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Continuous-velocity lattice-gas model for fluid flow

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Abstract. – A continuous-velocity lattice-gas model for fluid dynamics computations is constructed. The model combines a stochastic propagation scheme with a multi-particle collision rule that conserves mass, momentum and energy. It is demonstrated that the particle velocities have a Maxwell-Boltzmann distribution at equilibrium. A Chapman-Enskog analysis leads to the Navier-Stokes equation. Simulations support the results of the theoretical analysis and demonstrate that the model reproduces the observed behavior of flows for various values of the Reynolds number. The model also provides a means to investigate the statistical mechanical basis of macroscopic laws.

It is well known that idealized collision dynamics that preserves the mass, momentum and energy conservation laws can lead to the hydrodynamic equations on macroscopic scales. This is the strategy behind the the construction of the lattice-gas model of Frisch, Hasslacher and Pomeau (FHP) [1] for the simulation of the Navier-Stokes equations. In general, lattice-gas models provide stable simulation schemes that may be implemented efficiently on parallel machines. These models have been extended to investigate complex systems such as flow through porous media and phase separation phenomena [2-4]. Since lattice-gas models utilize a simplified description of phase space with discrete positions and velocities and employ an exclusion principle which restricts the number of particles at a site on the lattice, FHP lattice-gas dynamics has some peculiar features: the equilibrium distribution is Fermi-Dirac and energy relaxation processes cannot be treated since there is only a single speed in the model.

Other schemes have been devised to overcome some of these limitations. There exist multiple-velocity lattice-gas [5] and Boltzmann models [6]; these models extend the phase space by considering a finite, but sometimes large, collection of particle velocities on the lattice. There have also been extensive developments of lattice Boltzmann methods [7] which retain the discreteness of the phase space but work at the level of the real-valued particle distribution and are subject to the numerical instabilities of finite-difference schemes.

In this letter we construct a lattice-gas model which combines the stability of the lattice-gas automaton and the Maxwellian character of the particle velocity distribution. The method avoids some of the limitations of currently available lattice-gas models and can be extended easily to treat more complex systems than those considered here. We introduce a stochastic transition scheme and show that the macroscopic behavior of the system is described by the hydrodynamic equations: the Navier-Stokes equation for the velocity field and an energy evolution equation with an additional dissipative term. Several features distinguish the present model from conventional lattice-gas models [8]: the existence of a continuous vector velocity parameter, stochastic particle propagation and the abandonment of the exclusion principle so that there is no restriction on the number of particles per site. In view of these properties of the model, a statistical mechanical analysis allows one to establish an H-theorem with Maxwell-Boltzmann stationary distribution, the Onsager reciprocal relations and the Galilean invariance of the macroscopic equations.

We consider a system consisting of a set of particles on the sites of a regular lattice. Each particle is characterized by its position, mass, momentum and energy. There is no restriction on the number of particles at a site. The position of a particle is given by its discrete coordinates on the lattice and is changed during the streaming transformation which depends only on the particle momentum. The other attributes of a particle may be changed only during collisions with other particles or external fields. In the discrete space we may separate particles into groups according to their positions. The collision transformation acts on such groups independently and, in general, requires information on attributes of all particles residing at a site. It is natural to assume that collisions satisfying conservation laws may be built from a knowledge of the conserved quantities only.

The streaming operator moves the particles on the lattice stochastically with probabilities determined by the particle velocity. More specifically, propagation of a particle with velocity $\mathbf{v}$, expanded into a sum over lattice generators, $\mathbf{v} = \sum_i v_i \mathbf{e}_i$, is determined by a set of translations along the lattice generators given by integer random numbers $\xi_i(v_i)$: $\mathbf{n} = \sum_i \xi_i(v_i)\mathbf{e}_i$. To relate the particle propagation to the value of the particle momentum, we require that the expectation value of the particle displacement (in a unit time interval) is given by the particle velocity, thus constraining the choice of ξ_i:

$$E\big(\xi_i(v_i)\big) = v_i. \tag{1}$$

Symmetry requires that the random numbers ξ_i be identically distributed for all i. We employed random numbers with the following distribution:

$$P\big(\xi(v) = n\big) = \begin{cases} \{v\}\,, & n = [v] + 1, \\ 1 - \{v\}\,, & n = [v], \\ 0\,, & \text{else}, \end{cases} \tag{2}$$

where $\{v\}$ and $[v]$ are fractional and integer parts of v, respectively. It is straightforward to verify that eq. (1) holds for the above choice of random numbers.

The stochastic streaming rule using the choice of random numbers in eq. (2) has the following simple physical interpretation (cf. fig. 1). Consider an ensemble of uniformly distributed particles with identical velocities $\mathbf{v} = (v_x, v_y) = (1 + \{v_x\}, \{v_y\})$ in two dimensions. Deterministic streaming transfers particles from the shaded domain to the similarly shaded, translated domain. The probability of particle transfer to cell 1 is given by the area of intersection of cell 1 with the translated cell: $A = \{v_x\}(1 - \{v_y\})$. The same quantity gives the probability of

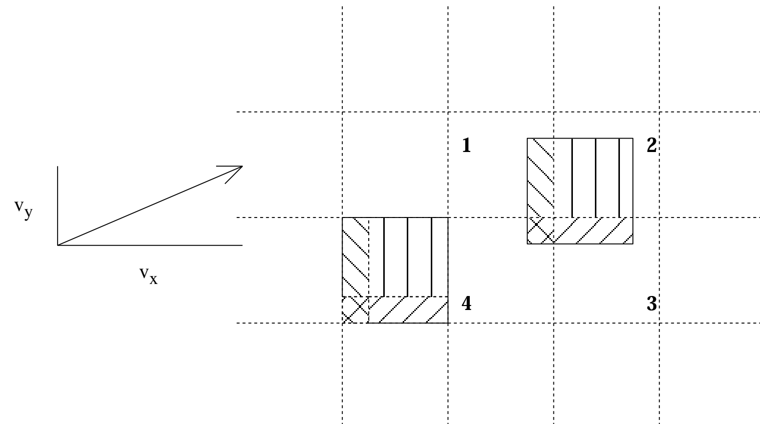

Fig. 1. – Pictorial representation of the streaming transformation in the stochastic model.

particle transfer using the stochastic streaming rule in eq. (2). The stochastic streaming rule yields, on average, the same result as deterministic streaming of an ensemble of particles.

A collision transformation is a process that acts on a group of particles at a site but does not change their positions. We considered a class of such schemes which depend only on gross quantities such as total momentum, energy and mass and an additional random rotation matrix. This class of collision rules still provides for very rich phenomenology. The schemes we use are based on the fact that rotations of the velocities in the frame moving with the velocity of the center of mass do not change the excess kinetic energy and thus the total energy. We implemented collision transformations according to the following formula:

$$\mathbf{v}_i' = \mathbf{V} + \sigma\big(\mathbf{v}_i - \mathbf{V}\big),$$

where $\mathbf{v}_i$ and $\mathbf{v}_i'$ are the pre- and post-collision velocities of the colliding particles, respectively, and $\mathbf{V}$ is the velocity of the center of mass of the colliding particles. The random rotation matrix σ may differ from site to site but is the same for all particles at a site. The values of the transport coefficients depend on the details of the collision model and, in the case of a monatomic ideal gas, are defined by the choices of collision matrices. The selection of a set of random rotations $\{\sigma_i\}$ that transform a vector $\mathbf{v}$ into an orthogonal vector, $(\mathbf{v}^{\mathrm{T}}, \sigma_i \mathbf{v}) = 0$, yields the smallest value of the shear viscosity coefficient in the Boltzmann approximation, a useful condition when one wishes to simulate high-Reynolds-number flows.

The system behavior under consecutive applications of the streaming and collision transformations in the Boltzmann approximation is described in terms of the 1-particle reduced probability distribution P_1. Action of the streaming operator on the probability distribution is

$$\mathcal{S}P_1(\mathbf{l}, \mathbf{v}) = \sum_{\mathbf{r}} W(\mathbf{r}, \mathbf{v}) P_1(\mathbf{l} - \mathbf{r}, \mathbf{v}), \tag{3}$$

where $\mathbf{l}$ and $\mathbf{r}$ are lattice coordinates and W is the transition probability matrix corresponding to random process defined by (2). The above formula is conveniently rewritten with the use of the cumulant expansion:

$$\sum_{\mathbf{r}} W(\mathbf{r}, \mathbf{v}) \exp[-\mathbf{r} \cdot \nabla] = \sum_{j=0}^{\infty} \frac{\mathsf{m}_j}{j!} \odot (-\nabla)^j = \exp\left[\sum_{j=1}^{\infty} \frac{\kappa_j}{j!} \odot (-\nabla)^j\right], \tag{4}$$

where $\odot$ denotes tensor contraction, m_j are the moments, κ_j, the cumulants and the second identity serves as a definition of the cumulant expansion. We use formal expressions for translation operators in space and in time as $f(\mathbf{r}+\mathbf{l}) = \exp[\mathbf{l}\cdot\nabla]f(\mathbf{r})$ and $f(t+1) = \exp[\partial_t]f(t)$, respectively. We may then rewrite (3) with the use of (4) in terms of a cumulant expansion in terms of powers of ∇:

$$\mathcal{S} = \exp\left[\sum_{j=1}^{\infty} \frac{\kappa_j(\mathbf{v})}{j!} \odot [-\nabla]^j\right]. \tag{5}$$

Thus, the evolution equation for the 1-particle probability density in the Boltzmann approximation takes the following form:

$$\exp[\mathcal{X}]P_1(\mathbf{l},\mathbf{v},t) = \mathcal{C}(P_1), \tag{6}$$

$$\mathcal{X} = \frac{\partial}{\partial t} - \sum_{j=1}^{\infty} \frac{\kappa_j(\mathbf{v})}{j!} \odot [-\nabla]^j,$$

where the collision operator $\mathcal{C}$ is defined by

$$\mathcal{C}(P_1)(\mathbf{v}_1') = \sum_{n=1}^{\infty} \frac{e^{-\rho}}{(n-1)!} \int \mathrm{d}\sigma \int \cdots \int \prod_{i=1}^{n} \mathrm{d}\mathbf{v}_i \delta\big(\mathbf{v}_1' - \mathbf{V} + \sigma[\mathbf{v}_1 - \mathbf{V}]\big) \prod_{i=1}^{n} P_1(\mathbf{v}_i),$$

and ρ is the expectation value of the particle number at a site. The Boltzmann H-theorem holds for this evolution and the stationary distribution of particle velocities is Maxwellian:

$$P_{\mathsf{m}}(\mathbf{v}) = \left(\frac{1}{2\pi T}\right)^{d/2} e^{-|\mathbf{v}-\mathbf{c}|^2/2T},$$

where T, d and $\mathbf{c} = \langle \mathbf{v} \rangle$ are the temperature in energy units, the system dimension and the expectation value of the particle velocity, respectively.

The Chapman-Enskog procedure applied to eq. (6) leads to a system of evolution equations for the expectations of the conserved quantities (*i.e.* density, momentum and energy). After a change of variables $\mathbf{w} = \mathbf{c} - D\nabla \log \rho$ (see below) we arrive at the following system of hydrodynamic equations:

$$\partial_t \rho + \nabla_i w_i \rho = 0, \tag{7}$$

$$\rho \partial_t w_i + \rho w_j \nabla_j w_i = -\nabla_i p - \nabla_j \pi_{ij}, \tag{8}$$

$$\rho \partial_t u + \rho w_i \nabla_i u = -p \nabla_i w_i - \pi_{ij} \nabla_i w_j - \nabla_i J_i - D\big[\rho \nabla_i w_j \nabla_j w_i + p \Delta \log \rho\big], \tag{9}$$

where we have used the equation of state $p = \rho T$ and the caloric equation $u = c_v T$ with $c_v = d/2$. The stress tensor and heat flux have the usual expressions:

$$\pi_{ij} = -\eta\big(\nabla_i w_j + \nabla_j w_i - \frac{2}{3}\delta_{ij}\nabla_k w_k\big) - \eta_v \nabla_k w_k \delta_{ij},$$
$$J_i = -\lambda \nabla_i T,$$

where η, η_v and λ are the shear and bulk viscosities and thermal conductivity coefficients, respectively.

As a consequence of the stochastic character of the streaming operator additional dissipative terms appear in the Chapman-Enskog analysis in the second order. Equations (7)-(9) are identical to the phenomenological hydrodynamic equations with the exception of the last term

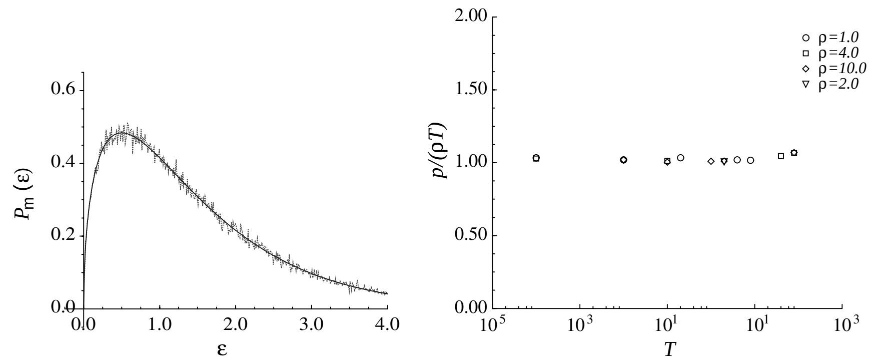

Fig. 2. – The left panel shows numerical and theoretical energy probability distribution densities. The solid line shows the Maxwell energy profile. The dotted line is obtained from numerical simulations. In the right panel the equation of state of the lattice-gas model is presented.

in eq. (9) which accounts for the additional contribution to the entropy production due to this effect. The additional terms come through averaging of the second cumulant $\kappa_2(\mathbf{v})/2$. We may show that this averaging yields a constant diagonal tensor $D\delta_{ij}$. Indeed, $\kappa_2(v_x)$ can be expressed as a sum of oscillatory functions:

$$\{v_x\}(1-\{v_x\}) = \frac{1}{6} - \sum_{k=1}^{\infty} \frac{\cos(2\pi k v_x)}{\pi^2 k^2}, \tag{10}$$

and only the first term gives a significant contribution when averaged over a smooth distribution. Thus, for a shifted Maxwell distribution and the values of parameters used in simulations the value of D is nearly independent of the average particle velocity and the correction to the zeroth-order approximation, $D = 1/12$, is of order 10^{-10}. The negligible value of the correction ensures the Galilean invariance of the resulting macroscopic equation.

The change of variables from $\mathbf{c}$ to $\mathbf{w}$ involving $D\nabla \log \rho$, which was used to obtain the Navier-Stokes equation, can be understood from the comparison of the first-order correction to deterministic streaming due to non-uniform density (cf. fig 1),

$$\left[\{v_x\} + \frac{1}{2}\kappa_2(v_x)\nabla_x \log \rho\right] \left[1 - \{v_y\} - \frac{1}{2}\kappa_2(v_y)\nabla_y \log \rho\right],$$

with the corresponding expression for stochastic streaming: $\{v_x\}(1-\{v_y\})$.

To study the stationary properties of the system we performed simulations of the lattice-gas model with the parameters $\rho = 6.0$ and $T = 1.0$, on a cubic lattice with dimensions $40 \times 25 \times 25$ with periodic boundary conditions giving a total of 1.5×10^5 particles. Initially particles were distributed uniformly in the domain. We assigned initial velocities to the particles from the set $\{\pm\sqrt{3}\mathbf{e}_x, \pm\sqrt{3}\mathbf{e}_y, \pm\sqrt{3}\mathbf{e}_z\}$. Thus, the initial energy distribution is given by a Dirac delta-function: $P_0(\varepsilon) = \delta(\varepsilon - 3/2)$. After several steps the energy distribution is thoroughly randomized. In general the rate of relaxation to the Maxwell distribution is high and the assumption of the local Gaussian character of the probability distribution holds. In fig. 2 (left panel) we show the energy probability distribution after 100 automation steps. The solid line depicts the Maxwellian energy distribution:

$$P_{\mathsf{m}}(\varepsilon) = \frac{2}{T\sqrt{\pi T}}\sqrt{\varepsilon}e^{-\varepsilon/T},$$

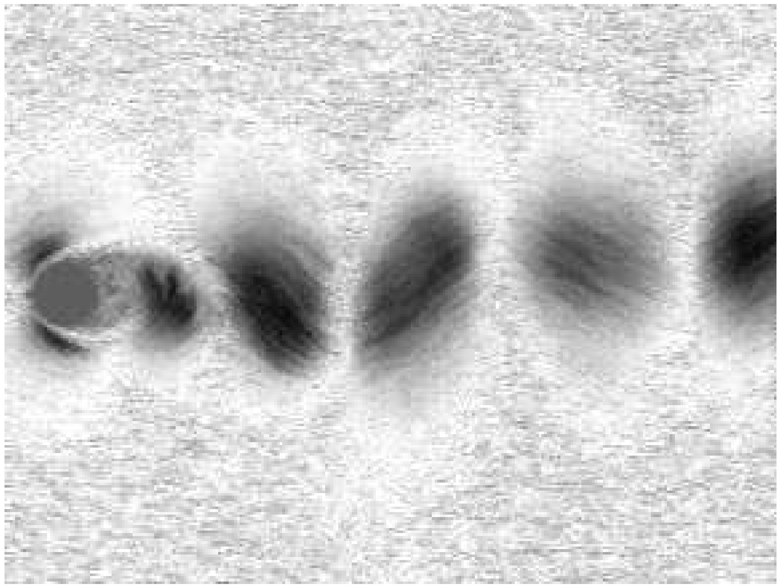

Fig. 3. – Simulation of a two-dimensional von Karman street. Shading indicates deviation of the y-component of the velocity field from the uniform flow.

while the dotted line represents the results of numerical simulations. There is good agreement between the theoretical prediction and the numerical results. The Maxwell distribution is spherically symmetric and, thus, leads to a symmetric pressure tensor.

We have verified that the equations of state of the model are those of an ideal gas. We carried out a series of simulations on a two-dimensional 100×100 square lattice for different values of the temperature and density. We imposed periodic boundary conditions in one direction, and no-slip boundary conditions in the other direction by inverting the velocity of a particle colliding with a wall. The pressure was computed as the total momentum transferred to a wall during an automaton step divided by the wall length. In fig. 2 (right panel) we present the results of simulations where we observe, as expected for a non-interacting gas, that the ratio $p/(\rho T)$ is independent of particle density and is equal to unity for a wide range of temperatures. The deviation from unity for large values of temperatures, when the velocity is comparable with the system linear dimensions, has its origin in the non-Boltzmann properties of the boundary collision rule.

In fig. 3 we present the results of simulations of von Karman streets for the flow past a disk with diameter $L = 44$ length units. The particle density is $\rho = 11$. In the figure, a fragment with dimensions 600×400 of a larger system (1200×400) is shown. At short distances from the object, a steady oscillatory flow is established after a transient time; however, a flow tail grows indefinitely until it occupies the entire system length. The system is driven at the $x = 0$ boundary where we assign values to particle velocities from the Maxwell distribution with $T = 1.5$ and $c_x = 0.5$. For the orthogonal scattering rule used in the simulations the viscosity coefficient is given by the expression

$$\eta = D\rho + \rho T \frac{1 - e^{-\rho}}{2(e^{-\rho} - (1 - \rho))}, \tag{11}$$

and thus for the simulation conditions the Reynolds number is $\mathrm{Re} = \rho c_x L/\eta \approx 94$. In experiments on fluid flow for such values of the Reynolds number the existence of von Karman streets is documented (for example, see fig. 4.12.6 of [9]).

The minimum value of the kinematic viscosity coefficient for our model is 1/12 which compares favorably with the best value 3/40 for the FHP-III model [8]. Moreover, due to lattice effects, the hydrodynamics of lattice gas models with a discrete set of velocities is described by the Navier-Stokes equations only in the small velocity limit ($\|u| \ll 1$). Thus, the present kinetic scheme allows one to study flows with higher Reynolds numbers compared to conventional lattice-gas models. Another advantageous feature of the model is the reduction of noise in measurement of the macroscopic densities. We may estimate the fluctuations in the momentum at a node for the present kinetic scheme and FHP-III model by $\langle\langle v_x^2\rangle\rangle = T/\rho$ and $\langle\langle v_x^2\rangle\rangle = c_s^2/\rho = 1/8.16$, respectively. Here ρ is the particle density at a node and c_{s} is the sound speed. For densities $\rho > 8.16$ we find a decrease in fluctuations of the velocity field with respect to the FHP-III model.

The present lattice-gas model provides a simple alternative scheme that accounts for the Maxwellian distribution of velocities and is easily extended to treat a wide class of physical and chemical problems. Our focus in this letter was on the documentation of the statistical mechanical and macroscopic properties of the model; the hydrodynamic flow calculations demonstrated the feasibility of simulating fluid flows. We remark that Green-Kubo formulae can be derived for the transport coefficients and as part of this derivation one may establish Onsager relations for the transport coefficients. The existence of flux-flux autocorrelation expressions for the transport coefficients provides an alternative route for the study of the transport properties of the system. For more complex systems or geometries that are difficult to treat by standard methods the inherent stability of the lattice-gas method can be an asset.

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