Use of the Boltzmann Equation to Simulate Lattice-Gas Automata

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We discuss an alternative technique to the lattice-gas automata for the study of hydrodynamic properties, namely, we propose to model the lattice gas with a Boltzmann equation. This approach completely eliminates the statistical noise that plagues the usual lattice-gas simulations and therefore permits simulations that demand much less computer time. It is estimated to be more efficient than the lattice-gas automata for intermediate to low Reynolds number $R \lesssim 100$.

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In this Letter we describe a simulation technique that can be used in some situations as an alternative to the lattice-gas automaton. The latter has been proposed as a new technique[1] for the numerical study of the Navier-Stokes equation and is based on the simulation of a very simple microscopic system, rather than on the direct integration of partial differential equations. Particles hop between the sites of a regular lattice and may have collisions only on the lattice sites. The collision process is deterministic and is controlled by a set of collision rules chosen so that, for instance, they conserve the number of particles and linear momentum. The transition from the microscopic to the macroscopic description of the lattice gas automata (LGA) is done by defining coarse-grained conserved densities, e.g., momentum density, obtained by averaging their microscopic equivalents on subregions of the lattice. The presence of microscopic conservation laws then reappears in the macroscopic dynamic as hydrodynamic modes and, if the underlying regular lattice has been properly chosen, one can argue that the form of the hydrodynamic equations is very similar to that found for simple fluids.

Many authors[2-4] have tested the validity of the lattice-gas scheme by simulating specific flow configurations that are analytic solutions to the Navier-Stokes equation. All these simulations required a rather massive use of computer resources because the microscopic dynamic of the LGA is intrinsically noisy[5,6] and to obtain reasonably resolved coarse-grained densities it is necessary to average over a combination of large subregions of the lattice, long times, and numerous initial conditions.

We would like to point out that the hydrodynamic properties of the lattice-gas automata can be determined very efficiently by using an alternative technique. What we suggest is to translate the LGA into a related Boltzmann model. The Boolean site populations of the LGA then become real numbers between 0 and 1 representing their average value and their time evolution controlled by a Boltzmann equation (BE)[7] derived from the lattice-gas model.

It is clear that what we have just described is not equivalent to the LGA since, by factorizing the LGA collision operator on the one-particle distribution functions, we completely neglected all the effects due to the correlations between the particles. Nevertheless, the Boltzmann model shares many features with the LGA. In particular, it has the same hydrodynamic behavior, even though some details, such as the transport coefficients, can be slightly different. This implies that basically all the peculiarities of the LGA, e.g., the lack of Galilean invariance, are inherited by the BE. Also, the Boltzmann gas is, like the LGA, a stable numerical scheme since its time evolution satisfies an H theorem.[8] We note that the BE approximations of the LGA are very common in the literature.[8-10] However, their use was previously restricted to analytical calculations and not to actual numerical simulations.

There is a feature of the LGA that it is not shared by the Boltzmann model, namely, the noise. In the latter approach we directly study the time evolution of the mean values of the one-particle distribution functions and we therefore completely bypass the statistical averaging step needed in the LGA simulations. We may then obtain accurate results even when using small lattices (say 8×8 sites in two dimensions).

The Boltzmann scheme is obviously applicable to any lattice-gas automaton and in particular it can be used for the testing of 2D and 3D models. For the purpose of the present Letter we constrain ourselves to the case of the original 2D lattice gas on an hexagonal lattice. In this model, the particles have momenta chosen from the vector

$$\mathbf{C}_a = \left[\cos\left(\pi\frac{a-1}{3}\right), \sin\left(\pi\frac{a-1}{3}\right)\right], \quad a = 1, \ldots, 6.$$

The microscopic densities corresponding to the number of particles and momentum conservation are, respectively, $n(\mathbf{r},t) = \sum_a f_a(\mathbf{r},t)$, and $g_l(\mathbf{r},t) = \sum_a C_{a;l} f_a(\mathbf{r},t)$, where $f_a(\mathbf{r},t)$ is the Boolean population field that indicates the presence (1) or absence (0) of a particle moving with momentum $\mathbf{C}_a$ at site $\mathbf{r}$ and time step t, and we use $i,j,k,l,\ldots$ to label Cartesian coordinates. The time evolution of the particle populations can then be

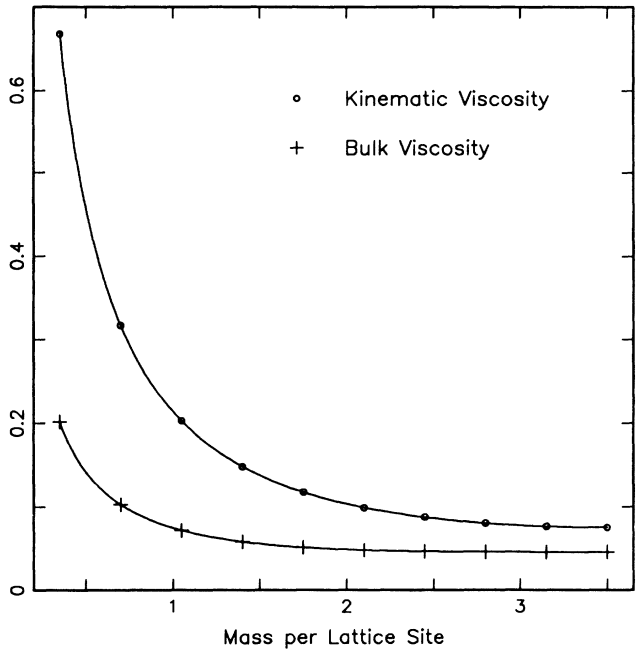

FIG. 1. Transport coefficients as a function of the density for the Boltzmann gas. The data were obtained by relaxation measurements. The wavelength of the waves used is $L=64\sqrt{3}$. The set of rules used is the FHP-III defined in Ref. 2. The solid lines are the Chapman-Enskog values.

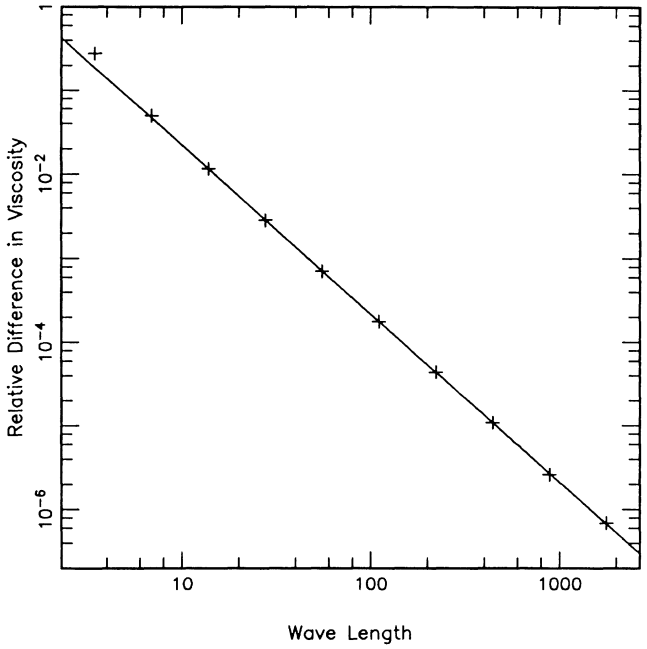

FIG. 2. Relative discrepancy between the measured kinetic viscosity and the corresponding Chapman-Enskog value as a function of the shear wave wavelength L. The straight line is fitted on all the points except the two leftmost. The slope of the fit is -2.009. It is not exactly -2 because of higher-order corrections for the very small wavelength. These corrections are particularly evident for the first two points.

written, with the assumption that the particles first hop in the direction of their velocities and then they are subject to collisions, as

$$f_a(\mathbf{r},t+1)=f_a(\mathbf{r}-\mathbf{C}_a,t)+T_a(\{f_b(\mathbf{r}-\mathbf{C}_b,t)\}),$$

where T_a is the microscopic collision operator,[8] that is the Boolean algebra expression that corresponds to the chosen set of collision rules. In the BE approximation of the previous equation we understand $f_a(\mathbf{r},t)$ as a continuous variable between 0 and 1 and replace the Boolean operations in T_a with the appropriate arithmetic operations.

The theory of the Boltzmann equation for the lattice gas has been extensively treated in Refs. 8–10 and various authors[2,8] have given formulas for the transport coefficients based on the Chapman-Enskog[7] approximation. As a straightforward application of this new tool we computed the values of the bulk and kinematic viscosities of the Boltzmann gas by studying the decay of shear and sound waves of wavelength L. The set of collision rules used is FHP-III described in Ref. 2. This set includes all the possible collisions that conserve a number of particles and their total momentum. Because of the simulation geometry we can suppress one of the dimensions and run on a $L\times 1$ lattice. The simulation data are then compared with the Chapman-Enskog predictions indicated as solid lines in Fig. 1. The agreement between the two, better than one part in 10^3 for $L>40$, is not surprising, but it is interesting to note that we can obtain hydrodynamic behavior even with very small lattices. To support this claim we plot in Fig. 2 the discrepancy between the kinematic viscosity measured from the simulation and ν_{CE}, the Chapman-Enskog prediction, as a function of L. In this plot the average number of particles per site is $\rho=2.1$. The above defined discrepancy is proportional to $(\lambda/L)^2$, where λ is the mean free path of the gas, as can be easily predicted, but the interesting result is that the simulation gives values of ν accurate to better than 5% even for a lattice as small as 4×1.

The last plot we present is a test of the rotational symmetry[11] of sound waves in a small system of 33×33 lattice sites with average density $\rho=2.1$ particles per site. We increase the mass of the central site, the "origin," by less than 1%. A "cylindrical" sound wave then develops.[12] In Fig. 3 we plot the resulting radial density profile after 16 microscopic time steps. The solid line is obtained by our interpolating with a cubic spline, the density measured along a straight line passing through the origin in the direction of one of its nearest neighbors. We then plot a symbol for each site of the lattice at the appropriate mass density and radial distance from the origin. As expected, all the symbols lay very close to the solid line. The short-wavelength oscillation close to the

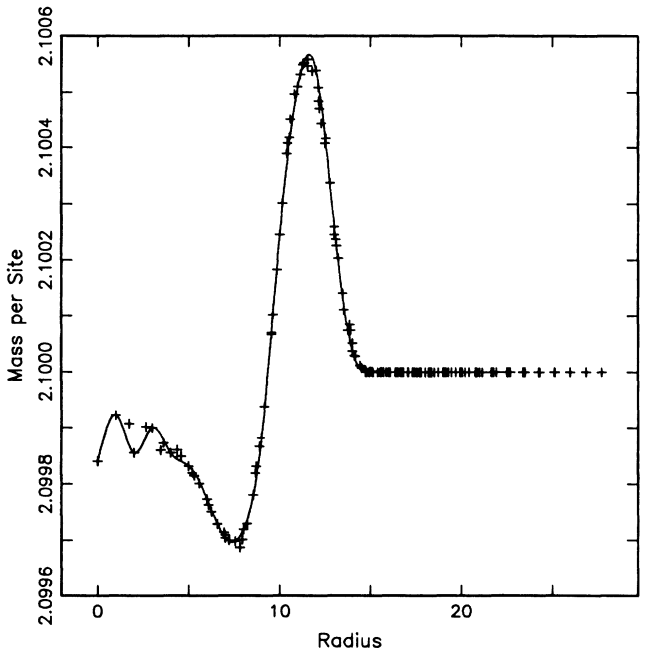

FIG. 3. Radial density distribution of a cylindrical sound wave 33×33 lattice sites, 16 time steps after initial disturbance, see text. The solid line is obtained by our interpolating the mass density along a line passing through the site initially excited and one of its nearest neighbors. For each site of the lattice we mark a point corresponding to its radial distance from the origin (the locus of the original disturbance) and its mass density.

origin is due to a peculiar lattice effect, common to both the LGA and the Boltzmann model, which has very interesting consequences that we will discuss elsewhere.[13,14]

Unfortunately the Boltzmann scheme described here does not seem to be an optimal tool for the study of highly turbulent flows. In fact, let us consider the simulation, using the LGA, of an incompressible, two-dimensional, flow of Reynolds number R. We require resolution η in the velocity field and spatial resolution χ. If we introduce L, v, ν, and l as, respectively, a characteristic length, velocity, viscosity, and linear dimension of the coarse-graining subregions, we have $R=vL/\nu$,[15] $\eta > \delta v/v$, and $\chi > l/L$. Since the flow is assumed to be incompressible we also have the constraint $L > Rv/c_s$, where c_s is the speed of sound of the gas. Using standard arguments we can evaluate

$$\eta > \frac{\delta v}{v} \approx \frac{C_0}{vl(\tau/\tau_s)^{1/2}}, \tag{1}$$

where $(C_0\rho)^2 = 3\rho(7-\rho)/49$ is the variance of the momentum fluctuation per site[6] while τ/τ_s is the number of independent samples obtained by averaging over a time τ. Assuming that the physical process relevant to the destruction of correlations in a region of size l is sound wave propagation, we get $\tau_s \approx l/c_s$. How large can τ be? It is the smallest resolved time scale $\tau = l/v$, and therefore $\tau/\tau_s \approx (c_s/v)LR^{-1}$. Substituting in Eq. (1) we get another constraint on L:

$$L > \left[\frac{C_0}{\eta\chi(vc_s)^{1/2}}\right]^2 R^{-1}. \tag{2}$$

The previous equation, together with the incompressibility constraint, defines a transition Reynolds number $R_1 = C_0/\eta\chi\nu$ below which the minimum size of the lattice is determined mainly by the requirement of velocity resolution rather than the required Reynolds number. We can now estimate the current amount of computer work, W_l, needed to perform the simulation. We have $W_l = L^2T$, where $T = L/v$ is the largest eddy turnover time. Therefore $W_l = L^4/\nu R$ and, for $R > R_1$,

$$W_l > \frac{1}{\nu}\left(\frac{\nu}{c_s}\right)^4 R^3, \tag{3}$$

while

$$W_l > \frac{1}{\nu}\left(\frac{\nu}{c_s}\right)^4 R_1^3\left(\frac{R}{R_1}\right)^{-5} \tag{4}$$

otherwise. The work required by the Boltzmann equation is instead, for all R,

$$W_b = \xi_w \frac{1}{\nu}\left(\frac{\nu}{c_s}\right)^4 R^3, \tag{5}$$

where ξ_w is the work needed to update a site of the Boltzmann lattice measured in units of LGA site updates. From Eqs. (3)–(5) we see that, for $R < R_w$, $R_w = \xi_w^{-1/8} R_1$ and it is more convenient to use the Boltzmann equation. An analogous calculation for memory space considerations gives the upper bound $R_s = \xi_s^{-1/4} R_1$ where ξ_s is the memory requirement per BE site in units of memory needed for a site of the LGA. At density $\rho = 2.1$ particles per site and for $\eta = \chi = 0.1$ we get $R_1 \approx 340$. In the simulations discussed in this Letter $\xi_w = 50$, $\xi_s = 32$ giving $R_w \approx 200$, $R_s = 142$. See Ref. 15. We have just shown that the BE is, for $R < R_s$, more efficient than the LGA. Also, for asymptotically large Reynolds numbers the standard numerical techniques are more economical[16] than the LGA. However, there are indications,[17] that the crossover point is much greater than R_s. Thus there is a window in the Reynolds number in which the LGA schemes are computationally superior.

In conclusion, we have presented a very simple tool for some hydrodynamic simulations and for the testing of the hydrodynamic properties of an LGA. This tool is particularly efficient for low Reynolds number simulations.

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[15]The Reynolds number defined here is not the relevant one for comparisons between the LGA (or the BE for what it matters) simulation and real simple fluids flows. In fact, because of the non-Galilean invariance of the LGA it should be multiplied by a density-dependent coefficient which is anyhow irrelevant to our comparisons since it afflicts both models.

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