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The Bird algorithm is a computationally efficient method for simulating dilute gas flows. However, due to the relatively large transport coefficients at low densities, high Rayleigh or Reynolds numbers are difficult to achieve by this technique. We present a modified version of the Bird algorithm in which the relaxation processes are enhanced and the transport coefficients reduced, while preserving the correct equilibrium and nonequilibrium fluid properties. The present algorithm is found to be two to three orders of magnitude faster than molecular dynamics for simulating complex hydrodynamical flows.

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Microscopic simulation of fluids is a promising tool for understanding the onset of instabilities in nonequilibrium systems [1,2]. Complex hydrodynamic phenomena such as shock waves [3], flow past an obstacle [4], and Rayleigh-Bénard instability [5,6] have been successfully simulated through molecular dynamics (MD) simulations. The next challenge is the microscopic simulation of high Reynolds number flows, yet traditional MD simulations of such flows seem beyond the reach of present day computers.

One possibility is to consider dilute systems for which there exist algorithms that are much faster than comparable MD simulations. The most efficient algorithms are undoubtedly the lattice gas cellular automata (LGCA) or the lattice Boltzmann (LB) method, which indeed allow the simulation of relatively high Reynolds number flows [7] and other instabilities [8,9]. Our main interest, however, is to use microscopic simulations as an "experimental" tool to check the validity of theoretical approaches or to account for cases where high-precision laboratory experiments are difficult or impossible to perform. This requires a method whose validity goes beyond that of macroscopic hydrodynamics, and which is also able to reproduce the correct fluctuation spectrum. This last requirement is crucial since most of the existing theories about turbulence are essentially statistical theories [10]. So far, it is not clear whether the LGCA or the LB method contains more information than the macroscopic Navier-Stokes equations [11].

A more suitable method which fully satisfies all the above requirements, is the Bird algorithm designed to simulate the Boltzmann equation [12]: It agrees with all experimental data concerning rarefied gas dynamics, including peculiar situations where hydrodynamics fail; it is in perfect agreement with Landau-Lifshitz fluctuating hydrodynamics, even in extreme nonequilibrium conditions [13]; and it reproduces correctly the data obtained through hard sphere molecular dynamics in strong shock wave conditions (Mach number >100), a domain far beyond the validity of Navier-Stokes equations [14]. Yet, although the Bird algorithm runs about three orders of magnitude faster than MD in comparable situations, its global performance is significantly reduced when applied to the simulation of high Reynolds number flows. There are two major reasons that this occurs.

First, one is typically interested in simulating strictly subsonic flows; otherwise, the shock waves generated in the system make the analysis and the theoretical interpretation of the results extremely difficult. The Reynolds number is proportional to the mean flow velocity and it is therefore limited by the value of the sound speed. Since the latter is about three times smaller in dilute gases than in liquids, the maximum possible value of the Reynolds number in subsonic flows remains also about three times smaller in dilute gases, and there seems to be no way to increase this ratio.

Second, the Reynolds number is inversely proportional to the kinematic viscosity coefficient, and the latter proves to be significantly larger in dilute gases than in dense fluids. This property is a serious handicap which clearly limits the usefulness of the Bird algorithm in simulating high Reynolds number flows, unless one can find a way to modify the values of the transport coefficients. In other words, the question arises: is it possible to set up an algorithm allowing the simulation of a fluid with adjustable transport coefficients, while remaining strictly within the Boltzmann limit? The main purpose of this Brief Report is to show that indeed such an algorithm can be constructed.

The method we proposed is directly based on the Bird algorithm. To understand its basic steps, we first summarize Bird's method: As with usual molecular dynamics methods, the state of the system is the set of particle posi-

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tions and velocities,

$$\{\mathbf{r}_i,\mathbf{v}_i\},\ i=1,\ldots,N\ ,$$

where N is the total number of particles. The evolution of the system is integrated in time steps Δt, typically a fraction of the mean collision time for a particle. Within a time step, the free flight motion and the particle interactions (collisions) are assumed to be decoupled. The free flight motion for each particle i is computed as

$$\mathbf{r}_i(t+\Delta t)=\mathbf{r}_i(t)+\mathbf{v}_i(t)\Delta t\ ,$$

along with the appropriate boundary conditions. After all the particles have been moved, they are sorted into spatial cells, typically a fraction of a mean free path, λ, in length. A set of representative collisions, for the time step Δt, is chosen in each cell. For each selected pair, a random impact parameter is generated and the collision is performed. After the collision process has been completed in all cells, the particles are moved according to their updated velocities and the procedure is repeated as before.

The resulting velocity distribution function obeys a Boltzmann-like equation [15]:

$$(\partial_t+\mathbf{v}\cdot\partial_{\mathbf{r}})f(\mathbf{v},\mathbf{r},t)=B(ff')\ , \tag{1}$$

where B represents a "model" collision operator. Since the free flight motions of the particles are computed exactly, the left hand side of (1) is exact. As a consequence, the nondissipative parts of the resulting hydrodynamic equations are also exact. The nature of the dissipative terms, on the other hand, depends directly on the way the collision processes are modeled. Since B conserves energy and linear momentum, these dissipative parts are necessarily in the form of the divergence of a dissipative flux. Therefore, no matter how B is modeled, the general structure of the hydrodynamic equations is preserved. The Bird algorithm also gives the correct transport coefficients, as predicted by Chapman-Enskog theory [16], and the correct fluctuation spectrum, as given by Landau-Lifshitz fluctuating hydrodynamics [13].

Suppose now that we modify B, while preserving its conservation properties. The resulting hydrodynamics will still be correct, except for the fact that the transport coefficients will no longer agree with their Boltzmann expressions. We shall take advantage of this in the following way.

The values of the transport coefficients in dilute gases are directly related to the balance between two processes: collisions and free flights. During the collision step, the velocity distribution approaches locally a Maxwellian distribution. The free flight motions of the particles, on the other hand, destroy this local Maxwellian. These conflicting processes determine the "relaxation time" τ of the system. The kinematic viscosity of the fluid is directly proportional to this relaxation time, as $\nu\approx\tau k_B T$, where k_B and T are the Boltzmann's constant and temperature, respectively. A similar relation holds for the thermal diffusivity coefficient. Note that, in general, τ is a function of the local temperature.

Now suppose that we increase the time step used for the collisions by a scaling factor S_c, while keeping it unchanged for the free flight step. The local velocity distribution function will then be S_s times "closer" to its local equilibrium value and, in turn, the resulting relaxation time and transport coefficients will also be S_s times smaller than their Boltzmann values. Of course, the effective time step allowed for the collisions $S_s\Delta t$ cannot exceed the mean collision time per particle, since otherwise a given particle will experience, on average, more than one collision per time step. To be consistent, we must choose an integration time step S_s times smaller than its normal value, which in turn increases the CPU time of the computer program by a similar amount. Moreover, since the mean free path λ is proportional to the relaxation time, decreasing the latter is equivalent to decreasing the former. In other words, we need more accurate spatial resolution that can be achieved by multiplying the number of elementary cells by S_s in each spatial direction, which in turn requires more memory space for the program. This is the price to be paid for this algorithm to be meaningful. Nevertheless, the "enhanced-relaxation" Bird algorithm still remains much faster than MD in comparable situations.

The above arguments are heuristic and need to be carefully checked. To do so, we have performed extensive computer experiments in a variety of near equilibrium situations. The conclusion was that the present algorithm preserves the thermodynamic properties of the system (equation of state, sound speed, etc.), it reproduces the correct equilibrium fluctuation spectrum, and the transport coefficients are indeed reduced by the scaling factor S_s [17]. Here, we concentrate on nonlinear hydrodynamic regimes in the case of the Rayleigh-Bénard instability.

In a fluid heated from below, the transition from conductive to convective behavior is governed by the Rayleigh number Ra, defined as [18]

$$\mathrm{Ra}=\frac{\alpha\Delta T g L_z^3}{\nu\lambda_T}\ , \tag{2}$$

where L_z is the distance between the horizontal plates, λ_T the thermal diffusivity coefficient, α the thermal expansion coefficient, g the acceleration field, and ΔT the temperature difference between the lower and upper horizontal walls. The critical value of the Rayleigh number is about 660 for stress-free boundary conditions [6].

For the simulation, we consider an assembly of 40 000 particles confined in a box whose dimensions are set to $L_y=1\lambda$, $L_z=L_x=10\lambda$. The fluid is subjected to an adverse external gravitational acceleration g in the z direction. To ensure a nearly uniform spatial distribution of particles, we set $g=k_B\Delta T/m$. Nonequilibrium constraints are imposed by stochastic horizontal walls that act as thermal reservoirs: Each time a particle strikes a horizontal wall, it is reinjected into the system conserving its tangential velocity component, while having its normal velocity component sampled from an equilibrium distribution at the wall's temperature. This thermalization mechanism simulates optimally stress-free boundary conditions [5,6]. The vertical sides are modeled as specularly

reflecting walls (insulating stress-free boundary conditions). The wall temperatures are set so that $\Delta T/T_a = 1$, where T_a is the average temperature. For $S_s = 1$ (the normal Bird algorithm), the system is below the convection threshold since the Ra$\cong$65.2. Since $\nu, \lambda_T \propto 1/S_s$, using $S_{sc} = 10$, we have Ra$\cong$6520, well above its critical value.

After a short transient time of about 1000 collisions per particle (CPP), the system evolves to a stable convective roll. After a relaxation period of 10 000 CPP, statistics are taken over ten sequences of 20 000 CPP. This procedure allows an estimation of statistical errors; measured velocities and temperature are accurate to about 8%.

To verify our results from the Bird simulation, we compare them with those obtained from the Navier-Stokes equations. Because of the complexity of this problem (non-Bousinesq fluid, state-dependent transport coefficients, mixed boundary conditions, etc.), we solve the full macroscopic hydrodynamic equations numerically using standard techniques [6]. Figure 1 illustrates the x component of the velocity profile versus z. The convective velocity profile measured in the enhanced-relaxation Bird simulation is in quantitative agreement with hydrodynamic theory. The same quantitative agreement is observed for all other hydrodynamic variables (temperature, pressure, etc.).

One important question remains: What are the advantages of using the present algorithm for the study of hydrodynamic instabilities, instead of traditional hard disk or hard sphere MD? The answer depends very much on the sensitivity of the simulated flows to the compressibility of the fluid since, as discussed earlier, the flow must remain strictly subsonic.

Best performances are obtained in situations where the sound speed is difficult to reach, such as, for example, in buoyancy induced convections (Rayleigh-Bénard instability). Detailed analysis shows that in this case the enhanced-relaxation Bird algorithm runs about three orders of magnitude faster than the corresponding hard disk MD. For instance, reaching a Rayleigh number as high as 80 000 through hard disk simulation requires about 15 days of CPU time on an IBM 3090 supercomputer [19]; the enhanced-relaxation Bird algorithm simulation of the same situation requires only an hour of CPU time on a typical RISC workstation.

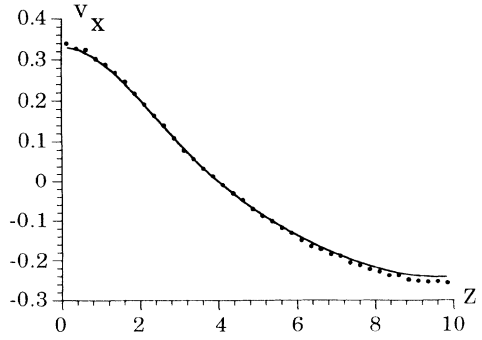

FIG. 1. Horizontal component of the velocity profile (scaled by the sound speed) at $x = L_x/2$ versus z (scaled by the mean free path) for Rayleigh-Bénard convection. The solid circles are from Bird simulation with $S_{sc} = 10$; the solid line represents the solution of hydrodynamic equations.

For the simulation of shear-induced instabilities, the relative gain does not exceed two orders of magnitude in computational speed, mainly because in this case the sound speed can be reached quite easily. Moreover, the CPU time of the simulation increases very rapidly with the Reynolds number (as Re^{α}, with $4 > \alpha > 3$). We are thus still limited to flows with moderate Reynolds number (Re$\sim$20 in three-dimensional flows). We are presently using the enhanced-relaxation Bird method to study two-dimensional Kolmogorov flow [20] and have been able to observe the first few instabilities (Re$\approx$200) using modest computational resources (RISC workstations).

At this point one may ask: "Are there other modifications to the Bird algorithm that would allow us to reach higher Reynolds number?" There are various ways to increase the Reynolds number in a simulation: increase the flow velocity, increase the system size, or decrease the fluid viscosity. Since one is principally interested in subsonic problems, the flow velocity is limited by the sound speed. Unfortunately, since the Bird algorithm is based on the Boltzmann equation, we are restricted to simulating a dilute gas so the speed of sound is fixed by the ideal gas law and the ratio of the specific heats, $\gamma = C_p/C_v$.

One way to increase the system size is to increase the collisional cell size, holding the number of particles fixed. We know that, as a rule of thumb, collisional cells in the Bird algorithm should be a fraction of a mean free path in size. However, numerical experiments indicate that cells as large as two mean free paths may often give accurate results [21]. One might also obtain better computational efficiency by using a cell-subcell hierarchy [22]. While these techniques might increase the Reynolds number by one order of magnitude, their applicability still needs to be established.

It is also possible to increase the Reynolds number by finding other ways of lowering the transport coefficients. For example, alternative collision rules (which preserve conserve quantities) have been tried. Collision rules that violate detailed balance are found to dramatically reduce the transport coefficients. Unfortunately, they also produce unphysical artifacts in the flows [23]. Still, it may be expected that the various ideas presented above, combined with the enhanced-relaxation Bird algorithm, will eventually lead to new ways of efficient simulation of high Reynolds number flows at the microscopic level.

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