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How the Lattice Gas Model for the Navier-Stokes Equation Improves When a New Speed is Added

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Abstract. The original lattice gas automaton model requires a density-dependent rescaling of time, viscosity, and pressure in order to obtain the Navier-Stokes equation. Also, the corresponding equation-of-state contains an unphysical velocity dependence. We show that an extension of this model which includes six additional particles with a new speed overcomes both problems to a large extent. The new model considerably extends the range of allowed Reynolds number.

1. Introduction

It has been shown theoretically and numerically by Frisch, Hasslacher, and Pomeau [1] and others [2–4] that the lattice gas or cellular automaton (CA) is an effective numerical technique for solving Navier-Stokes equation and many other types of partial differential equations. The important properties of the local interaction between lattice gas particles and efficient memory utilization make the lattice gas an ideal method for massively parallel computers.

Most of the recent lattice gas studies of two-dimensional hydrodynamic problems are based on a hexagonal lattice in which the stress tensor is isotropic up to fourth order in the speed. Due to both the discreteness of the lattice and the limited range of velocities, the lattice gas model is not Galilean-invariant. The limitation of previous models to a single, nonzero speed causes two problems.

The first problem is that $g(n)$, the coefficient of the convective term in the Navier-Stokes momentum equation, is not equal to 1, as it should be in a physical system. This problem can be overcome by a density-dependent rescaling of time, viscosity, and pressure. This rescaling decreases the Reynolds number, requiring additional computational time and storage.

The second problem is that the equation-of-state depends on the macroscopic speed in the form $p = p_o(n,T) + p_1(n,T)u^2$. Here n is the particle density, T is the temperature, and u is the field speed. Recently it has been

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demonstrated that a nonzero value of p_1 in the equation-of-state can cause unphysical oscillations in kinetic energy decay [5]. All the previous models have p_1 directly proportional to $g(n)$. Thus $p_1 = 0$ implies $g(n) = 0$. This means that one cannot overcome these two problems simultaneously for previous models.

In this paper, we present one type of multispeed, multimass lattice gas model which allows $g(n) = 1$ and $p_1 = 0$ simultaneously. This model is an extension of the hexagonal lattice in two dimensions.

2. A general multispeed model

We consider, in general, N types of particles with different speed and mass. The spatial lattice is triangular. Many particles with different speeds can occupy the same point at the same time. When the particles occupy the same site, a momentum-conserving collision can occur and change the particle directions and speeds. Examples of such scatterings are shown in figure 1. We assume $N \geq 3$. Let m^σ be the masses of particles, $\vec{e}_a^\sigma$ the particle velocity, and ϵ_a^σ the kinetic energy for type σ particles; $\epsilon_a^\sigma = 1/2|\vec{e}_a^\sigma|^2$. σ denotes the type of particle, $1 \leq \sigma \leq$ N-1, and a indicates the velocity directions. $1 \leq a \leq 6$ for hexagonal lattices. $\sigma = 0$ indicates the rest particles. We have $\vec{e}_a^\sigma = |c^\sigma|(\cos\frac{2\pi a}{6}, \sin\frac{2\pi a}{6})$; here $|c^\sigma|$ is the speed of the σ particles. Thus we now consider a lattice gas model with more than two speeds.

Three kinds of collisions are allowed. The first kind of collision includes all collisions between the same type of particles. We may identify these collisions by the notation of 2R, 2L, 3S, and so on, used by Wolfram [6]. The second kind of collision includes collisions between different types of particles, but conserves the number of each type of particle. We can design more than three body collisions. The third type of collision rules allows a change of the number of each type of particle. All collisions can conserve mass, momentum, and energy.

Let the Boolean field $S_a^\sigma(\mathbf{x}, \mathbf{t})$ be the particle number of the σ type particle at site $\mathbf{x}$, and moment $\mathbf{t}$, with velocity $\vec{e}_a^\sigma$. $f_a^\sigma =< S_a^\sigma >$ is the ensemble averaged particle distribution. The kinetic equation for the particle distribution f_a^σ may be chosen to be

$$\frac{\partial f_a^\sigma}{\partial t} + \vec{e}_a^\sigma \cdot \nabla f_a^\sigma = \Omega_a^\sigma, \tag{2.1}$$

where Ω_a^σ represents the change rate of f_a^σ due to collisions.

We define the macroscopic mass density, n, fluid momentum field, $n\vec{u}$, and particle internal energy $n\epsilon$ by the following equations:

$$\sum_{a,\sigma} m^\sigma f_a^\sigma = n, \tag{2.2}$$

$$\sum_{a,\sigma} m^\sigma f_a^\sigma \vec{e}_a^\sigma = n\vec{u}, \tag{2.3}$$

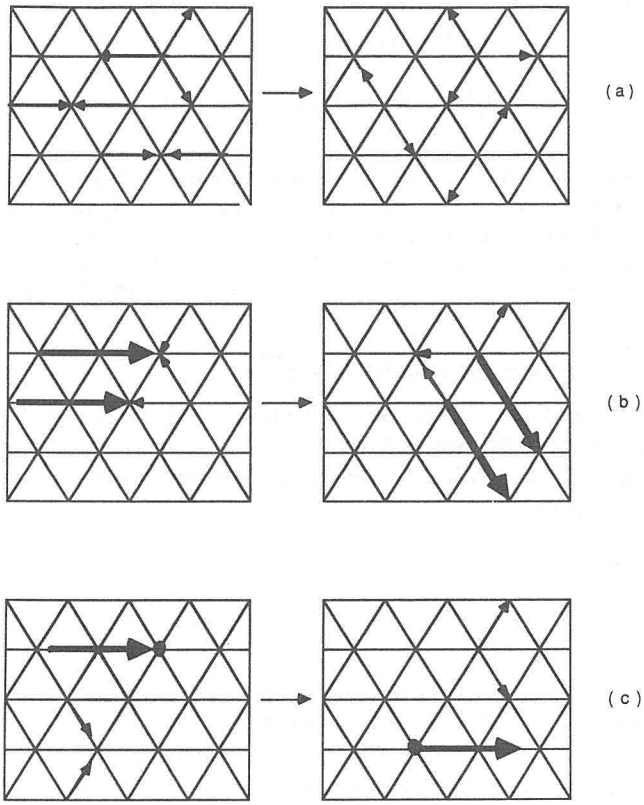

Figure 1: Some collision rules for the 13-bit lattice gas model. The length of the arrows is proportional to speed. Speed one particles have a unit mass. Speed two particles have 1/2 unit mass. The left side refers to the states before a collision. The right side refers to the states after the collision. (a) describes collisions between same type particles, (b) describes collisions between different types, and (c) shows collisions which change the number of each type of particle.

$$\sum_{a,\sigma} m^\sigma f_a^\sigma (\vec{e}_a^\sigma - \vec{u}) \cdot (\vec{e}_a^\sigma - \vec{u}) = n\epsilon. \tag{2.4}$$

We may define the temperature T of the lattice gas as

$$\epsilon = \frac{i}{2} k_B T, \tag{2.5}$$

where i is the number of degrees of freedom and k_B is the Boltzmann constant.

The conservation of mass, momentum, and energy require the following:

$$\sum_{a,\sigma} m^\sigma \Omega_a^\sigma = 0, \qquad \sum_{a,\sigma} m^\sigma \Omega_a^\sigma \vec{e}_a^\sigma = 0,$$
$$\sum_{a,\sigma} m^\sigma \Omega_a^\sigma (\vec{e}_a^\sigma)^2 = 0. \tag{2.6}$$

In order to obtain the hydrodynamic equation, we assume the local collisions cause the system to approach the local thermodynamic equilibrium state. According to the Chapman–Enskog expansion method, the equilibrium state corresponds to the zero order of collision term in kinetic equation (2.1), i.e, $\Omega_a^{\sigma(0)} = 0$. This leads to the Fermi-Dirac equilibrium distribution

$$f_a^{\sigma(0)} = \frac{1}{1 + \exp[m^\sigma(\alpha + \beta \vec{e}_a^\sigma \cdot \vec{u} + \gamma \epsilon_a^\sigma)]}, \tag{2.7}$$

where α, β, and γ are Lagrange multipliers which are determined by the definitions (2.2), (2.3), and (2.4).

Taking moments of (2.1), we obtain the following continuity, momentum, and energy equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot n\vec{u} = 0, \tag{2.8}$$

$$\frac{\partial n\vec{u}}{\partial t} + \nabla \cdot \hat{\Pi} = 0, \tag{2.9}$$

$$\frac{\partial (n\epsilon)}{\partial t} + \nabla \cdot (n\epsilon\vec{u}) + \nabla \cdot \vec{q} + \hat{P} : \nabla\vec{u} = 0, \tag{2.10}$$

where $\hat{\Pi}$ is the symmetric tensor of order 2, $\hat{\Pi}_{\alpha\beta} = \sum_{a,\sigma} m^\sigma f_a^\sigma (\vec{e}_a^\sigma)_\alpha (\vec{e}_a^\sigma)_\beta$, $\vec{q}$ is the heat flux, $(\vec{q})_\alpha = \sum_{a,\sigma} m^\sigma f_a^\sigma \frac{1}{2}(\vec{e}_a^\sigma - \vec{u})^2 (\vec{e}_a^\sigma - \vec{u})_\alpha$, and $\hat{P}$ is the pressure tensor, $\hat{P}_{\alpha\beta} = \sum_{a,\sigma} m^\sigma f_a^\sigma (\vec{e}_a^\sigma - \vec{u})_\alpha (\vec{e}_a^\sigma - \vec{u})_\beta$.

To obtain the solutions for $\hat{\Pi}$, $\vec{q}$, and $\hat{P}$, we expand $f_a^{\sigma(0)}$ to third order in speed, assuming $|\vec{u}| \ll c_{min}$, and expand $\alpha = \alpha_0 + \alpha_1 u^2, \beta = \beta_0 + \beta_1 u^2$, and $\gamma = \gamma_0 + \gamma_1 u^2$. Here c_{min} is the minimum nonzero "light" speed. The velocity expansion of $f_a^{\sigma(0)}$ then has the form

$$\begin{aligned} f_a{}^{\sigma(0)} &= d_a{}^\sigma - d_a{}^\sigma(1 - d_a{}^\sigma)[m^\sigma \beta_0 \vec{e}_a^\sigma \cdot \vec{u} + m^\sigma(\alpha_1 + \gamma_1 |\vec{e}_a^{\sigma 2}|)u^2] \\ &+ \frac{d_a^\sigma}{2}(1 - d_a^\sigma)(1 - 2d_a^\sigma) m^{\sigma 2} \beta_0{}^2 (\vec{e}_a^\sigma \cdot \vec{u})^2 \\ &- d_a^\sigma(1 - d_a^\sigma) m^\sigma \beta_1 (\vec{e}_a^\sigma \cdot \vec{u}) u^2 \\ &+ d_a^\sigma(1 - d_a^\sigma)(1 - 2d_a^\sigma) m^{\sigma 2} \beta_0 (\alpha_1 + \gamma_1 |\vec{e}_a^\sigma|^2) u^2 \\ &- \frac{1}{6} d_a^\sigma (1 - d_a^\sigma)(1 - 6d_a^\sigma + 6d_a^{\sigma 2}) m^{\sigma 3} \beta_0{}^3 (\vec{e}_a^\sigma \cdot \vec{u})^3 + \cdots, \end{aligned} \tag{2.11}$$

where d_a^σ is the equilibrium particle distribution when $\vec{u} = 0$,

$$d_a^\sigma = \frac{1}{1 + \exp[m_\sigma(\alpha_0 + \gamma_0 |\epsilon_a^\sigma|)]}. \tag{2.12}$$

Because d_a^σ does not depend on a, we can simplify $d_a^\sigma = d_\sigma$ and $\epsilon_a^\sigma = \epsilon_\sigma$. The coefficients β_0, β_1, α_1, and γ_1 in equations (2.11) and (2.12) are functions of n and ϵ which will be determined from the definitions of (2.2), (2.3), and (2.4).

For the models in which the rest particle does not have the internal energy, we can obtain

$$\hat{\Pi}_{\alpha\beta}^{(0)} = ng(n,\epsilon)u_\alpha u_\beta + p\delta_{\alpha\beta}, \tag{2.13}$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol, $g(n,\epsilon)$ is the coefficient of the convective term,

$$g(n,\epsilon) = \frac{\beta_0^2 M}{D(D+2)n}\sum_\sigma m^{\sigma 3} d_\sigma(1-d_\sigma)(1-2d_\sigma)|c^\sigma|^4, \tag{2.14}$$

and

$$p = p_0 + p_1 u^2, \tag{2.15}$$

where M is the number of distinct velocity directions and D is the space dimension,

$$p_0 = \sum_\sigma m^\sigma d_\sigma |c^\sigma|^2 \frac{M}{D} = n\epsilon, \tag{2.16}$$

and

$$p_1 = \frac{n}{2}(1 - g(n,\epsilon)). \tag{2.17}$$

In equation (2.17), note that $p_1 = 0$ when $g(n,\epsilon) = 1$. This very desirable coincidence is the direct result of including an additional speed in the model.

Equation (2.16) is the equation-of-state for the ideal gas.

Up to $O(u^2)$, the heat flux vector can be written

$$q_i^{(0)} = h(n,\epsilon)n\epsilon u_i, \tag{2.18}$$

where $h(n,\epsilon) = \frac{\sum_\sigma m^\sigma d_\sigma(1-d_\sigma)|c^\sigma|^4}{2\sum_\sigma m^\sigma d_\sigma(1-d_\sigma)|c^\sigma|^2\epsilon} - 2$.

Note that FHP-I and FHP-II models are degenerate cases of equations (2.14) and (2.16). After simple algebra, we obtain $g(n,\epsilon) = \frac{3-n}{6-n}$ and $\epsilon = \frac{1}{2}$ for FHP-I, and $g(n,\epsilon) = \frac{7(7-2n)}{12(7-n)}$ and $\epsilon = \frac{3}{7}$ for FHP-II. These results agree with reference [9].

Now we consider the isothermal incompressible fluid limit in the above multispeed models. We want to recover the Navier-Stokes equation with no unphysical terms at some fixed temperatures. Note that if ϵ and n both are constant, the energy equation is automatically satisfied. We know that mass density n and energy ϵ are defined by (2.2) and (2.4). Thus, for a given mass density, we can vary the temperature by varying the ratios of different types of particle to mass density $k_\sigma = d_\sigma/n$. The temperature is determined by

these ratios. The quantities, d_σ, we consider here are the equilibrium values, determined by the equation (2.12).

If all the particles are in statistical equilibrium, the collisions between the different types of particles should satisfy the detailed balance condition. After eliminating α_0 and γ_0 in (2.12), we have

$$\tilde{d}_i^{\,x}\tilde{d}_k^{\,y} = \tilde{d}_j^{\,z}, \tag{2.19}$$

which is required by the principle of the detailed balance. $\tilde{d}_i = \frac{d_i}{1-d_i}$, $x = \frac{1}{m_i(\epsilon_i-\epsilon_j)}$, $y = \frac{1}{m_k(\epsilon_j-\epsilon_k)}$, and $z = \frac{1}{m_j}[\frac{1}{\epsilon_j-\epsilon_k} + \frac{1}{\epsilon_i-\epsilon_j}]$. Note here we have $N+1$ variables but only N equations. The internal energy is still a free parameter. We may add the equation of $g(n,\epsilon) = 1$, or equivalently, $p_1 = 0$ and ask whether physical solutions exist for these equations. The physical solutions require the conditions $1 \geq d_\sigma \geq 0$ and $\epsilon_{max} \geq \epsilon \geq 0$. Here σ varies from 0 to N-1 and ϵ_{max} is determined by the model geometry. For the physical solution of equations, we may write $d_\sigma = d_\sigma(n)$ and $\epsilon = \epsilon(n)$. We show later that physical solutions exist.

Because the lattice gas model has density fluctuations, we cannot exactly satisfy the equation $g(n,\epsilon) = 1$. Instead, we can write down the velocity dependence of $n = n_0 + n_1u^2$ and $\epsilon = \epsilon_0 + \epsilon_1 u^2$. Consequently we have $g(n,\epsilon) = 1 + O(u^2)$ and $p_1 = O(u^2)$. One can show that these u^2 corrections contribute terms of order u^4 to the Navier-Stokes equation. Hence the order of accuracy of the Navier-Stokes equation is unchanged by corrections of order u^2 in the density and internal energy.

3. A simple example: The three-speed model

To illustrate our theoretical results, we examine the three-speed, multimass model. The particles have speeds 0, 1, and 2 and masses 3/2, 1, and 1/2 respectively. The collisions between different types particles are given by figure 1. Up to the second order of $|\vec{u}|$, we obtain the equilibrium distributions d_0, d_1, and d_2 and the energy ϵ as a function of density n. We have four variables from the four equations,

$$\begin{aligned}
\frac{3}{2}d_0 + 6d_1 + 3d_2 &= n,\\
3d_1 + 6d_2 &= n\epsilon,\\
(\frac{1-d_1}{d_1})^2 &= (\frac{1-d_0}{d_0})(\frac{1-d_2}{d_2}),\\
nd_1(1-d_1)(1-2d_1) + 2d_2(1-d_2)(1-2d_2)&\\
= 12[d_1(1-d_1) + d_2(1-d_2)]^2.&
\end{aligned} \tag{3.1}$$

In figure 2, we show the numerical solution of d_0, d_1, and d_2 when $n \leq 2.5$. Other allowed physical solutions appear for $3 \leq n \leq 4.5$ and $7 \leq n \leq 10.5$. For other values of n, some d_i becomes unphysically negative.

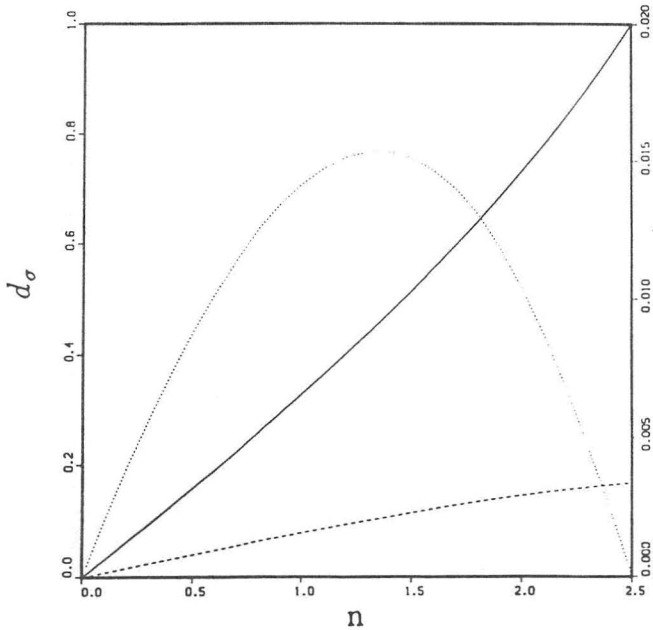

Figure 2: $\epsilon(n)$ plots for $g = 0.9$ (dash), 1.0 (solid), 1.2 (dot), 1.5 (chain dash), and 2.0 (chain dot). This figure illustrates the range of g for which physical solutions exist.

In figure 3, the solid line shows those values of ϵ and n for which $g = 1$. Physical solutions exist all along this line. We also plot physically allowed $\epsilon(n)$ for other values of g. There are two reasons to be interested in the dependence of the solution of g. First, one would like the $\epsilon(n)$ to be slowly varying with g, so that small density fluctuations cause small changes in g. We see that this is true. Second, we could carry out the usual g-scaling of time, viscosity, and pressure and obtain a corresponding change in the Reynolds number, $Re = gul/\nu$. Here u is a characteristic velocity, l is a characteristic length, and ν is the viscosity. In previous calculations, g is about 1/3. Having $g = 1$ allows at least a factor of 3 higher Reynolds number. Letting g be higher than one and scaling allows higher Reynolds numbers if the viscosity is unchanged. It is expected that the viscosity can be less in multispeed models because more collisions are allowed.

In figure 4, we give the numerical results of this 13-bit model for the energy decay in the Kolmogorov flow compared with the FHP-I model [5]. We find that the oscillation in kinetic energy decay greatly decreases because

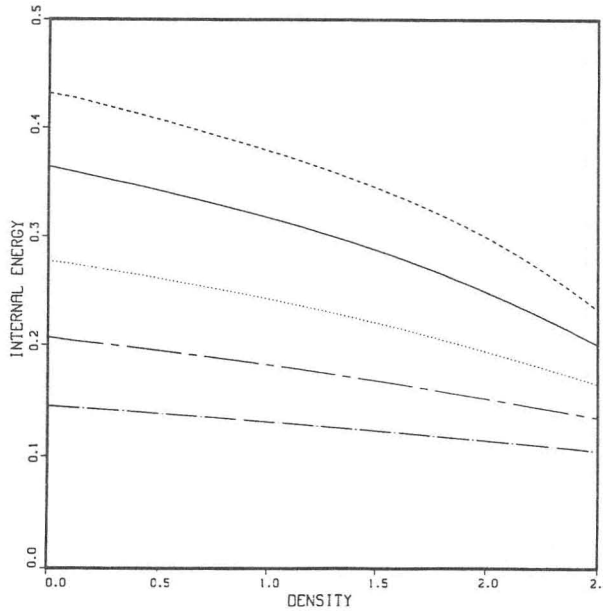

Figure 3: Equilibrium distributions for speed zero (solid), speed one (dash), and speed two (dot, right vertical coordinate) when $g(n, \epsilon) = 1$. This figure demonstrates the existence of physical solutions when g, the coefficient of the $\vec{u} \cdot \nabla \vec{u}$ term, is unity.

p_1 equals to zero in the present model. The internal energy decay rate is within three percent of the theoretical prediction.

4. Conclusions

The multispeed lattice gas automaton model is the simple extension of FHP lattice gas model by adding more speeds. This method leads to thermohydrodynamic equations. One important result of the additional flexibility is that we can have $g(n) = 1$ and $p_1 = 0$ to second-order accuracy in the speed u. The expense of adding more bits to the model is offset by the increase in the allowed range of Reynolds number. The extension of this work to three-dimensional hydrodynamics is straightforward.

5. Acknowledgments

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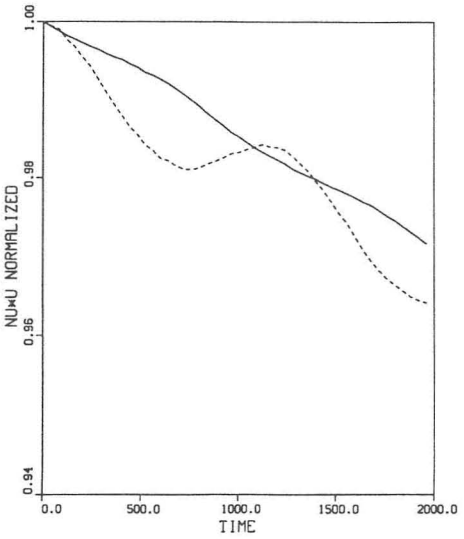

Figure 4: The streamwise kinetic energy for Kolmogorov flow. $u_0 = 0.3\sin(y)$. The solid curve is the 13-bit result with $n = 2.0$ and $\epsilon = 0.25$. The dashed curve is the 6-bit result when $n = 1.8$ and $\epsilon = 0.5$. The unphysical oscillation presented in the 6-bit result is reduced significantly in the 13-bit result because the u^2 term in the pressure has been eliminated.

References

[1] U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.*, **56** (1986) 1505.

[2] D. Boghosian and D. Levermore, *Complex Systems*, **1** (1987) 17.

[3] T. Shimomura, Gary D. Doolen, B. Hasslacher, and C. Fu, *Los Alamos Science* special issue, 1987.

[4] H. Chen, S. Chen, Gary D. Doolen, and Y.C. Lee, *Complex Systems*, **2** (1988) 259.

[5] J.P. Dahlburg, D. Montgomery, and G. Doolen, *Phys. Rev.*, **A36** (1987) 2471.

[6] S. Wolfram, *J. Stat. Phys.*, **45** (1986) 471.

[7] T. Hatori and D. Montgomery, *Complex Systems*, **1** (1987) 734.

[8] S. Chen, M. Lee, Gary D. Doolen, and K. Zhao, "A lattice gas model with temperature," *Physica D*, **37** (1989) 42.

[9] D. d'Humières and P. Lallemand, *Complex Systems*, **1** (1987) 599.