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1989 Europhys. Lett. 9 663

(http://iopscience.iop.org/0295-5075/9/7/009)

EUROPHYSICS LETTERS 1 August 1989

Europhys. Lett., 9 (7), pp. 663-668 (1989)

Boltzmann Approach to Lattice Gas Simulations.

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(received 6 April 1989; accepted in final form 26 May 1989)

PACS. 47.10 – General theory.
PACS. 02.70 – Computational techniques.
PACS. 51.10 – Kinetic and transport theory.

Abstract. – An alternative simulation procedure is proposed for lattice hydrodynamics, based on the lattice Boltzmann equation instead of on the microdynamical evolution. The averaging step, used by the latter method to derive macroscopic quantities, is suppressed, as well as the associated fluctuations. The collision operator is expressed in terms of its linearized part, and condensed into a few parameters, which can be selected, independently of a particular collision rule, to decrease viscosity as much as desired.

Lattice gases have been proposed in recent years as a technique for the numerical simulation of hydrodynamics flows [1-3]. Since their collision and evolution rules are relatively simple and local, they are ideally adapted to the massively parallel computer architectures that are expected to dominate large-scale simulation in the coming decades and, since a global H-theorem can usually be proved from the kinetic-theory nature of the microscopic evolution of the particles, they are also intrinsically unconditionally stable. However, their memory and processing requirements are higher than those of other conventional numerical schemes, and increase faster with Reynolds number [4]. As a consequence, lattice gas methods are not considered at present an attractive numerical alternative. In this paper, we discuss a new approach [5] that removes some of these limitations, without removing the parallel nature of the schemes, restoring some of their competitiveness with respect to conventional numerics.

One of the main difficulties of lattice gas methods is the high level of fluctuations associated with the necessarily limited number of lattice points that can be used with the present computational resources [4]. Normalizing the length with the distance between nearest lattice neighbours (or its 3D projection for pseudo-4D models) [1-3], and the time with the elementary-particle flight time, the r.m.s. velocity fluctuation associated to a single lattice site is a constant, $O(1)$, which depends on the details of the model. Usually, the results are averaged over «boxes» of size λ, containing $n = \lambda^D$ sites, where D is the

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dimensionality of the space, decreasing the fluctuations by a factor of $n^{-1/2}$. Without any further loss of resolution, it is also possible to average over the flow residence time in a box, λ/Vg, where V is a macroscopic reference velocity for the fluid, and g is the standard velocity scaling factor for the lattice gas [1-3]. Converting the reference velocity to a Mach number, M, the result is a relative fluctuation level $v'/V \simeq \lambda^{-(1+D)/2} M^{-1/2}$.

Assume that we fix admissible values for the relative velocity fluctuations, v'/V, and for the spatial resolution λ, related to the smallest velocity and spatial scales that need to be resolved in the flow. The fluctuation estimate in the previous paragraph leads to a lower limit for the linear size, L, of the required lattice, $L > L_\lambda = k(\lambda/L)^{-(1+D)/D}(v'/V)^{-2/D} Re^{-1/D}$. The constant k depends on the details of the model, and on the particle density. It takes the value of 0.60 for the 2D FHP-III set of collision rules and 0.84 for the 24-particle pseudo-4D FCHC model, using in both cases the density resulting in minimum gas viscosity (see [1, 6] for the definition of these models). Also, the Reynolds number, Re, is related to M by the efficiency factor $R_* = Re/ML$, which is a measure of the inverse of the lattice gas viscosity and which depends only on the parameters of the microdynamical model. Since the Mach number is limited to low values, $M < M_0 = 0.3 \div 0.4$, by the requirement that the macroscopic behaviour of the lattice gas approaches the Navier-Stokes equations [1], another lower limit to L is given by $L > L_0 = Re/R_* M_0$. Usually it can be assumed that $v'/V < Re^{-\alpha}/G$, and $\lambda/L < Re^{-\beta}/G$, where α and β depend on the type of flow and are discussed below, and G is a separation factor between the required solution and the estimates for the smallest flow scales. Taking into account that the amount of computational work increases like L^{1+D}, the extra work used to control the fluctuations is

$$W = (L_\lambda/L_0)^{1+D} = KRe^{(1+D)[2\alpha(1+D)(\beta-1)]/D}, \qquad K = (kR_* M_0)^{1+D} G^{(3+D)(1+D)/D}. \tag{1}$$

As an example, for 2D turbulent flows one can take [7], $\alpha = 1/2$, $\beta = 1/2$, and, using the FHP-III model, and $M_0 = 0.3$, $W \simeq 0.07 G^{15/2} Re^{-3/4}$. For 3D homogeneous turbulence [8], $\alpha = 1/4$, $\beta = 3/4$, and, for the FCHC model, $W \simeq 10 G^8 Re^{-2/3}$. In both cases, the extra work needed to suppress the fluctuations decreases with Reynolds number, and becomes unimportant as $Re \to \infty$ [3, 4]. However, there is a critical value Re_c, below which the smoothing of the fluctuations becomes expensive. In the two previous examples $Re_c \simeq 0.026 G^{10}$ for the 2D case, and $Re_c \simeq 33 G^{12}$ in 3D. These values are very sensitive to the value chosen for the separation parameter G, but, for moderate values $G = 2 \div 4$, Re_c become $27 \div 27\,000$ for 2D flows and $10^5 \div 5 \cdot 10^8$ in 3D. These are high Reynolds numbers, outside the range of present simulations, especially in 3D, and show that much of the present lattice gas work is limited by the necessity of smoothing the macroscopic variables.

One possible solution is to use the Boltzmann equation for the lattice gas, instead of following the microscopic evolution of its individual molecules. In this way, one deals with one-particle distributions functions, which represent ensemble averages over a conceptually infinite number of equivalent systems and which are, therefore, free from fluctuations (1). The Boltzmann equation for a lattice gas is [1]

$$N_i(\boldsymbol{x} + \boldsymbol{c}_i,\ t+1) = N_i(\boldsymbol{x},\ t) + \Omega_i(\boldsymbol{N}), \tag{2}$$

(1) Many interesting features of the lattice gas microdynamics may not be captured by the Boltzmann approach, including those associated with the decay of the correlations and the accompanying divergence of the Green-Kubo formulae in 2D (see *e.g.* [9-11]). However, insofar as the Navier-Stokes equations come out from the Boltzmann equation, under the conditions well established now by the general theory, this furnishes a convenient starting point for the description of macroscopic behaviour, *i.e.* to establish the basis for a numerical method for solving the Navier-Stokes equations.

where Ω is the collision operator, $0 \leqslant N_i \leqslant 1$, $i = 1, \ldots, b$, are the mean particle populations in the b possible states per lattice site, and $\boldsymbol{c}_i$ are the corresponding particle velocities. For 2D triangular lattices (FHP), $b = 6$ or 7, for 4D face-centred hypercubic ones (FCHC), $b = 24$ or 25. The variable $\boldsymbol{x}$ runs over the discrete lattice sites, and eq. (2) is a finite-difference equation that can be solved exactly, within the computer precision, by using the same procedure commonly applied to describe the microdynamical evolution of the gas particles, but replacing the Boolean variables that represent the presence or absence of particles, by the real-valued mean populations.

For small Knudsen and Mach numbers, the collision operator, $\Omega(\boldsymbol{N})$, can be simplified by expanding the distribution function about its local equilibrium value

$$\boldsymbol{N} = \boldsymbol{N}^{\mathrm{eq}} + \boldsymbol{N}^{\mathrm{ne}}. \tag{3}$$

$\boldsymbol{N}^{\mathrm{eq}}$ is the equilibrium distribution function, which depends only on the local values of the gas density ρ and velocity $\boldsymbol{v}$, and which can be expanded in powers of the velocity components as $\boldsymbol{N}^{\mathrm{eq}}(\rho, \boldsymbol{v}) = \boldsymbol{N}_0^{\mathrm{eq}} + \boldsymbol{N}_1^{\mathrm{eq}} + \ldots$, where $\boldsymbol{N}_j^{\mathrm{eq}}$ is $O(|\boldsymbol{v}|^j)$. The nonequilibrium part, $\boldsymbol{N}^{\mathrm{ne}}$, is, at most, $O(\boldsymbol{N}_2^{\mathrm{eq}})$ for the nonlinear hydrodynamics flow regime [1, 2]. Expanding now the collision operator, we get

$$\Omega(\boldsymbol{N}) = \Omega^{(0)} + \Omega^{(1)} \cdot (\boldsymbol{N}_1^{\mathrm{eq}} + \boldsymbol{N}_2^{\mathrm{eq}} + \boldsymbol{N}^{\mathrm{ne}}) + \frac{1}{2} \boldsymbol{N}_1^{\mathrm{eq}} \cdot \Omega^{(2)} \cdot \boldsymbol{N}_1^{\mathrm{eq}} + \ldots, \tag{4}$$

where $\Omega^{(j)} = \partial^j \Omega 1 / \partial \boldsymbol{N}^j$ are constants evaluated at $\boldsymbol{N} = \boldsymbol{N}_0^{\mathrm{eq}}$. By using the property $\Omega(\boldsymbol{N}^{\mathrm{eq}}) = 0$, eq. (4) can be simplified, without loss of accuracy, to

$$\Omega(\boldsymbol{N}) = \Omega^{(1)} \cdot (\boldsymbol{N} - \boldsymbol{N}_0^{\mathrm{eq}} - \boldsymbol{N}_2^{\mathrm{eq}}) + \ldots, \tag{5}$$

which involves only the first derivative of the collision operator. This derivative is a $b \times b$ matrix that, after the symmetries of the lattice and the mass and momentum conservation conditions are imposed, has only two independent parameters for 2D FHP models without resting particles, and three for either the 2D FHP models with resting particles or for the 24 particles FCHC pseudo-4D model.

The expressions for $\boldsymbol{N}_0^{\mathrm{eq}}$ and $\boldsymbol{N}_2^{\mathrm{eq}}$ can be found in [1, 2]. Being parts of the equilibrium distribution function, they depend only on the local density and velocity, defined in terms of $\boldsymbol{N}$ by

$$\rho = \sum_{i=1}^{b} N_i, \qquad \rho \boldsymbol{v} = \sum_{i=1}^{b} N_i \boldsymbol{c}_i. \tag{6}$$

In fact, $\boldsymbol{N}_0^{\mathrm{eq}}$ is a constant, equal to the common value, $d_0 = \rho_0 / b$, of the mean populations for all the states in the absence of motion. The solution of the Boltzmann equation proceeds as follows: given $\boldsymbol{N}(\boldsymbol{x}, t)$ for all the lattice sites at a given time, eq. (6) determines the local values for ρ and $\boldsymbol{v}$; next, $\boldsymbol{N}_2^{\mathrm{eq}}$ is computed and used in the simplified form of the collision operator, eq. (5), and the updating is completed by moving the resulting distributions to the neighbouring sites in the lattice, as implied by eq. (2). Note that no assumption is made about the form of the nonequilibrium part $\boldsymbol{N}^{\mathrm{ne}}$.

A global H-theorem exists for the Boltzmann equation with the simplified collision operator. The new entropy, expressed per lattice site, is

$$S = -\sum_{i=1}^{b} \hat{N}_i^2 + \frac{1 - 2d_0}{d_0 (1 - d_0)} \frac{D^2}{b^2 c^4} \sum_{i=1}^{b} \hat{N}_i \left(\sum_{j=1}^{b} \boldsymbol{c}_i \cdot \boldsymbol{c}_j \hat{N}_j \right)^2, \tag{7}$$

where $\hat{N}_i = N_i - d_0$. The equilibrium state, maximizing S with the constraints of mass and momentum conservation, is just the two-term expansion of the equilibrium distribution function for the complete Boltzmann equation, which was the same truncation used to obtain the simplified collision operator. This entropy does not change, globally, during the particle displacement phase of the lattice gas evolution, and increases during the collisions, provided that the eigenvalues of $\Omega^{(1)}$ verify the conditions $-2 < \sigma \leqslant 0$. In fact, the only part of S that changes during the collisions depends only on the nonequilibrium part of N, and is proportional to $-\sum_{i=1}^{b} N_i^{ne^2}$, which increases under the above eigenvalue conditions, except for strict equilibrium. It can also be shown that, both for 2D triangular and pseudo-4D FCHC lattices, the above conditions on the eigenvalues guarantee the local linear stability of the scheme, independently of any particular collision rules chosen.

To test these ideas, we implemented this method for two- and three-dimensional flows. In 2D, we chose the flow about a circular cylinder [12], over a range of Reynolds numbers, based on the diameter, between 10 and 80, with a Mach number smaller than 0.3, and leading either to stationary or to unsteady flows, depending on the Reynolds number. The simplified operator matrix was derived from the FHP-III set of collision rules, to allow comparisons with direct microscopic lattice gas simulations, which were also carried out. In both the steady and unsteady cases, the Boltzmann simulation agreed well with previously published experimental and numerical (finite difference) results. As an example of 3D flow we chose a symmetric delta wing at incidence, for Reynolds numbers up to several hundreds. The collision operator was derived from the optimal 24-particle FCHC set of rules [6, 13, 14]. The detachment and rolling-up of vortex sheets from the leading edge of the wing was observed.

It was found that (for an IBM 3090 vector computer) the computational cost of substituting the Boolean operations of the direct simulation by the floating point ones of the Boltzmann model, was a factor of 30 in computer time, and nearly the same one in computer storage. From eq. (1), taking into account this overhead factor, and using $G = 4$, the break-even Re_c for the Boltzmann method in the 2D calculation is about 300, suggesting that the use of the new procedure would be moderately advantageous even in this 2D case. In fact, it turned out to be much more important than this estimate suggests. In trying to determine the Reynolds number for the bifurcation to unsteadiness, the lack of spurious fluctuations of the Boltzmann model allowed us to approach the bifurcation in a controlled way, while, using the FHP model, it was impossible to maintain steady flows, even well below the bifurcation Re, due to the intrinsically high forcing from the microscopic fluctuations.

Actually, the Boltzmann approach and, in particular, the compact way in which the collision operator is represented in terms of a small matrix, simplifies the way to the optimization of lattice gas methods. The viscosity coefficient for the macroscopic evolution equation, which should be as small as possible to increase the Reynolds number attainable for a given lattice and Mach number, is a linear function of the inverse of a particular eigenvalue of the linearized collision operator [1], and vanishes when the eigenvalue is equal to -2. The optimization seeks to carry that eigenvalue as close to -2 as possible.

Usually, this is done through the manipulation of the collision rules. These are characterized by the matrix of transition probabilities between all the possible microscopic configurations at a given lattice site across a collision. These probabilities are nonnegative quantities restricted by the constraints of conservation of particle number and momentum, by the invariance under the symmetry group of the lattice, and by the conditions of normalization and semi-detailed balance [1, 2]. The eigenvalue determining the viscosity is a linear symmetric function of the probability matrix [1, 15], and the optimization can be reduced to a sequence of linear programming problems.

The optimization of the collision rules for the FHP 2D lattice model is discussed in [16], and that of the pseudo-4D FCHC lattice, in [6, 13, 14]. In both cases the optimum efficiency turns out to be moderate, $R_* < 10$. In the case of the FHP model, it is attained for a set of collision probabilities which can be implemented easily in microscopic simulations, but this is not necessarily so for other lattices. In general the optimal probabilities are fractional numbers, whose microscopic implementation implies a stochastic simulation for each collision, plus the storage of part of the transition matrix in the computer. This matrix can be very large (up to 2^{24} entries for current implementations of the FCHC model [6]), offsetting most of the storage advantage of the microscopic simulation scheme against the Boltzmann approach. In the latter the complete dynamics of the collision step is summarized in the much smaller collision matrix, $\Omega^{(1)}$, whose implementation complexity is independent of the detailed probability values. From the point of view of the use of lattice gases as a numerical simulation tool, this might turn out to be one of its greatest advantages.

Moreover, in the Boltzmann approach, it is possible to select the simplified operator matrix, $\Omega^{(1)}$, in a more general way, in terms of the reduced set of parameters described above, and independently of whether they are derivable from any particular set of collision rules. As long as the eigenvalue condition is satisfied, the H-theorem and the linear stability results guarantee that the scheme is numerically stable, and the extra freedom allows us to make the pertinent eigenvalue as close to -2 as desired, decreasing the viscosity coefficient and increasing the efficiency of the scheme beyond the optimum values attainable in the microscopic simulation. Of course, as the viscosity coefficient is decreased in this way, the flow becomes increasingly unstable, and more susceptible to truncation errors in the computation, but this is a real *physical* effect, as opposed to the instabilities found in classical numerical schemes.

In conclusion, the fluctuations, due to the limited number of lattice sites used in the averaging step of typical microdynamical lattice gas simulations, are suppressed by dealing with the one-particle distribution functions in the Boltzmann approximation. This procedure increases the amount of work and storage required per lattice site, and would be inadvisable in the limit of $Re \to \infty$, in which the scale separation renders fluctuations irrelevant [1, 3], if R_* were the same. Even in that case, for finite Reynolds numbers below some threshold, the new method presents advantages over direct microscopic simulations. In addition, in the new approach, the implementation of different collision rules can be replaced by the tuning of a few parameters in the simplified collision operator, increasing the flexibility of the method, and allowing much higher R_*, thus making the break even point as high as desired. Most of the advantages of direct lattice gas simulations are retained: suitability for massively parallel computations and easy handling of complex boundaries, as well as freedom from the truncation errors found in classical numerical methods, with only the Mach number and the Knudsen number determining how closely the Navier-Stokes equations are reproduced.

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The numerical simulations cited in the text were supported in part by IBM ECSEC in Rome, by the CIEMAT in Madrid and by IBM Spain.

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