Journal of Statistical Physics, Vol. 103, Nos. 5/6, 2001

Irreversibility in a Reversible Lattice Gas

James E. Broadwell[1, 2]

Received May 8, 2000; revised August 17, 2000

A simple lattice gas model, a microscopically reversible cellular automaton, is described and shown to exhibit thermodynamic irreversibility in processes similar to those in real gases. The model, which has no random elements, develops a long-lasting equilibrium state within a Poincaré cycle. This state is an attractor resulting from the nonlinear nature of the collective particle collisions and motions. The results illustrate how the Second Law of Thermodynamics applies to real systems governed by reversible microscopic dynamics.

KEY WORDS: Irreversibility; lattice gases; nonlinear dynamics; statistical mechanics

1. INTRODUCTION

In his book on the foundations of statistical mechanics, Lawrence Sklar[(1)] writes concerning the apparent conflict between the reversible laws thought to govern dynamics at the molecular level and the observed irreversibility of real systems:

"Although some aspects of the theory are well understood and universally accepted, such crucial areas as the correct approach to the introduction into the theory of irreversibility and the approach to equilibrium and the proper statistical mechanical definition of entropy are the subject of intense and seemingly interminable controversy."

[1] Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California 91125.

[2] Present address: 8 Muirfield Road, Half Moon Bay, California 94019. e-mail: genejeb@ix.netcom.com

Richard Feynman devotes one of his chapters on thermodynamics to an exploration of the paradox,[2] and in their Statistical Mechanics Landau and Lifshitz state that there is "a contradiction, a very deep one" in the foundations of statistical mechanics.[3] They reject the critical role assigned to initial conditions in the standard theory, writing: "It is quite uncertain at present whether one can deduce the law of increase of entropy formulated in such a way on the basis of classical physics."

More recently, Roger Penrose writing about the statistical asymmetry of the universe proposes a drastic resolution of this apparent contradiction with symmetrical microscopic laws:[4] "In my own judgement, there remains the one ('obvious') explanation that the precise physical laws are actually *not* time-symmetric!"

In several recent papers Joel L. Lebowitz presents a detailed study of the issue.[5–7] He remarks in ref. 6 that "...it is quite surprising that there is still so much confusion about the 'problem of irreversibility'," and expresses the opinion that there are no grounds for the controversies—that Boltzmann's explanations of the matter are completely satisfactory. He attributes the continuing controversy to a lack of appreciation of Boltzmann's responses to his early critics and of his later writings.

Lebowitz's view is supported in this paper by exact results from a system of the kind that Boltzmann considered in this later work,[8, 9] i.e., a microscopically reversible system within perfectly elastic walls. Such a system satisfies the conditions that a valid entropy-decreasing motion can result if the velocities of all particles in the system are reversed, and the system is cyclic, conditions that Loschmidt and Zermelo pointed out were not satisfied in Boltzmann's early work. The model illustrates how what are called irreversible processes, expansion into vacuum for example, arise in such a system. Thus the results from the model are in general accord with the Boltzmann predictions for real gas systems.

Although the model motions resemble those of real gases in several respects, there are significant differences. For this reason the work is not to be viewed as an attempt to approximate real gas behavior; instead it is a study of a selfcontained model in which fundamental concepts underlying the thermodynamics of gases can be examined more easily. Of course, the hope is that the results will add to our understanding of real gas behavior. Thus the model shares the purpose of the Ehrenfest wind-tree model.[10]

The remainder of the paper is organized as follows:

Section 2. Model description

Section 3. Model results

Section 4. Discussion and conclusion

2. MODEL DESCRIPTION

(a) Basis of the Model

The model is a lattice gas version, a cellular automaton, of the discrete velocity gas model introduced in Broadwell.[11, 12] The simplicity of that model allows exact solution of the model Boltzmann equations for several flows, including Couette and Rayleigh flow and shock waves. Shock wave solutions are also presented in Caflisch[13] and Cornille.[14, 15] The remarkable similarity of these model solutions to those of more realistic models and the similarity of the model H-function behavior to that given by the Boltzmann equation suggest that an examination of the thermodynamic behavior of the related lattice gas might be instructive. The lattice version of the model was formulated by Hardy and Pomeau[16] and some of its thermodynamic properties discussed by them and by Hardy *et al.*[17] Wolfram presents a comprehensive treatment of the kinetic and hydrodynamic theory of general cellular automata.[18]

(b) The Model

The two-dimensional lattice gas model consists of indistinguishable particles that move on a two-dimensional square lattice in the x–y plane with four fixed velocities. (The restriction to four velocities is an element in common with the Ehrenfest wind-tree model to which the discrete velocity gas is distantly related.) Particles move and collide according to the following rules. In each time step all particles move to the adjacent site and then some collide. Collisions, which turn the collision partners through ninety degrees, take place if and only if two particles with oppositely directed velocities occupy the same site and the collision destination velocity locations are empty. Particles are excluded from having the same velocity at the same site. Particles pass through each other between sites.

Each step is reversible, with the result that if at some time all particle velocities are reversed, the initial state with all the velocities reversed is recovered. Furthermore, since the number of configurations is finite and each move and collision produces a new state, a return to the initial condition is guaranteed. Stated another way, the system cannot enter a closed loop in phase space that does not include the initial condition.

3. MODEL RESULTS

Model results are presented in the following for three processes: (1) equilibration at constant area from arbitrary initial particle configurations,

(2) expansion into a vacuum, and (3) equilibration at constant area through expansion and shock waves. In some of the following, particles moving N, E, S, and W will be denoted by the numerals 1–4.

3.a. Constant Area Particle Re-Arrangement

The model is used first to address the motion of particles from prescribed initial conditions in lattice areas of increasing size, first steps towards the thermodynamic limit. Figure 1(a) is the particle number history for the 5×5 lattice where for clarity only two of the population histories are shown. The initial condition consists of East moving particles at every site and a particle directed South at the (3, 3) site. In these figures and in the subsequent discussions, the particle velocity, lattice spacing, and time step are taken to be unity.

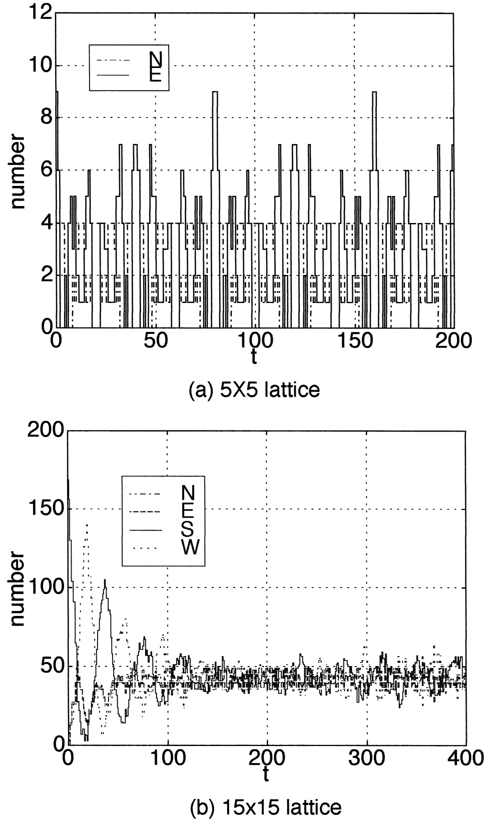

Fig. 1. Particle number history for two lattices.

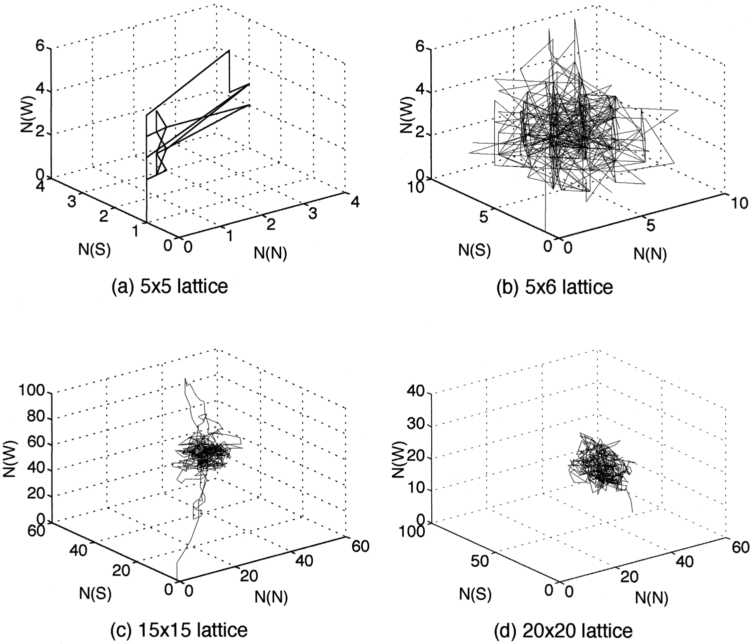

Fig. 2. Particle number history demonstrating the emergence of an equilibrium state.

The velocity fields for the 5×5 lattice show that the system returns to the initial configuration in 81 steps as Fig. 1(a) suggests. This lattice with ten particles has approximately 10^{11} possible microstates so the model is far from ergodic. The return or recurrence time of the 5×6 lattice is approximately 10^4 and is too long to be conveniently computed for any larger lattice.[3]

Figures 1 and 2 show that as the lattice size increases (towards the thermodynamic limit) a long lasting equilibrium state emerges in which the populations in the four directions are equal. With further increase in size the relative magnitude of the fluctuations continues to decline and the length of the equilibrium state increases. The oscillations at early time in Fig. 1(b) are the motions required to remove the mean horizontal momentum in the initial condition. The results in Fig. 2(d), discussed later, are for initial conditions with no mean momentum. (There are fewer particles in this case than in the 15×15 lattice so the fluctuations are larger.)

[3] All the computer results reported here were obtained on a desktop computer.

The Boltzmann H-function for the lattice gas is the discrete representation of

$$H = \int_V d\tau_r \int_{-\infty}^{\infty} d\tau_v f(\vec{v}, r, t) \ln f(\vec{v}, r, t)$$

where $\vec{r}$ is the position vector, $\vec{v}$ is the particle velocity vector, and $d\tau_r$ and $d\tau_v$ the differential volumes in position and velocity space. The model expression is

$$H(t) = \sum n(i) \ln n(i) A$$

where A is the area, N the number of particles, and $n(i) = N/A$ is number density of the ith-particles. As is conventional, the area is dropped in the following cases when it is constant.

The H-function, a step function, is shown in Fig. 3 for the processes discussed above. We see that the emerging equilibrium state is one of

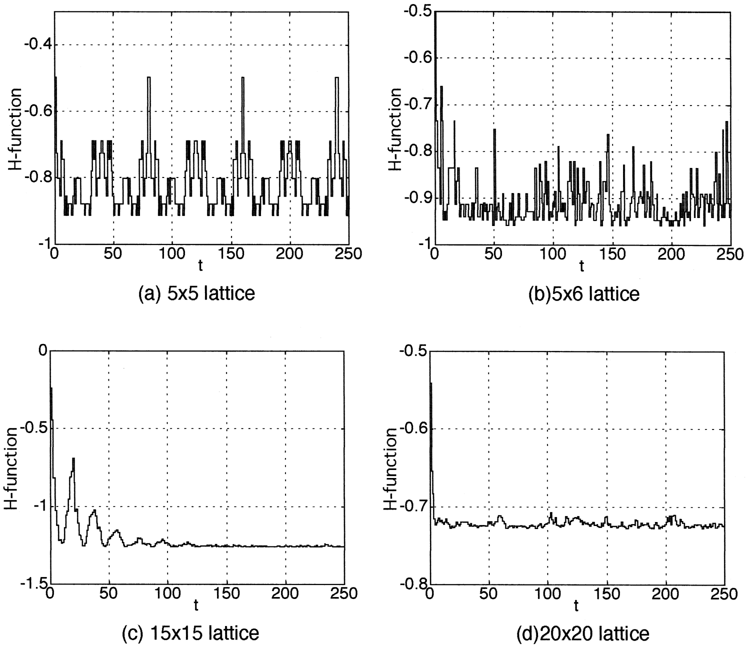

Fig. 3. H-function for particle rearrangement.

minimum H with fluctuations that decline with lattice size. (Note the scale change in the vertical axis.) Boltzmann proved that when there are no spatial gradients the H-function falls monotonically to its minimum value. This behavior is illustrated in Fig. 3(d) in which the initial field consists of equal numbers of North and South particles, an arrangement in which there is no mean velocity in either direction, and no gradients are generated.

When the lattice is large enough for the continuum approximation to be appropriate the model replicates the Boltzmann proof that H must decline from non-equilibrium conditions. In this circumstance the equations for the discrete velocity gas[11] are applicable and are:

$$\begin{aligned}
\frac{\partial n_1}{\partial t}+\frac{\partial n_1}{\partial y}&=\theta(n_2 n_4-n_1 n_3)\\
\frac{\partial n_2}{\partial t}+\frac{\partial n_2}{\partial x}&=\theta(n_1 n_3-n_2 n_4)\\
\frac{\partial n_3}{\partial t}-\frac{\partial n_3}{\partial y}&=\theta(n_2 n_4-n_1 n_3)\\
\frac{\partial n_4}{\partial t}-\frac{\partial n_4}{\partial x}&=\theta(n_1 n_3-n_2 n_4)
\end{aligned} \tag{1}$$

where θ the collision frequency. When there are no spatial gradients it can be shown from these equations that

$$\frac{dH}{dt}=\theta(n_1 n_3-n_2 n_4)(\ln n_2 n_4-\ln n_1 n_3)$$

so that, as in Fig. 3(d),

$$\frac{dH}{dt}\leqslant 0$$

Noting that the collision term $n_1 n_3$ is the inverse of $n_2 n_4$ and *vise versa*, we can see the similarities between these equations and the full Boltzmann and H- function equations.

These examples of particle rearrangement are models of thought experiments only: particle configurations cannot be prescribed. The next two examples in contrast, where only macroscopic conditions initial conditions are imposed, are idealizations of possible real experiments.

3.b. Expansion into a Vacuum

Consider a configuration in which the particles are initially contained in the left half of a "vessel" 40 units high and 80 units long. The gas is in equilibrium with an initial number density distribution as shown in Fig. 4 at t = 0. From this state the gas expands into the "vacuum" and comes to rest through a series of compression and expansion waves, the early stages of which are shown at t = 20 and t = 120. Equilibrium is reached at approximately t = 1500 when the mean density becomes uniform as is illustrated by the distribution at t = 10, 000.

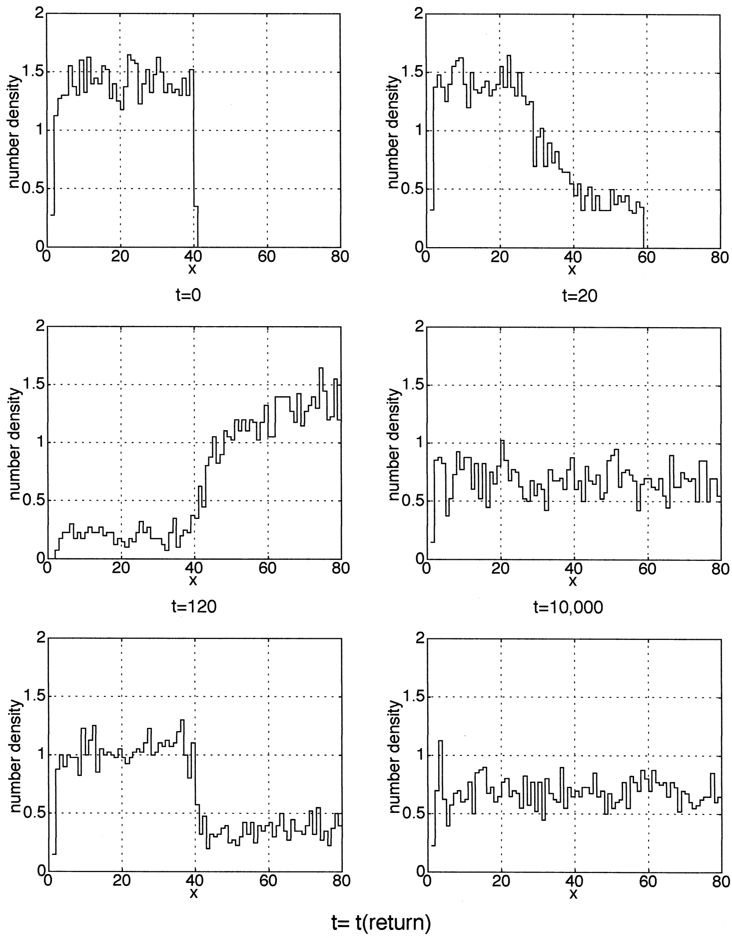

Fig. 4. Particle number density distribution, expansion into vacuum, 40 × 80 lattice.

If at t = 10, 000 all particle velocities are reversed, the gas returns to the initial state in the reverse direction along the forward path, and the initial density distribution is recovered. If, however, at the reversal just one particle is not correctly reversed, the return to the initial state is destroyed as the density distribution at the return time t(r) indicates. The two return states, Fig. 4(e) and Fig. 4(f), result when errors are introduced at different, randomly chosen, locations in two different runs. The computation illustrates the instability of paths towards non-equilibrium states, the significance of which has been discussed by Lebowitz.[5] Nadiga *et al*[19] have also demonstrated this instability with a nine-velocity lattice gas model.

Since both directions along the path are equally valid dynamical motions, the instability backwards towards the initial non-equilibrium state can serve just as well to show that any interaction with the environment, always present in any real system, will destroy the return to the initial state as the system moves *forward* in time.

In this example $H = \sum n(i) \ln n(i)$ $A = \sum N(i) \ln n(i)$ in which the number of particles, N, is constant and at equilibrium $N(i) = 1/4N$ and $n(i) = 1/4n$. Thus since the particle density falls by one half, the change in H is $-N \ln 2$.

3.c. Shock and Expansion Waves

The model can treat another idealization of a possible real experiment, one in which dissipation takes place within shock waves. Consider a lattice for which the boundaries at x = 0 and x = L are at first made periodic so that East and West moving particles that leave at one boundary enter at the other. The gas is given a mean velocity to the right by assigning more E, (2), particles than W, (4), particles in the expression for mean x-direction velocity, $u = q[n(2) - n(4)]/n$, where q is the particle velocity (taken to be unity) and n the total particle number density.

After the gas (with the mean velocity) equilibrates, the boundaries at x = 0 and L are made reflective (as if walls were inserted) and the gas comes to rest through a series of shock and expansion waves as indicated in Fig. 5. After many passages of the waves through the system, the gas comes to rest with the equilibrium particle density distribution shown at t = 5000.

Since H for the initial non-uniform particle distribution is larger than that for an equal distribution, the change in H in the process is negative as in the previous cases. Adding significance and relevance to these results is another parallel with monatomic gases described by the Boltzmann equation: the shock waves in Fig. 5 are described by model hydrodynamic equations derived from the model Boltzmann equations, Eq. 1.[13, 20, 21]

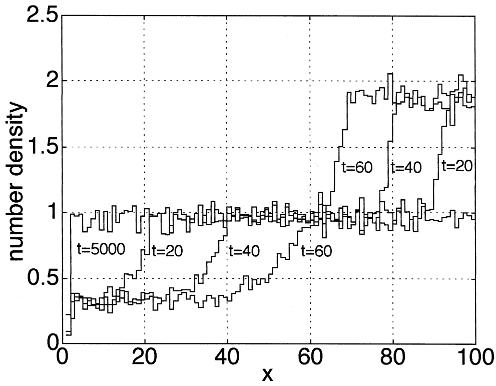

Fig. 5. Particle number density distribution, expansion and shock waves, 100×200 lattice.

4. DISCUSSION AND CONCLUSIONS

To discuss the above described results it is necessary to recall that in the present context "reversible" has two different meanings. In molecular dynamics it means that the reversal of time in the equations of motion has no effect; in thermodynamics a process is said to be reversible if at its conclusion the system and its surroundings can be returned to their initial macrostates by (idealized) macroscopic operations.

An illustration of this confusing usage is Feynman's remark about molecular mixing, ref. 2, p. 46–7. "So the mixing is completely reversible, and yet it is irreversible." Likewise, the expansion into a vacuum and the expansion and shock wave flow are reversible in the first sense but irreversible in the second. (The systems cannot be returned from the equilibrium state to the initial conditions by macroscopic operations such as compression with a piston and energy transfer by heat conduction.) The time for the "automatic" return is, of course, too long to be relevant for real systems.

With the two meanings of reversible in mind, the results can be summarized by stating that the reversible, deterministic lattice gas system has been shown to develop, within a closed cycle, a long-term equilibrium state towards which it evolves from non-equilibrium conditions. Despite the microscopic reversibility and the cyclic nature of the system, the lattice motions exhibit two of the canonical, thermodynamically irreversible, processes that take place in real gases.

In view of the similarities between the model Boltzmann and H-function equations and the full Boltzmann counterparts it not surprising that the model results provide general support to Boltzmann's views about the behavior of gas systems. The fluctuations of H in the equilibrium state and its long persistence are in accord with his description, expressed in probabilistic terms, of the behavior of that function.[8] In fact all the results of this paper are consistent with Boltzmann's own summary statement:[9] "We proved that it [the H-function] continually decreases as a result of the motion of the gas molecules among each other. The one-sidedness of this process is clearly not based on the equations of motion of the molecules. For these do not change when the time changes its sign. This one-sidedness rather lies uniquely and solely in the initial conditions."

The behavior in the thermodynamic limit, the Boltzmann–Grad limit, of two related models should be mentioned. Caprino *et al*[22] analyze a system of particles moving stochastically on a two-dimensional lattice, and Uchiyama[23] studies a system of diamonds moving freely in two-dimensional space. The diamonds are so oriented that collisions deflect collision partners through ninety degrees. In the first reference the one-particle distribution function is proved to converge, in the limit, to a solution of Eq. 1, while in the second the solution does not come out. The present model has not been so analyzed.

ACKNOWLEDGMENTS

Donghee Han wrote the computer program for this work at Stanford University. The speed and flexibility of the program made possible the efficient exploration of the ideas and findings reported here. The author is pleased to thank him for his collaboration. He also thanks Donald Baganoff for his work in a preliminary study of the lattice gas. The author is grateful for the hospitality of the Mechanical Engineering Department at Stanford during the course of the work.

REFERENCES

1. L. Sklar, *Introduction to Physics and Chance, Philosophical Issues in the Foundations of Statistical Mechanics* (Cambridge University Press, Cambridge, 1993).
2. R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics*, Vol. 1 (Addison–Wesley, Reading, Mass., 1963).
3. L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, Addison–Wesley, Reading, MA, 1958).
4. R. Penrose, Singularities and time-asymmetry. *General Relativity: An Einstein Centenary*, S. W. Hawking and W. Israel (Eds.) (Cambridge University Press, Cambridge, 1979).
5. J. L. Lebowitz, Macroscopic laws, microscopic dynamics, time's arrow and Boltzmann entropy, *Physica A* **194**:1 (1993).
6. J. L. Lebowitz, in *Lecture Notes in Physics*, 25 Years of Non-Equilibrium Statistical Mechanics, Proceedings, Sitges, Barcelona, Spain 1994, J. J. Brey, J. Marro, J. M. Rubi, and M. San Miguel, Eds. (Springer, 1995).

7. J. L. Lebowitz, Microscopic Origins of Irreversible Macroscopic Behavior, *Physica A* **263**:516 (1999).
8. L. Boltzmann, On Certain Questions of the Theory of Gases, *Nature* **51**:413 (1895).
9. L. Boltzmann, *Lectures on Gas Theory* (University of California Press, Berkeley and Los Angeles, 1964), pp. 442.
10. P. Ehrenfest and T. Ehrenfest, *The Conceptual Foundation of the Statistical Approach in Mechanics* (Cornell University Press, Ithaca, New York, 1959).
11. J. E. Broadwell, Study of rarefied shear flow by the discrete velocity method, *J. Fluid Mech.* **19**:401 (1964).
12. J. E. Broadwell, Shock structure in a simple discrete velocity gas, *Phys. Fluids* **7**:1243 (1964).
13. R. E. Caflisch, Navier–Stokes and Boltzmann shock profiles for a model of gas dynamics, *Comm. Pure Appl. Math.* **32**:521 (1979).
14. H. Cornille, Exact solutions of the Broadwell model in $1+1$ dimensions, *J. Phys. A: Math. Gen.* **20**:1973 (1987).
15. H. Cornille, Positive $(2+1)$-dimensional exact shock waves solutions to the Broadwell model, *J. Math. Phys.* **30**(4):789 (1989).
16. J. Hardy and Y. Pomeau, Thermodynamics and Hydrodynamics for a Modeled Fluid, *J. Math. Phys.* **13**:1042 (1972).
17. J. Hardy, O. de Pazzis, and Y. Pomeau, Molecular dynamics of a classical lattice gas: Transport properties and time correlation functions, *Phys. Rev. A* **13**:1949 (1976).
18. S. Wolfram, Cellular Automaton Fluids: Basic Theory, *J. Stat. Phys.* **45**:471 (1986).
19. B. T. Nadiga, J. E. Broadwell, and B. Sturtevant, *Study of a Multispeed Cellular Automaton. Rarefied Gas Dynamics: Theoretical and Computational Techniques*, E. P. Muntz, D. P. Weaver, and D. H. Campbell, Eds., Vol. 118 (Progress in Astronauts and Aeronautics, AIAA Washington, D. C., 1989).
20. R. E. Caflisch and G. C. Papanicolaou, The fluid-dynamical limit of a nonlinear model Boltzmann equation, *Comm. Pure Appl. Math.* **32**:589 (1979).
21. S. K. Godunov and U. M. Sultangazin, On discrete models of the kinetic Boltzmann equation, *Uspekhi Mat. Nauk* **26**:3 (1971). Also *Russ. Math. Surv.* **26**:1 (1971).
22. S. Caprino, A. DeMasi, E. Presutti, and M. Pulvirenti, A derivation of the Broadwell equation, *Comm. in Math. Phys.* **135**:443 (1991).
23. K. Uchiyama, On the Boltzmann–Grad Limit for the Broadwell Model of the Boltzmann Equation, *J. Stat. Phys.* **52**:331 (1985).