIC FLUCTUATIONS AND THE DIRECT SIMULATION MONTE CARLO METHOD

Alejandro L. Garcia

Dept. of Physics, San Jose State Univ.

San Jose, CA 95192-0106

ABSTRACT: The use of particle simulations in the study of hydrodynamic fluctuations in nonequilibrium systems is reviewed. Some results for Rayleigh-Bénard convection measured by a Direct Simulation Monte Carlo program are presented.

I. INTRODUCTION

One of the early problems to which electronic computers were applied was the measurement of the statistical properties of fluids.[1] Computer simulations of particle dynamics are attractive since microscopic details, such as correlation functions, are available. The first molecular dynamics (MD) programs dealt with only equilibrium systems but the combination of new algorithms and advanced computer technology has expanded the field to include nonequilibrium systems. This work ranges from simple systems (constant shear or heat flux) to the more recent work in complex flows; these proceedings present a good sampling of this spectrum: Prof. Hoover shows us how to work with nonequilibrium systems of no more than three particles; on the other hand, there are papers describing van Karman vortex shedding behind an obstacle and Rayleigh-Bénard convection.

Microscopic fluctuations are often studied using Molecular dynamics (MD) simulations; the characteristic length scale for their correlations is a few atomic diameters. In experiments, these microscopic fluctuations are measured by neutron scattering. At larger length scales one enters the hydrodynamic regime where the fluctuations are observable by light scattering.[2] At equilibrium, the Landau-Lifshitz theory accurately predicts the experimentally observed spectrum. A few years ago it was realized that in a highly nonequilibrium system the hydrodynamic correlation functions would be slightly modified from their equilibrium form. Specifically, it was predicted [3] (and later observed [4]) that the Brillouin peaks are asymmetric when the fluid is subjected to a strong temperature gradient. This effect is caused by the fact that the static density-velocity correlation function, $\langle \delta\rho(r)\delta v(r') \rangle$ is nonzero in the presence of the temperature gradient. Several good reviews of this work have appeared [5,6].

Microscopic Simulations of Complex Flows
Edited by M. Mareschal, Plenum Press, New York, 1990

This paper is divided into two parts. In the first part, I review the use of particle simulations in the study of hydrodynamic fluctuations in simple nonequilibrium systems. The latter half of the paper discusses the more recent work on complex flows, specifically Rayleigh-Bénard convection. An important branch of simulation work is excluded here: the coupling of hydrodynamic and chemical fluctuations. This exciting and rapidly advancing field is discussed, at least partly, in the contributions by Michel Mareschal and Florence Baras in this volume.

Given the informal atmosphere of the meeting I decided to organize the review part of the paper around a theme: the hunt for the elusive $\langle \delta T(x,t)\delta T(x',t)\rangle$ correlation. Since this static correlation is not readily accessible experimentally, it has been primarily studied by computer simulation. I have purposely made this a personal account; putting in some background behind the work and including details not found in the original papers. It has been my privilege and pleasure to know many of the people who have worked on these computer simulations; I only hope that the reader finds the style of the presentation more interesting than distracting.

II THE HUNT FOR THE ELUSIVE $\langle \Delta T(X)\Delta T(X')\rangle$ CORRELATION

a) Master Equation models

In the early 80's, Prigogine's group began studying thermo-chemical problems (such as combustion) using the Master Equation formalism. Gregoir Nicolis and Malek Mansour introduced a simple way of deriving a Master equation for the one-dimensional thermal conduction problem.[7] The corresponding Langevin equation is derived using only the properties that a) in the deterministic limit it reduces to the Fourier law and b) that the transition rate between states obeys detailed balance at equilibrium. They obtained the following interesting result; for a fluid contained between thermal plates at x=0 and x=L, the static correlation of temperature fluctuations has the form

$$\langle \delta T(x)\, \delta T(x')\rangle = \frac{k_B T_0^2}{C_v}\,\delta(x-x') + \{\delta T(x)\, \delta T(x')\} \qquad (1)$$

where

$$\{\delta T(x)\, \delta T(x')\} \equiv \frac{k_B \gamma^2}{C_v\, L}\, x\, (L-x') \qquad (2)$$

and $x \leq x'$; C_v is the specific heat per unit length, γ is the imposed temperature gradient ($\gamma \equiv (\Delta T/L)$) and k_B is Boltzmann's constant. The first term on the r.h.s. is the equilibrium contribution to the temperature fluctuations modified by the fact that the average temperature, $T_0(x)$, is a function of location. The term $\{\delta T(x)\, \delta T(x')\}$ is the nonequilibrium contribution to the correlation function; this term is illustrated in Figure 1. Note that this

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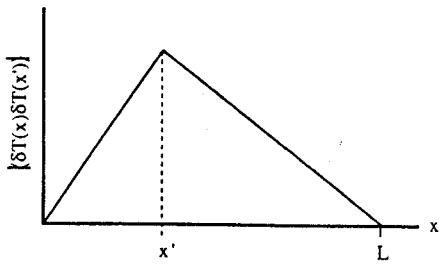

FIGURE 1. Sketch of $\langle \delta T(x) \delta T(x') \rangle$ as defined in equation (2).

I was still a graduate student at the University of Texas when Prof. Nicolis showed me a preprint of that paper. He asked me if it would be possible to measure $\langle \delta T(x) \delta T(x') \rangle$ using a Monte Carlo simulation of the Master equation presented in the paper.[8] Unfortunately, as they point out in the paper, the transition rate in their model has some unphysical properties. The difficulty arises from the approximation that the thermal diffusivity is strictly constant; only if one includes the (weak) dependance it has on temperature is a proper transition rate possible.

I was, however, already familiar with another model which did not have this problem. Nicolis, Baras and Malek-Mansour [9] had derived the Master equation for a dilute gas when the transport is Knudsen flow between cells. (Knudsen flow occurs when two containers are connected by an aperture which is only a few mean free paths in diameter) They derived an expression for the fluctuations in a single cell connected to two reservoirs at different temperatures; I had already confirmed this result by a simple Monte Carlo simulation. Using a similar program with a chain of cells connected by Knudsen apertures, I observed the long-range, linear correlation of temperature fluctuations predicted by equation (1).[10] While this result was encouraging, the Knudsen system was only a curious but unrealistic model.

b) Molecular Dynamics

About the same time that I was getting these results on the Knudsen system, Michel Mareschal and Eddie Kestemont were visiting Texas for a few months. They came to study the same problem by a different approach, using a molecular dynamics simulation of 3000 hard disks under a strong temperature gradient. Working first on our VAX and then on the Cyber, they made runs of some 2 million collisions each for various temperature gradients. The system was only some 220 molecular diameters in length and the temperature gradients were very large ($g \approx 10^8$ K/cm). Measurements of the moments of the local velocity distribution, however, were in very good agreement with a Gaussian distribution; this shows that local thermal

equilibrium is maintained even under such extreme nonequilibrium conditions [11].

Mareschal and Kestemont measured $\langle \delta T(x)\, \delta T(x') \rangle$ and found, in agreement with (1), that the nonequilibrium temperature fluctuations were proportional to the square of the imposed temperature gradient [12]. Unfortunately, they did not have enough statistics to accurately measure the spatial dependence of the correlations; i.e. they did not reproduce Figure 1. The problem is complicated by the slow relaxation of the lowest order modes in the system. One thing was clear: observation of these subtle effects required long run times. In my Knudsen flow model, I needed to run for over 10^8 events to get the correlation function to about 10% error. A few years later, Lar Hannon would run another MD program and attempt to measure $\langle \delta T(x)\, \delta T(x') \rangle$ only to find that even the supercomputer resources at IBM Kingston were insufficient [13].

c) Direct Simulation Monte Carlo

While finishing my dissertation, I was trying to find a realistic system for which I could hope to observe $\langle \delta T(x) | \delta T(x') \rangle$. By chance, my thesis advisor, Jack Turner, was serving as a consultant on an aerospace project involving the evaporation of a solid into vacuum. The problem was being studied using an algorithm called Direct Simulation Monte Carlo (DSMC) method. This simulation was introduced by G.A. Bird in the early 70's and it is widely used in rarefied gas dynamics [14]. Turner showed me the problem; lent me a copy of Bird's book and asked me to look it over.

After learning the algorithm, I realized that the evaluation of collisions is very similar to the Master Equation formulation of Kac for a homogeneous gas [15]. However, the motion of the particles is computed deterministically from their positions and velocities. The two processes are combined by "splitting": at each time step the particles are moved and a few undergo collisions. If the timestep is sufficiently small the DSMC correctly models a dilute gas (see Prof. Bird's contribution in these proceedings). One of the main advantages of DSMC is that it runs over 100 times faster than comparable MD codes. When I came to Brussels in early 1985, I suggested to Malek Mansour and Michel Mareschal that we try using Bird's method to measure the nonequilibrium temperature fluctuations.

The initial results from the simulation were very encouraging.[16] The DSMC reproduced the equilibrium fluctuations perfectly, including the finite size corrections. In the nonequilibrium system, the peak of the measured density-velocity static correlation function was linearly proportional to the temperature gradient, in agreement with theory and light scattering experiment. [5] Finally, the measured $\langle \delta T(x) | \delta T(x') \rangle$ was in good agreement with Figure 1 although the error bars were still unsatisfactorily large.

d) Landau-Lifshitz theory

While the Cyber labored away, we began working on the theory using fluctuating hydrodynamics. The fluctuating Fourier equation is obtained from the Landau-Lifshitz theory when one assumes that the temperature

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fluctuations are uncoupled from the density and velocity fluctuations. The solution of this equation for the temperature gradient problem also gives (1) [17,18]. For a dilute gas, however, the equations for density, velocity and temperature are coupled making the problem far more complicated. However, we expected that the results for $\{\delta T(x)|\delta T(x')\}$ would be qualitatively similar.

While much theoretical work had been done on the temperature gradient problem, most was motivated by light scattering experiments in liquids. Our computer simulation differed significantly from these experiments in several ways. (1) The system was extremely small (10 mean free paths) so finite size effects were very important. (2) To get an observable effect we used an extremely large temperature gradient. Since our medium was a dilute gas the density variation was also large. (3) We could measure all hydrodynamic quantities while light scattering only probed the density-density time correlation function.

After various attempts to analytically solve the Landau-Lifshitz equations for a dilute gas, Malek Mansour hit on solving them numerically. Our first effort was to numerically integrate the fluctuating Fourier equation since we knew the exact solution. Discretizing in space, the partial differential equation reduces to a set of ordinary stochastic differential equations.[19] I remember that we had the simulation of this Langevin equation running in a few days and good results after about a week. Euphorically confident, we then tried to write a similar Langevin simulation for the dilute gas equations and quickly hit an impasse. It was not so easy to properly handle the boundary conditions; specifically, there could be no boundary condition on the density.

The second attempt at numerically solving the fluctuating hydrodynamic equations involved using the static correlation equations. For a Langevin equation of the form,

$$\frac{dc_i}{dt} = f_i(c_1,...,c_n) + F_i(t) \tag{3}$$

where $F_i(t)$ is a white noise with variance,

$$\langle F_i(t)\, F_j(t')\rangle = Q_{ij}\, d(t - t') \tag{4}$$

then

$$\frac{d}{dt}\langle c_i(t)\, c_j(t)\rangle = \langle f_i(c_1,...,c_n)\, c_j(t)\rangle + \frac{1}{2} Q_{ij} \tag{5}$$

Applying this identity to the linearized fluctuating hydrodynamic equations yields a coupled set of equations for the static correlations.[19,20] Malek noticed that the equation for $\{\delta T(x)|\delta T(x')\}$ is closed without having to specify any boundary conditions for the density. After discretizing in space, the problem reduces to solving a set of simultaneous linear equations.

In early 86, Malek and I went to upstate New York as invited scientists. It was an exciting time to be in IBM Kingston; Lar Hannon had recently found vortex formation in the flow behind an obstacle and Dennis Rapaport was beginning to work with him on this problem [21]. Using the ICAP supercomputer, we could make new DSMC simulations using much larger systems (50 mean free paths between the thermal plates).

As mentioned above, our data from smaller systems (10 mean free paths) gave temperature correlations as in Figure 1. The larger system showed richer behavior; the correlations took the form shown in Figure 2. The agreement with the numerical solution of the correlation equations was excellent.[20] In fact, we first obtained Figure 2 from the correlation equations and it was so unexpected we spent a long time trying to find the bug in the program. Only later, when the DSMC simulation gave the same result did we realize that we were really observing multimodal behavior.

While in Kingston, Malek resolved the problem of how to numerically solve the full equations without specifying boundary conditions for the density. This difficulty with the boundary conditions is overcome by using a half-grid formulation. The density is specified on grid points which lie between the grid points for the velocity and temperature. The density grid contains only interior points (no points on the boundary) so no boundary conditions are needed for density.

The hydrodynamic correlation functions in the temperature gradient problem are now well known. The Couette flow problem (constant shear) has received similar attention and again, the results from DSMC simulations agree very well with fluctuating hydrodynamic theory.[22] A recent application of these results has been the testing and validation of Cellular Automata (CA) simulations. Chopard and Droz developed a two-speed CA model and measured the hydrodynamic fluctuations in the temperature gradient problem. Unfortunately, their preliminary results are inconclusive.[23]

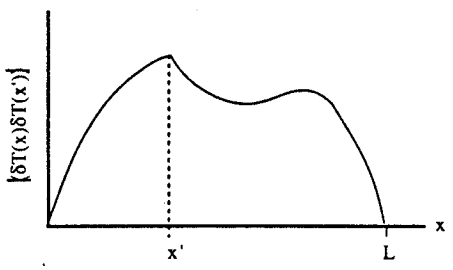

FIGURE 2. Schematic picture of $\langle \delta T(x) \delta T(x') \rangle$ as observed in larger systems.

III. RAYLEIGH-BENARD CONVECTION

Recent work has shown that particle simulations may be used to study complex flow problems. Rayleigh-Bénard convection is a paradigm instability; at a critical Rayleigh number there is a bifurcation between the states of purely conductive heat flow and buoyancy-driven convection. [24] The nature of the hydrodynamic fluctuations near this transition point has been studied theoretically by a variety of methods.[25] Ahler's group has

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performed several careful experiments and have measured the variation in the heat flux near the onset of convection.[26] Quantitative comparison, however, between fluctuating hydrodynamics calculations and laboratory experiments reveal significant, unaccountable discrepancies.[27] Furthermore, many theoretical predictions for the fluctuations near the convective threshold remain untested due to experimental difficulties.

Mareschal and Kestemont showed that it was possible to observe the Rayleigh-Bénard instability using Molecular Dynamics [28]; this work has been duplicated by other groups [29,30]. The observed density, velocity and temperature fields agree very well with those predicted by the standard Navier-Stokes equations.[31,32]

The DSMC method may also be used to study this problem but only at the expense of working with large systems. The dimensionless number characterizing the instability is the Rayleigh number,

$$R = \frac{\alpha\gamma g L^4}{\nu\kappa} \qquad (6)$$

where g is the gravitational field, L is the depth of the system, $\gamma \equiv \Delta T/\Delta z$ is the uniform temperature gradient, $\alpha \equiv 1/\rho\ [\partial\rho/\partial T]_p$, is the coefficient of volume expansion, κ is the thermometric conductivity and ν is the kinematic viscosity.

The critical Rayleigh number depends on the boundary conditions at the walls; in the limit of large aspect ratio the critical Rayleigh number is 1708 for no-slip boundaries and 658 for slip boundaries. In the simulation described below, I used slip boundaries but the aspect ratio was unity raising the critical Rayleigh number to about 780.

For a dilute gas, the density profile is a function of the temperature profile as, $\rho \propto T^{-a}$, where $a = 1 - mg/k_B\gamma$, m is the particle mass. Taking the value of the gravitational field as $g = k_B\gamma/m$ the density is approximately constant throughout the system. The thermometric expansivity, thermal conductivity and kinematic viscosity may be written as

$$\alpha = 1/T \quad ; \quad \nu = 2/5\ \kappa \qquad (7)$$

$$\nu = \frac{10}{32} l \sqrt{2\pi k_B T/m} \qquad (8)$$

where λ is the mean free path. From the above

$$R = \frac{256}{125\pi} (\Delta T/T)^2\ (L/\lambda)^2 \approx 0.652\ (\Delta T/T)^2\ (L/\lambda)^2 \qquad (9)$$

Even with an extremely strong temperature gradient $\Delta T/T$ will be of order one; to achieve the critical Rayleigh number one needs a system with a length of about 35 λ (for slip boundaries and an aspect ratio of one). Because the DSMC method needs about 10 particles per computational cell and that the cells be no larger than about a mean free path, we need to use over 12,000 particles. This is to be compared with Molecular Dynamics where convection may be observed in a system as small as 1500 particles.[32]

I ran a large DSMC simulation with 50,000 particles in a square box $50\lambda \times 50\lambda \times 1\lambda$ in size (i.e. the aspect ratio equals one). The sidewalls are slip, insulating walls; a particle striking them rebounds elastically. The top and bottom walls are semi-slip, thermal walls; a particle striking them is thermalized in the directions perpendicular to the convective flow (y and z directions) while its velocity in the x-direction is unchanged. Similar boundary conditions were used by Mareschal and Kestemont in their MD simulations of Rayleigh-Bénard.[28]

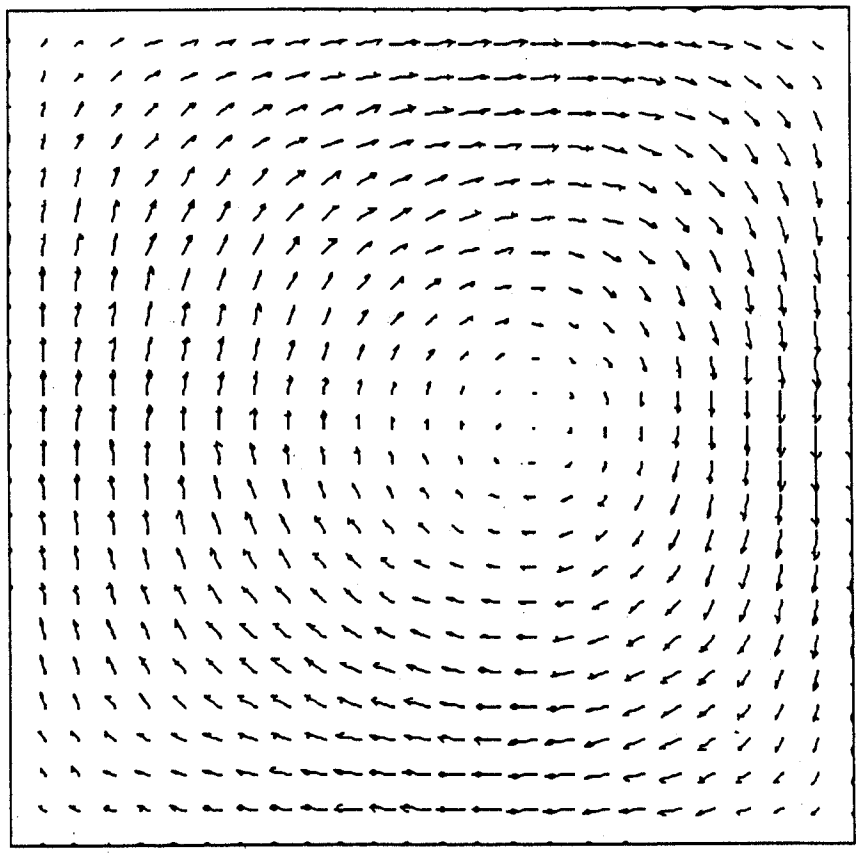

FIGURE 3. Velocity field from the DSMC simulation of the Rayleigh-Bénard problem. See the text for the parameters used in the simulation.

The top and bottom temperatures are 0.5 and 2.0, respectively [33]. Because of the temperature jump at the boundary, the effective boundary temperatures are .636 and 1.874. The gravitational field is g = 0.1; as mentioned above, the imposed gravitational field is chosen to maintain the density approximately constant. The Rayleigh number is approximately 1300, almost twice the critical Rayleigh number. The system was run for about 200 million collisions; a noticeable roll developed after about 40 million collisions. After about 150 million collisions the system reached a steady state and statistics were accumulated over the last 40 million collisions. On a SUN 4/260 the program processed about 2.2 million collisions per CPU hour.

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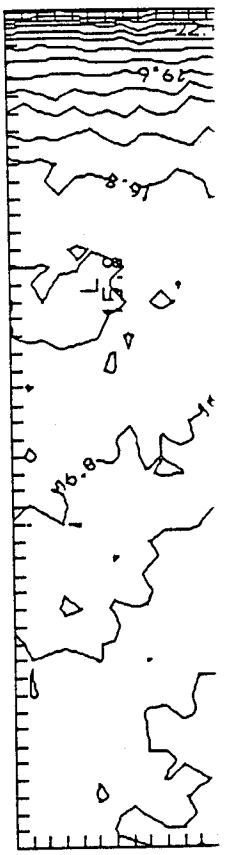

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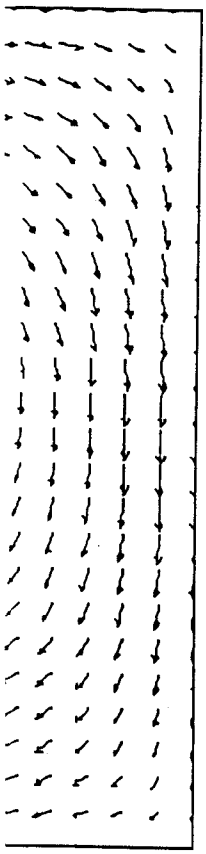

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The observed average flow field is illustrated in Figure 3. Note that the roll is not symmetric since the density is lower in the hot, rising fluid and higher in the cold, falling fluid. Conservation of mass requires that the hot stream be wider than the cold stream. [34] The fluid is highly non-Bousinessq; this can be seen from the fact that the contours of constant density (Figure 4) look very different from the contours of constant temperature (Figure 5).

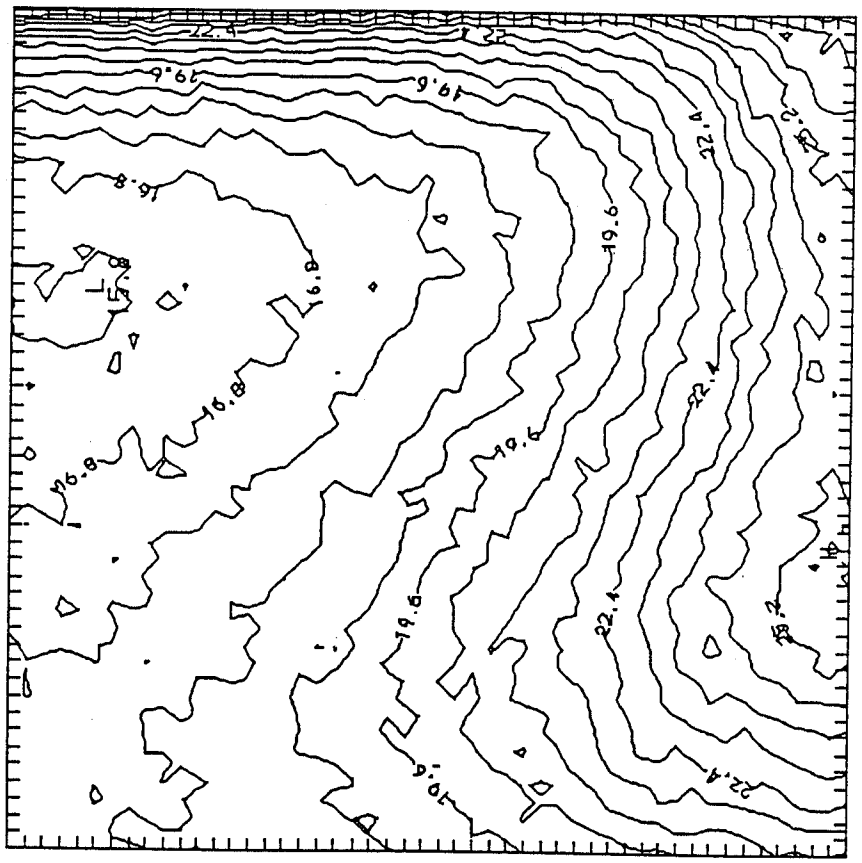

FIGURE 4. Contour plot of the density field from the DSMC simulation of the Rayleigh-Bénard problem. Compare with Figure 5; note that the isotherms are not parallel to the isopycnal lines.

The full Navier-Stokes equations for a dilute gas were solved numerically and the resulting solutions agree closely with the average density, velocity and temperture fields measured in the DSMC simulation. My earlier DSMC runs showed only mediocre agreement with the Navier-Stokes integrator because: 1) I was using half as many particles (only 10 per cubic mean free path) and 2) I was only thermalizing the velocity in the direction perpendicular to the wall. This led to a considerable temperature jump at the wall. A complete discussion of these results will appear elsewhere.

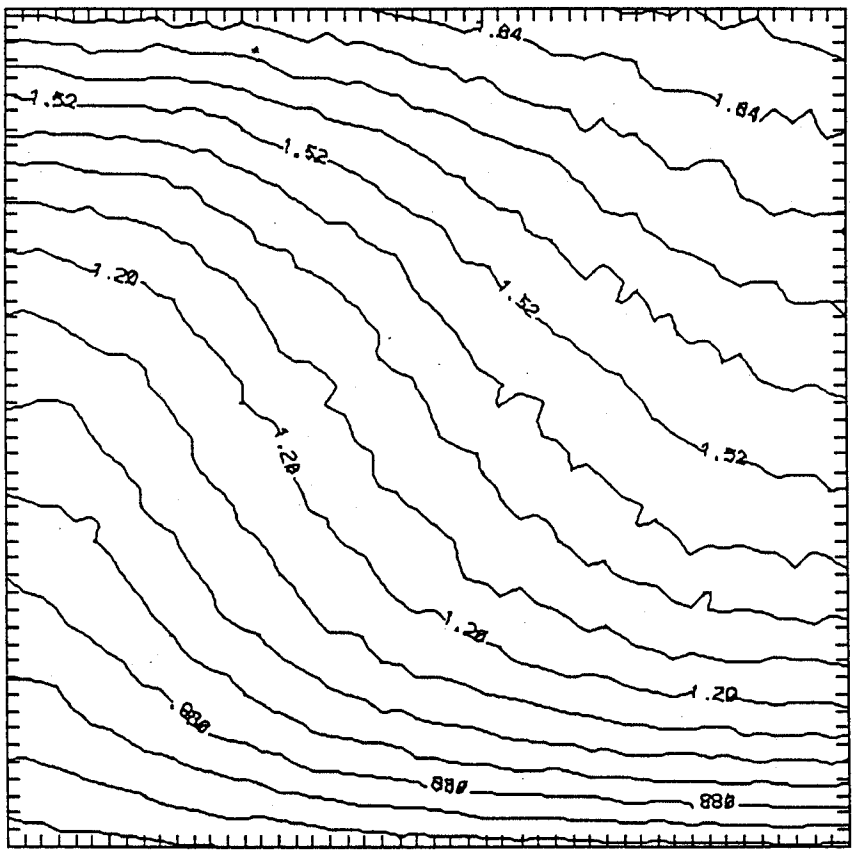

FIGURE 5. Contour plot of the temperature field from the DSMC simulation of the Rayleigh-Bénard problem. Compare with Figure 4; note that the isotherms are not parallel to the isopycnal lines.

The next step in this research is the study of the hydrodynamic fluctuations in the Rayleigh-Bénard problem. Due to the considerable computational effort involved in the simulations it is difficult to get reliable results to compare with theoretical predictions. Towards this end, Cecile Penland and I are beginning to use some of the sophisticated data analysis methods developed in climatology.

ACKNOWLEDGEMENTS

It was my pleasure to collaborate with Michel Mareschal, Malek Mansour, Florence Baras, John William Turner, Andreas Puhl and Eddie Kestemont on the work present in this paper. I wish to thank Prof. Prigogine for his encouragement and insightful suggestions. Special thanks to Malek Mansour for the use of his Navier-Stokes integrator and for his unsolicited remarks whenever my programs wouldn't run.

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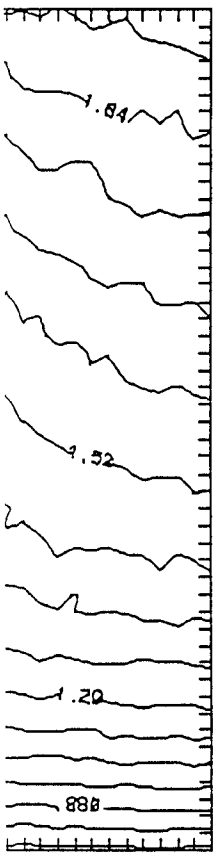

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33. The temperature is scaled such that at temperature T=1, the most probable molecular speed equals one. See reference 14 for more details.

34. I wish to thank Malek Mansour for this comment.

A SIMPLE MODEL OI

M. Malek I

Faculté des

Campus Pl

1 INTRODUCTION

For the theoret ideal laboratory for t scheme, etc... A nice a microscopic model, wit of the boundary condi performed which, with tures nevertheless som instance, hard sphere velopment of MD[1]. A the trajectory of a sing studied through MD[2].

With the ever g been focused recently c ior, such as shock wav bilities[5,6,7]. The main complex behavior, for w form. One example is near an instability thre for the case of Bénard i of magnitude between t hydrodynamics[8,9]. Th namic instabilities and 1971, many theoretical

Microscopic Simulations of Complex F
Edited by M. Mareschal, Plenum Press