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Alejandro Garcia
San Jose State University, alejandro.garcia@sjsu.edu

G. Lie
IBM Corporation

E. Clementi
IBM Corporation

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Fluctuating Hydrodynamics in a Dilute Gas

M. Malek Mansour,[a] Alejandro L. Garcia,[a] George C. Lie, and Enrico Clementi
IBM Corporation, Kingston, New York 12401
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Hydrodynamic fluctuations in a dilute gas subjected to a constant heat flux are studied by both a computer simulation and the Landau-Lifshitz formalism. The latter explicitly incorporates the boundary conditions of the finite system, thus permitting quantitative comparison with the former. Good agreement is demonstrated.

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Fluctuating hydrodynamics is a stochastic formulation of standard fluid mechanics.[1] Spontaneous fluctuations of hydrodynamic variables are introduced into the transport equations by the addition of random components to the pressure and heat fluxes. Since these fluxes are not conserved quantities, the correlations between the random components are expected to be short ranged and short lived so that at hydrodynamic scales they are assumed to be Dirac-delta correlated. Their strengths are then chosen to yield the correct equilibrium thermodynamic fluctuations as derived from the Gibbs distribution. Nowadays there are various ways to derive the Landau-Lifshitz fluctuating hydrodynamics and there is general agreement about its validity, at least in near-equilibrium situations.[2]

Extension of the theory to nonequilibrium systems leads to predictions of the asymmetry of the Brillouin lines in a liquid subjected to a constant heat flux.[3-6] Kinetic theory provides further support for these predictions.[7,8] Although these theoretical results are in agreement with light-scattering experiments,[9,10] the importance of the nonlinearities[11] and the influence of the boundaries[12] remain under discussion (see also the work of Tremblay[13]). In any case, the question arises as to the applicability of the fluctuating-hydrodynamics formalism to systems under strong nonequilibrium constraints. One way to address these questions is through particle simulations.

In this article we study a dilute hard-sphere gas bounded by two parallel plates located at $y=0$ and $y=L$, using both the fluctuating-hydrodynamics formalism and a Boltzmann Monte Carlo particle simulation. The plates act as infinite reservoirs so that by fixing their temperatures one can impose the desired temperature gradient across the system. As can be checked easily from the macroscopic hydrodynamic equations, the heat flux in the stationary state is constant and the velocity is zero [note that there is no instability because we do not include external fields (gravity) in our formulation[14]]. To study the fluctuations, we first linearize the fluctuating-hydrodynamics equations around the macroscopic stationary state. Since we are mainly interested in the influence of nonequilibrium constraints and since the particle simulations with which we compare our results employ periodic boundary conditions in the x and z directions, we shall limit ourselves to reduced quantities, defined as

$$\delta A(y)\equiv\frac{1}{S}\int_0^{L_x}dx\int_0^{L_z}dz\,\delta A(x,y,z), \tag{1}$$

where A is any dynamical variable and $S\equiv L_xL_z$ is the wall cross section (note that the reduced variables are in fact the zero-wave-vector values of the "parallel" Fourier components of the dynamical variables). It is easy to check that the reduced equations for the x and z components of the velocity fluctuations decouple from the rest and are not influenced by the constraint. We will therefore concentrate our attention on the remaining equations for the reduced mass density $\delta\rho$, the y component of velocity δv, and the temperature δT, which turn out to be

$$\partial\delta\rho/\partial t=-\partial\rho_0\delta v/\partial y, \tag{2}$$

$$\rho_0\frac{\partial\delta v}{\partial t}=-R\frac{\partial}{\partial y}(T_0\delta\rho+\rho_0\delta T)+\frac{4}{3}\frac{\partial\eta_0}{\partial y}\frac{\partial\delta v}{\partial y}-\frac{\partial s_{yy}}{\partial y}, \tag{3}$$

$$\tfrac{3}{2}\rho_0R\frac{\partial\delta T}{\partial t}=-\tfrac{3}{2}R\rho_0\delta v\frac{\partial T_0}{\partial y}-P_0\frac{\partial\delta v}{\partial y}+\frac{\partial}{\partial y}\left(\delta\kappa\frac{\partial T_0}{\partial y}+\kappa_0\frac{\partial\delta T}{\partial y}\right)-\frac{\partial g_y}{\partial y}, \tag{4}$$

where the subscript 0 indicates *local* macroscopic quantities, R the Boltzmann constant divided by the mass, η_0 the shear viscosity, κ_0 the thermal conductivity, and P_0 the pressure. s_{yy} and g_y are the random components of the pressure and heat fluxes, respectively, with the following covariances[1]:

$$\langle s_{y,y}(y,t)s_{y,y}(y',t')\rangle=\tfrac{8}{3}k_BT_0(\eta_0/S)\delta(y-y')\delta(t-t'), \tag{5a}$$

$$\langle g_y(y,t)g_y(y',t')\rangle=2k_BT_0^2(\kappa_0/S)\delta(y-y')\delta(t-t'),\quad\langle s_{y,y}(y,t)g_y(y',t')\rangle=0. \tag{5b,c}$$

In writing Eqs. (2)–(4) we have made use of the closure relations for a dilute gas, $P(\rho,T)=R\rho T$ and $e(\rho,T)=3\rho RT/2$ where e is the internal energy density. If the force between the particles is purely repulsive and obeys a power law, then the transport coefficients are only functions of temperature as[15] $\eta_0=\eta_c T_0^s$ and $\kappa_0=\kappa_c T_0^s$, so that in Eq. (4) we can set $\delta\kappa=\alpha\kappa_0\delta T/T_0$. For a hard-sphere gas, the exponent α is $\frac{1}{2}$ and, from Chapman-Enskog theory, $\kappa_c/\eta_c=15R/4$.

There remains the problem of specifying the boundary conditions for Eqs. (2)–(4). If we assume that the state of the walls is statistically independent with respect to the system, then the boundary conditions for δT are

$$\delta T(y=0,t)=\delta T(y=L,t)=0. \tag{6}$$

The boundary conditions for δv follow from the conservation of the total particle number; the continuity equation yields

$$\rho_0(y)\delta v(y)\,|_{\text{boundaries}}=0. \tag{7}$$

This completes our specification of the boundary conditions.

It may seem strange that we do not have to specify any boundary conditions for $\delta\rho$. From a physical point of view, this comes from the fact that the state of the wall can only constrain the temperature and velocity of the gas at the wall, whereas the behavior of the density close to the wall is entirely determined by the internal dynamics of the system. From the mathematical point of view, it can be shown that for any given initial condition $\delta\rho(y,0)$, $\delta\mathbf{u}(y,0)$, $\delta T(y,0)$, the boundary conditions for $\delta\mathbf{u}$ and δT are sufficient to specify completely the solution of the system.[16]

Because the coefficients and the noise are both space dependent and because we are dealing with a finite system, it is no longer possible to use elementary transform methods to solve the above fluctuating-hydrodynamics equations (for large enough systems, an expansion in the wave number of the gradient can still be used[4,17]). An alternative approach would be a direct computer simulation of the Langevin equations (2)–(4). This is a useful method in the study of fluctuating-hydrodynamics equations in two or three dimensions.[18] Here, instead, we construct the evolution equations for the correlation functions and numerically solve these equations by relaxation.[19] The first step in this approach is the evaluation of the static correlation functions, which can then be used to compute the dynamical correlation functions as an initial value problem. In this short Letter we deal only the static correlation functions.

To proceed further, we appeal to a very useful identity of the theory of stochastic processes[20]; namely, given that

$$dc_i/dt=f_i(c_1,\ldots,c_n)+F_i(t),\quad i=1,2,\ldots,n, \tag{8a}$$

where the f_i's are arbitrary analytic functions of c_i's, and $F_i(t)$'s are multi-Gaussian white-noise processes with covariances

$$\langle F_i(t)F_j(t')\rangle=Q_{ij}\delta(t-t'), \tag{8b}$$

then

$$\langle c_i(t)F_j(t')\rangle\equiv\begin{cases}\frac{1}{2}Q_{ij}, & t=t',\\ 0, & t<t'.\end{cases} \tag{8c}$$

For finite n, this identity is easily proved by writing the Fokker-Planck equation corresponding to (8a) and from it deriving the second-moment equations. A comparison with the second-moment equations derived directly from (8a) then leads to the relation (8c). These relations remain valid for $n\to\infty$ although, from a strictly mathematical point of view, some special care is needed in the continuum case. Using the relation (8c), one can derive the evolution equations for the equal-time correlation functions. If one discretizes the spatial derivatives, the steady-state solution may then be obtained by relaxation methods.

The primary purpose of this work is to compare the predictions of the fluctuating-hydrodynamics theory with particle-simulation results (the nonequilibrium effects we are considering are too subtle to be readily studied by laboratory experiments). Molecular-dynamics simulations prove to be too slow and have, thus far, yielded only qualitative results.[21] We rely, instead, on results obtained by a Boltzmann Monte Carlo simulation originally developed for rarefied gas studies by Bird[22] (some limitations of this method are discussed by Meiburg[23]). We have considered a system containing 20000 particles between two thermal plates 50 mean free paths (λ) apart and held at different temperatures. Here we report the results for a temperature gradient of 0.04° per mean free path. Distances and velocities are scaled by λ and the most probable speed, $(2k_BT/m)^{1/2}$, respectively; the

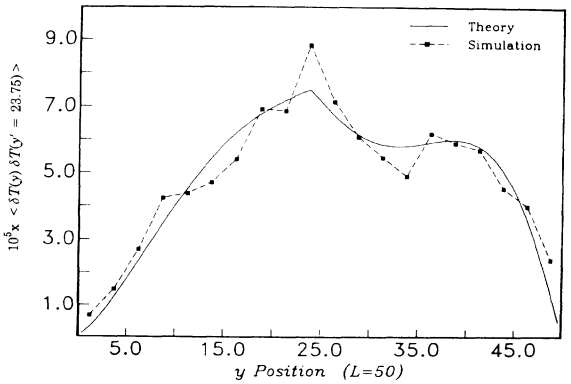

FIG. 1. Comparison of the temperature-temperature spatial correlation functions obtained from the fluctuating-hydrodynamics formalism (solid curve) and Boltzmann Monte Carlo particle simulation. Note that the local equilibrium delta-function contribution has been removed.

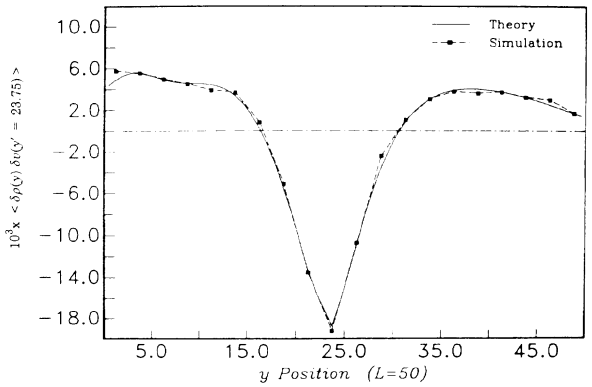

FIG. 2. Comparison of the density-velocity spatial correlation functions obtained from the fluctuating-hydrodynamics formalism (solid curve) and Boltzmann Monte Carlo particle simulation.

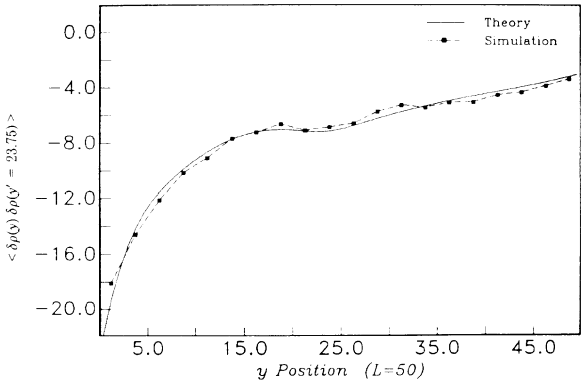

FIG. 3. Comparison of the density-density spatial correlation functions obtained from the fluctuating-hydrodynamics formalism (solid curve) and Boltzmann Monte Carlo particle simulation. Note that the local equilibrium delta-function contribution has been removed.

mass is set equal to 1 and k_B to $\frac{1}{2}$ (see the work of Garcia[24] for details). The statistical error is estimated to be about 10% for the temperature autocorrelation function (Fig. 1) and less than 5% for the other correlation functions (Figs. 2 and 3). The local equilibrium contributions to the correlation functions are removed and, as a result, larger errors are to be expected at the central peak. We note that there are no free parameters in the analysis; the solution of the correlation-function equations is entirely specified once the simulation parameters are given. These are, in the reduced units, $T(y=0)=1$, $T(y=L)=3$, and $\eta_c=5\pi^{1/2}\rho_{eq}/16$, where ρ_{eq} is N/L. Because of a small slip in the temperature profile, $T(y=L)$ is set equal to 2.95 in the hydrodynamic equations (2)–(4).

The program was run in parallel on two FPS264 array processors attached to the 1CAP2 system at IBM Kingston for 2×10^5 collisions per article. Figure 1 shows the temperature-temperature static correlation function which is clearly long ranged. Despite some statistical scatter, the simulation results show quite good agreement with the fluctuating-hydrodynamics results. The nonequilibrium contribution to the global temperature fluctuation (defined as the space average of the static temperature autocorrelation function) is found to be proportional to the square of the temperature gradient. Further studies with different system sizes indicate that for fixed temperature gradient it increases with the length of the system. These observations are in agreement with previous work on model systems.[25] In Figs. 2 and 3, we depict the density-velocity and density-density static correlation functions, respectively. Because of the conservation of the total mass, the static density autocorrelation function is strictly negative; its space integral compensates exactly for the local equilibrium contribution. Both curves show much better agreement with the fluctuating-hydrodynamics predictions. Similar agreement is found for all the static correlation functions investigated. For completeness, we are also studying the dynamic correlation functions and are experimenting with molecular-dynamics simulations for dense systems using more realistic interaction potentials.

Our present observations suggest that the fluctuating-hydrodynamics equations are valid at length scales of a few mean free paths even in the presence of strong nonequilibrium constraints, at least for a dilute gas (see also Alder and Wainwright[26]). Had the data shown otherwise then a strictly microscopic formulation in kinetic theory would have been the only recourse. We consider this a fortunate development which will encourage future work in this direction. For instance, recent large-scale molecular-dynamics results demonstrate the feasibility of the observation of macroscopic hydrodynamic phenomena such as vortex formation and shedding past an obstacle[23,27,28] in particle simulations. The next major step, of course, will be the study of fluctuations near hydrodynamic instabilities by computer simulations. Our results indicate that fluctuating hydrodynamics provides a promising way to tackle this problem, at least before and, probably, close to the instability.[14]

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[a]Permanent address: Service de Chimie Physique II,

Université Libre de Bruxelles, Campus Plaine, C.P. 231, 1050 Bruxelles, Belgium.

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