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A Cellular Automaton for a Solvable Boltzmann Equation

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Abstract. A probabilistic cellular automaton as an approximation of a solvable Boltzmann equation in one space and one time dimension is presented. First the model that was introduced by Ruijgrok and Wu [6,7] is revised in a Lorentz covariant form. Next, an appropriate cellular automaton is defined. By analogy with the Boltzmann approach, equations for the time dependence of ensemble averages of single-particle quantities are obtained by making the Stoßzahlansatz. The required nonlinearity is a consequence of the exclusion principle. In accordance with the Boltzmann equation, homogeneous as well as inhomogeneous equilibria are derived exactly. On the basis of intuition and symmetry considerations, a relationship between the two systems is found. By means of this relationship it is demonstrated that the ensemble averaged automaton approximates the Ruijgrok–Wu model up to first order of the lattice spacing, for all time scales. Simulations show that the Stoßzahlansatz is justified.

1. Introduction

In the last few years people have become increasingly interested in using cellular automata as discrete microscopic analogues of continuous many-particle systems (see for instance [1–4]).

First, cellular automata have a very simple structure [5]. Space is restricted to a (usually regular) lattice. The information available at each site is very limited, usually amounting to no more than a few bits. Time evolution is also discrete: at each time step all sites are updated according to the automaton rule. This rule has two important properties: locality (the state of the updated site depends only on its direct environment) and homogeneity (the same rule is applied at each site). These properties together with the fact that the application of the automaton rule involves only a few elementary bit operations make cellular automata ideal for parallel implementation.

Second, the interest in cellular automata has been stimulated by the knowledge that the form of the macroscopic equations of fluids is determined

largely by the microscopic conservation laws and symmetries. Therefore two physically quite different fluids can exhibit similar macroscopic behavior.

Therefore, cellular automata that have similar microscopic conservation laws and a maximum of symmetry resemblance with fluids provide a promising simulation technique for solving the Navier–Stokes equations. However, there are a number of discrepancies, one of them being Galilean invariance.

In this paper a probabilistic cellular automaton for a one-dimensional solvable Boltzmann equation is studied; this automaton is simple enough to analyze. This model, which was introduced by Ruijgrok and Wu in 1981 [6,7], is analyzed in section 2 in rather a comprehensive way, for the present approach is slightly different from the approach used in [6]. In section 3, an appropriate cellular automaton is constructed and analyzed. The relationship between the two systems is established in section 4. Symmetry considerations play an essential role. Simulations are discussed in section 5.

2. The Boltzmann equation

2.1 Definition

The model that Ruijgrok and Wu introduced (from now on abbreviated to R.W.) can be defined as follows. There is only one space dimension, and the only allowed velocities with which particles move are $+1$ (or just $+$) and -1 (or just $-$).There are three collision processes described in the table below. Here $p(s \to s')$ is the probability per unit time that a single particle or a pair of neighboring particles make a transition from the state s to the state s'.

s		s'	$p(s \to s')$
$+$	$\longrightarrow$	$-$	α
$-$	$\longrightarrow$	$+$	β
$+-$	$\longrightarrow$	$++$	1

(2.1)

These collisions cause a violation of detailed balance and of time reversal invariance. Here, however, these factors will not be regarded as essential ingredients for kinetic theory.

Let f_1 and f_2 be the distribution functions for the $+$ and $-$ particles respectively; then for each $\alpha, \beta > 0$ the Boltzmann equation is given by

$$\mathcal{B}_{\alpha,\beta}: \quad \begin{aligned} (\frac{\partial}{\partial t} + \frac{\partial}{\partial x})f_1 &= \ f_1 f_2 - \alpha f_1 + \beta f_2 \equiv \ \Omega(f_1, f_2) \\ (\frac{\partial}{\partial t} - \frac{\partial}{\partial x})f_2 &= -f_1 f_2 + \alpha f_1 - \beta f_2 \equiv -\Omega(f_1, f_2) \end{aligned} \tag{2.2}$$

Summing both equations leads to the continuity equation

$$\frac{\partial}{\partial t}(f_1 + f_2) + \frac{\partial}{\partial x}(f_1 - f_2) = 0 \tag{2.3}$$

This equation reflects conservation of particle number, which in this case coincides with energy conservation. It is the only conservation relation, for there is no conservation of momentum.

2.2 Symmetries

The functions $f_{1,2}$ are distributions and must therefore be nonnegative ($f_{1,2} \geq 0$). In principle $f_{1,2}$ have no upper bounds. However, due to the nonlinearity of the collision term Ω in equation (2.2), there is also a natural upper bound. This can be seen clearly from the transformation $\mathcal{R} : (f_1, f_2) \rightarrow (f_1', f_2')$:

$$\mathcal{R}: \quad \left.\begin{array}{l} f_1'(x,t) = (\alpha - \beta) - f_2(-x,t) \\ f_2'(x,t) = (\alpha - \beta) - f_1(-x,t) \end{array}\right\} \Rightarrow \mathcal{R}^{-1} = \mathcal{R}; \quad \mathcal{R}^2 = \mathcal{I} \qquad (2.4)$$

Because $\Omega' = \Omega$ and the advection terms in equation (2.2) interchange, it can be seen that the system is *invariant* under this transformation. In [6,7] it is shown that the system can give rise to interesting inhomogeneous equilibria when

$$\alpha > \beta. \qquad (2.5)$$

On the basis of physical arguments, we know that the evolution of a nonnegative initial distribution will always be nonnegative. Therefore in the region where $\alpha > \beta$, the symmetry transformation (2.4) shows

$$f_{1,2}(x,0) \in [0, \alpha - \beta] \, \forall x \in \Re \iff \begin{array}{l} f_{1,2}(x,t) \in [0, \alpha - \beta] \\ \forall x \in \Re, \ \forall t \geq 0 \end{array} \qquad (2.6)$$

So an initial distribution that is completely contained in the interval $[0, \alpha - \beta]$ will *never* leave this interval. This information is very useful for constructing an appropriate automaton where, besides the nonnegativity constraint, distributions are bounded by the completely filled state. To give an example: in 1987 Boghosian and Levermore [8] constructed a cellular automaton for Burger's equation

$$\frac{\partial}{\partial t} n + c \frac{\partial}{\partial x}(n - \frac{n^2}{2}) = \nu \frac{\partial^2}{\partial x^2} n$$

A similar transformation $\mathcal{R} : n \rightarrow n'$ that leaves the system invariant can be given:

$$n'(x,t) = 2 - n(-x,t)$$

This symmetry shows that the interval $n \in [0,2]$ is invariant under time evolution, which corresponds exactly to the allowed interval for the distributions of the automaton.

Information in the system cannot flow faster than the velocity of the particles. A group of linear coordinate transformations that leaves this concept invariant is the group of *Lorentz* transformations. Consider two frames S and S' moving with a relative velocity v, and let events be denoted by

coordinates $X \equiv (x,t)$ and $X' \equiv (x',t')'$ respectively; the relation between the two frames is then given by

$$\begin{pmatrix} x' \\ t' \end{pmatrix} = L_v \begin{pmatrix} x \\ t \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma v \\ -\gamma v & \gamma \end{pmatrix} \begin{pmatrix} x \\ t \end{pmatrix} \tag{2.7}$$

where

$$\gamma = \frac{1}{\sqrt{1-v^2}}$$

Physical quantities must transform such that the physics described by them is unaltered. Some simple calculations lead to the transformation rules

$$\begin{aligned} f_1' &= \frac{f_1}{k} & \alpha' &= k\alpha \\ f_2' &= k f_2 \quad \text{and} & \beta' &= \frac{\beta}{k} \end{aligned} \tag{2.8}$$

where

$$k = \sqrt{\frac{1+v}{1-v}}. \tag{2.9}$$

It follows that a Lorentz transformation L_v maps the Boltzmann equation $\mathcal{B}_{\alpha,\beta}$ onto the equation $\mathcal{B}_{k\alpha,\frac{\beta}{k}}$. Note that $\alpha\beta$ is an invariant under this group of transformations.

Not only Lorentz transformations but also the group of *scaling* transformations $\mathcal{S}$ leave the particle velocity invariant:

$$S_a: \quad \begin{aligned} x' &= \frac{x}{a} \\ t' &= \frac{t}{a} \end{aligned} \qquad a > 0 \tag{2.10}$$

Again the physical quantities must transform, such that the physics described by them is unaltered; so

$$\begin{aligned} f'(x')\,dx' = f(x)\,dx \quad &\Rightarrow \quad f_1' = a f_1, \quad f_2' = a f_2 \\ \alpha'\,dt' = \alpha\,dt \quad &\Rightarrow \quad \alpha' = a\alpha, \quad \beta' = a\beta \end{aligned} \tag{2.11}$$

It follows that S_a maps the system $\mathcal{B}_{\alpha,\beta}$ onto the system $\mathcal{B}_{a\alpha,a\beta}$. Note that α/β is an invariant under this group of transformations.

Combining the two transformation groups $\mathcal{L}$ and $\mathcal{S}$, and using the fact that the two groups commute, it follows that any two systems $\mathcal{B}_{\alpha_1,\beta_1}$ and $\mathcal{B}_{\alpha_2,\beta_2}$ can be related to each other by a unique transformation $S_a \circ L_v$ $(= L_v \circ S_a)$. Further, the nonnegativity condition $f_{1,2} \geq 0$ is conserved under both groups. Transformation $\mathcal{R}$ commutes with $\mathcal{S}$, but it does not commute with $\mathcal{L}$. Therefore one can derive a number of theorems analogous to equation (2.6), first by applying a Lorentz transformation, then by using transformation $\mathcal{R}$ to prove (2.6) in the transformed system, and finally by transforming the information obtained back to the original system. One should, however, be aware that initial condition problems are not Lorentz invariant.

2.3 Explicit solution

Equation (2.2) is to be solved with given $f_1(x,0)$ and $f_2(x,0)$. From the observation that the collision term Ω can be written as

$$\Omega(f_1,f_2) = (f_1+\beta)(f_2-\alpha)+\alpha\beta$$

one obtains more suitable equations by introducing the shifts

$$f_+ = \beta + f_1 \quad \text{and} \quad f_- = \alpha - f_2 \tag{2.12}$$

Let

$$m = \sqrt{\alpha\beta}$$

which is a scalar, i.e. it has the same value in each Lorentz frame. Then equation (2.2) transforms into

$$\begin{aligned}\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial x}\right) f_+ &= m^2 - f_+ f_- \\ \left(\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right) f_- &= m^2 - f_+ f_-\end{aligned} \tag{2.13}$$

The equation of continuity (2.3) allows us to introduce a function $H(x,t) > 0$, such that

$$f_+ = \left(\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right)\log H \quad \text{and} \quad f_- = \left(\frac{\partial}{\partial t}+\frac{\partial}{\partial x}\right)\log H \tag{2.14}$$

From the transformation rules (2.7) and (2.8), it is seen that H is also a scalar. Substitution of equation (2.14) into (2.13) and using the identity

$$\begin{aligned}\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right)\log H \;=\; & \frac{1}{H}\left(\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}\right)\log H \\ & -\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial x}\right)\log H\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right)\log H\end{aligned}$$

leads to a single equation for H:

$$(\partial^2 - m^2)H = 0 \tag{2.15}$$

where

$$\partial^2 \equiv \frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2} \tag{2.16}$$

is also a scalar. So redefinition (2.14) maps the *nonlinear* Boltzmann equation (2.2) onto the *linear* partial differential equation (2.15), which is manifest Lorentz covariant. In combination with initial conditions

$$H(x,0) \equiv A(x) \quad \text{and} \quad \frac{\partial}{\partial t}H(x,t) \equiv B(x,t) \tag{2.17}$$

the solution of (2.2) is given by

$$\begin{aligned} H(x,t) &= \tfrac{1}{2}(A(x+t)+A(x-t)) \\ &\quad + \tfrac{1}{2}mt\int_{-t}^{+t}\frac{I_1(m\sqrt{t^2-x'^2})}{\sqrt{t^2-x'^2}}A(x+x')\,dx' \\ &\quad + \tfrac{1}{2}\int_{-t}^{+t} I_0(m\sqrt{t^2-x'^2})B(x+x')\,dx' \end{aligned} \tag{2.18}$$

I_0 and I_1 denote modified Bessel functions. The functions A and B in (2.17) are determined by initial conditions $f_1(x,0)$ and $f_2(x,0)$. Define new variables f and g

$$\begin{aligned} f &= \tfrac{1}{2}(f_+ - f_-) = \tfrac{1}{2}(f_1+f_2) - \tfrac{1}{2}(\alpha-\beta) \\ g &= \tfrac{1}{2}(f_+ + f_-) = \tfrac{1}{2}(f_1-f_2) - \tfrac{1}{2}(\alpha+\beta) \end{aligned} \tag{2.19}$$

then using equation (2.14), the relation between f, g, and H is

$$\begin{aligned} f &= -\frac{\partial}{\partial x}\log H \\ g &= +\frac{\partial}{\partial t}\log H \end{aligned} \tag{2.20}$$

In particular for $t=0$ it is found that

$$A(x) = e^{-\int^x f(x',0)dx'} \quad \text{and} \quad B(x) = g(x,0)e^{-\int^x f(x',0)dx'} \tag{2.21}$$

Let

$$F = (f,g)$$

then F is a *vector*, i.e. it transforms in the same way as the coordinates X, so $F' = L_v F$. This can be proved by combining equations (2.8) and (2.19). Another example of a vector is the differential operator

$$\partial \equiv (\frac{\partial}{\partial x}, -\frac{\partial}{\partial t})$$

which can be derived from equation (2.7). The dot product of two vectors $X=(x,x_0)$ and $Y=(y,y_0)$ is defined by

$$X\cdot Y = x_0y_0 - xy$$

which is also a scalar. Equation (2.20) can now be written in the manifest Lorentz covariant form

$$F = -\partial \log H \tag{2.22}$$

2.4 Special solutions

In principle the Boltzmann equation (2.2) has been solved for any initial distribution, i.e. we have written its solution (2.18) in terms of known transcendental functions. However, solution (2.18) in combination with equations (2.12) and (2.14) has a very complex form. To unravel its complexity, in this section we will consider some important special cases: relaxation to equilibrium and shock waves.

Consider the system to be well mixed, so that there is no spatial dependence left. The evolution of the distribution $(f(x,0), g(x,0)) = (f_0, g_0)$ is found to be (by omitting the spatial dependence of equation (2.13))

$$f(t) = f_0 \quad \text{and} \quad g(t) = g^e \frac{1 - ae^{-2g^e t}}{1 + ae^{-2g^e t}} \tag{2.23}$$

where

$$g^e = \sqrt{m^2 + f_0^2} \quad \text{and} \quad a = \frac{g^e - g_0}{g^e + g_0}$$

The conservation of f is a direct consequence of particle number conservation. Each homogeneous initial distribution (f_0, g_0) relaxes exponentially toward a homogeneous equilibrium

$$F^e: \quad (f^e, g^e) = (f_0, \sqrt{m^2 + f_0^2}) \tag{2.24}$$

on a time scale $T = \mathcal{O}(1/g^e) = \mathcal{O}[1/(\sqrt{\alpha\beta})]$, i.e. of the order of a few collisions, which is a characteristic of the Boltzmann approach. All homogeneous equilibria lie on the hyperbola

$$g^{e2} - f^{e2} = m^2 \quad (\text{or } f_+^e f_-^e = m^2) \tag{2.25}$$

which can also be directly found by taking $\frac{\partial f_{1,2}}{\partial t} = \frac{\partial f_{1,2}}{\partial x} = 0$ in (2.2). From equations (2.19) and (2.25) it can be derived that the range of physical solutions, i.e., solutions for which $f_{1,2} \geq 0$, is given by

$$f^e \geq -\tfrac{1}{2}(\alpha - \beta) \tag{2.26}$$

The H^e corresponding to equilibrium F^e is found from (2.22)

$$H^e(X) = e^{F^e \cdot X} \tag{2.27}$$

Note that H obeys the linear equation (2.15). Therefore

$$H_{12}(X) = H_1 + H_2 = \exp^{F_1^e \cdot X - C_1} + \exp^{F_2^e \cdot X - C_2} \tag{2.28}$$

where C_1 and C_2 are constants, is again a solution of (2.15). It corresponds to a shock wave between the equilibria F_1^e and F_2^e. Let $f_1^e > f_2^e$, then for $x \to -\infty$, H_1^e dominates, corresponding to equilibrium F_1^e. For $x \to +\infty$,

H_2^e dominates, corresponding to equilibrium F_2^e. The transition between the two equilibria occurs when both H's are comparable, so

$$(F_2^e - F_1^e) \cdot X = C_2 - C_1 \tag{2.29}$$

This defines a path X^s in the $x - t$ plane moving with a velocity

$$v = \frac{g_2^e - g_1^e}{f_2^e - f_1^e} \tag{2.30}$$

which is identified with the velocity of the shock wave (2.28). For a shock wave to be physical, i.e. the corresponding distributions $f_{1,2}$ are nonnegative, it is a necessary condition that both asymptotic equilibria are physical. Consider the special case of a wave with zero velocity, so $g_1^e = g_2^e \equiv g^e$ (see equation (2.30)) and $f_e^1 = -f_2^e \equiv f^e = \sqrt{g^{e2} - m^2}$ (see equation (2.25)). From equations (2.12), (2.20), and (2.28), it is found that

$$\begin{aligned} f_+(x) &= g^e - f^e \tanh(f^e(x - x_0)) \\ f_-(x) &= g^e + f^e \tanh(f^e(x - x_0)) \end{aligned} \tag{2.31}$$

From the fact that $\tanh(\cdot) \in (-1, +1)$ it follows that the above mentioned condition is also sufficient for nonmoving shock waves. By transforming an arbitrary shock wave to its rest frame and using the fact that the physical region is invariant under such a transformation, one concludes that this condition is sufficient for all shock waves, so

$$H = H_1^e + H_2^e \text{ physical} \iff H_1^e \wedge H_2^e \text{ physical}$$

From equations (2.26) and (2.30) it is concluded that the range of the velocity of shock waves is

$$\frac{\beta - \alpha}{\beta + \alpha} < v < 1 \tag{2.32}$$

In particular nonmoving waves, which are inhomogeneous equilibria, can only occur when $\alpha > \beta$.

The superposition of more than two H^e's corresponds to solutions that represent shock wave interaction. For instance, consider

$$H_{123} = \sum_{i=1}^{3} e^{F_i^e \cdot X}, \quad f_1^e > f_2^e > f_3^e \tag{2.33}$$

For $t \ll 0$, there are two separate shock waves: H_{12} and H_{23}. At $t \approx 0$ the two waves interact, resulting in a single shock wave H_{13} for $t \gg 0$. From (2.30) and the fact that g^e as a function of f^e is convex (see equation (2.25)), it follows that two initially separated shock waves always interact eventually.

It is conjectured that the evolution (2.18) of any initial distribution is as follows: first on a time scale $\mathcal{O}[1/(\sqrt{\alpha\beta})]$, the system will relax toward a number of locally homogeneous equilibria connected by shock waves. Next these shock waves interact on a time scale that depends on their velocities and relative spatial separations, which finally results in a single shock wave.

3. The automaton

3.1 Definition

The automaton is a discrete version of the Boltzmann equation. It consists of a one-dimensional lattice that is updated at discrete time steps. Each lattice site can contain only two bits of information. A "right" bit represents the presence (bit= 1) or absence (bit= 0) of a right-moving (+) particle; a "left" bit denotes the presence (bit= 1) or absence (bit= 0) of a left-moving (+) particle. We will denote this right and left bit at lattice site k and just after timestep l by $b_1(k,l)$ and $b_2(k,l)$ respectively. Furthermore, at each site two bits $\alpha(k,l)$ and $\beta(k,l)$ denote the presence (bit= 1) or absence (bit= 0) of an α and β scatterer, which are set with a probability $\overline{\alpha}$ and $\overline{\beta}$ respectively. In the next section these averages $\overline{\alpha}$ and $\overline{\beta}$ will be related to α and β of the Boltzmann equation.

By analogy with the Boltzmann equation, the updating rule can be decomposed into two substeps: advection and collisions.

The collision substep determines how particles interact. This step *must* give rise to nonlinearities, for if it did not, all particles could be regarded as independent, thus noninteracting. Let the two bits $b'_1(k,l)$ and $b'_2(k,l)$ denote the state of site (k,l) just after this substep has been applied. This state can be a function of the states of adjacent sites and site (k,l) itself, just prior to the collision substep. In particular we will propose a rule whereby $b'_1(k,l)$ and $b'_2(k,l)$ depend only on the state (k,l) itself. The rule must locally conserve particle number, which requires that the empty state 00 and the totally occupied state 11 remain invariant. Only in the two cases where the site contains precisely one particle do we have the freedom to choose (dependent on the outcome of α and β) whether the particle should flip or not. Remembering the collisions (2.1), the following rule is proposed by the truth table:

$b_1(k,l)$	$b_2(k,l)$	$b'_1(k,l)$	$b'_2(k,l)$
0	0	0	0
0	1	$\beta(k,l)$	$!\beta(k,l)$
1	0	$!\alpha(k,l)$	$\alpha(k,l)$
1	1	1	1

(3.1)

The bit operation "!" denotes bitnegation, so $!0 = 1$ and $!1 = 0$.

The advection substep determines the particle flow: + particles are shifted one site to the right, − particles are shifted one site to the left. This leads to the rule

$$\begin{aligned} b_1(k+1,l+1) &= b'_1(k,l) \\ b_2(k-1.l+1) &= b'_2(k,l) \end{aligned} \tag{3.2}$$

The complete automaton rule is found by composing both substeps. Table 3.1 written as a Boolean expression gives:

$$\begin{aligned} b_1(k+1,l+1) = {} & (\beta \wedge (!b_1) \wedge b_2) \vee ((!\alpha) \wedge b_1 \wedge (!b_2)) \vee (b_1 \wedge b_2) \\ b_2(k-1,l+1) = {} & ((!\beta) \wedge (!b_1) \wedge b_2) \vee (\alpha \wedge b_1 \wedge (!b_2)) \vee (b_1 \wedge b_2) \\ & \text{at site } (k,l) \end{aligned} \tag{3.3}$$

where $\vee$ denotes the *inclusive or* and $\wedge$ the *and* operation on a pair of bits. This expression can be converted into an algebraic expression by the use of the conversions $x \vee y = x + y - xy$, $x \wedge y = xy$, and $!x = 1 - x$, which leads to

$$\begin{aligned} b_1(k+1,l+1) = {} & (1-\alpha)b_1 + \beta b_2 + (\alpha - \beta)b_1 b_2 \\ b_2(k-1,l+1) = {} & \alpha b_1 + (1-\beta)b_2 - (\alpha - \beta)b_1 b_2 \\ & \text{at site } (k,l) \end{aligned} \tag{3.4}$$

The nonlinear term $b_1 b_2$ is induced by the *exclusion principle*, i.e. no more than one particle can occupy the same state.

3.2 The ensemble average

To establish a relation with R.W. we must describe the dynamics of the automaton in terms of *ensemble averages*. A large set (ensemble) of systems is considered, each with initial conditions randomly chosen from a given distribution. Then the ensemble averages (or occupation numbers) $\overline{b}_{1,2}(k,l)$ denote the value of the bits $b_{1,2}(k,l)$ averaged over all systems. Updating equations for these averages can be obtained by averaging the automaton rule (3.4). Several averaged products appear in this expression. The Booleans $\alpha(k,l)$ and $\beta(k,l)$ are assumed to be generated by a "perfect" random generator, with averages $\overline{\alpha}$ and $\overline{\beta}$ respectively that are independent of k and l:

$$\overline{\alpha}(k,l) \equiv \overline{\alpha} \quad \text{and} \quad \overline{\beta}(k,l) \equiv \overline{\beta}$$

Therefore averages like $\overline{\alpha(k,l)b_1(k,l)}$ can be written as $\overline{\alpha}\overline{b_1}(k,l)$. However the averaged product $\overline{b_1(k,l)b_2(k,l)}$ cannot be replaced *a priori* by $\overline{b_1}(k,l)\overline{b_2}(k,l)$, for both quantities may be correlated. Therefore the updating equations for $\overline{b_1}$ and $\overline{b_2}$ will contain $\overline{b_1 b_2}$, which leads to a BBGKY hierarchy [9]. By analogy with the Boltzmann approach, we break this hierarchy by making the *Stoßzahlansatz*: particles that are just about to collide are considered to be uncorrelated, so

$$c(k,l) \equiv \overline{((b_1 - \overline{b_1})(b_2 - \overline{b_2}))}_{(k,l)} = (\overline{b_1 b_2} - \overline{b_1}\,\overline{b_2})_{(k,l)} \approx 0 \tag{3.5}$$

This ansatz (which will be tested by simulations) leads to the closed equations for $\overline{b_1}$ and $\overline{b_2}$:

$$\begin{aligned} \overline{b_1}(k+1,l+1) - \overline{b_1}(k,l) = {} & -\overline{\alpha}\,\overline{b_1} + \overline{\beta}\,\overline{b_2} + (\overline{\alpha} - \overline{\beta})\overline{b_1}\,\overline{b_2} \\ \overline{b_2}(k-1,l+1) - \overline{b_2}(k,l) = {} & +\overline{\alpha}\,\overline{b_1} - \overline{\beta}\,\overline{b_2} - (\overline{\alpha} - \overline{\beta})\overline{b_1}\,\overline{b_2} \\ & \text{at site } (k,l) \end{aligned} \tag{3.6}$$

3.3 Symmetries

The variables b_1 and b_2 are bits. Therefore their averages must be contained in the interval $[0,1]$. This can also be seen from the transformation:

$$\mathcal{P}: \left.\begin{array}{l} b_1'(k,l) = !b_2(-k,l) \\ b_2'(k,l) = !b_1(-k,l) \end{array}\right\} \Rightarrow \mathcal{P}^{-1} = \mathcal{P},\ \mathcal{P}^2 = \mathcal{I} \tag{3.7}$$

The reader can check that the automaton rule (3.3) or (3.4) is invariant under this transformation. Using an argument similar to that in section 2.2 it follows that an initial distribution that is contained in the unit interval $[0,1]$ will evolve completely within this interval.

Besides the symmetry $\mathcal{P}$ a second discrete transformation that leaves the system invariant can be defined:

$$\mathcal{A}: \left.\begin{array}{ll} b_1'(k,l) = b_2(k,l), & \alpha'(k,l) = \beta(k,l) \\ b_2'(k,l) = b_1(k,l), & \beta'(k,l) = \alpha(k,l) \end{array}\right\} \Rightarrow \mathcal{A}^{-1} = \mathcal{A},\ \mathcal{A}^2 = \mathcal{I} \tag{3.8}$$

This symmetry allows us to choose $\overline{\alpha}$ always larger than $\overline{\beta}$; from now on this will be always the case.

The space–time lattice can be divided into two types of sites: even sites, for which $k+l$ is even, and odd sites, for which $k+l$ is odd. The collection of each type constitutes a sublattice; the two in combination have a checkerboard structure (see figure 1). From (3.4) it is easily seen that quantities at sites are only affected by quantities at sites of the same kind. Therefore the automaton consists of two completely independent subsystems, each again defined by the rule (3.4), but restricted to one of the two sublattices. The cellular automaton for Burger's equation [8] has precisely the same structure.

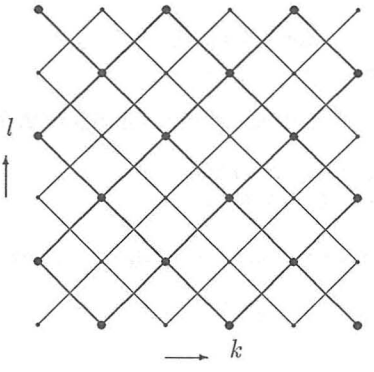

Figure 1: The spatial-temporal lattice divided into two sublattices.

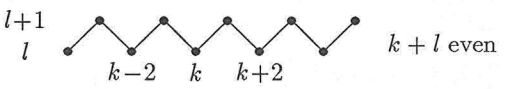

Figure 2: Structure of the sites (k) for the time-independent case.

3.4 Special solutions

More convenient equations are obtained by introducing the binary shifts

$$\begin{array}{lll} b_+ = (\alpha \wedge b_1) \vee (\beta \wedge !b_1) & = & (\alpha - \beta)b_1 + \beta \\ b_- = (\beta \wedge b_2) \vee (\alpha \wedge !b_2) & = & (\beta - \alpha)b_2 + \alpha \end{array} \tag{3.9}$$

so $b_\pm \in \{0,1\}$. Updating rule (3.4) in terms of these new variables reads

$$\begin{array}{ll} b_+(k+1,l+1) - b_+(k,l) = & (\alpha\beta - b_+b_-) \\ b_-(k-1,l+1) - b_-(k,l) = & (\alpha\beta - b_+b_-) \\ & \text{at site } (k,l) \end{array} \tag{3.10}$$

The ensemble averages $\overline{b_+}$ and $\overline{b_-}$ of b_+ and b_- are given by

$$\begin{array}{l} \overline{b_+} = (\overline{\alpha} - \overline{\beta})\overline{b_1} + \overline{\beta} \\ \overline{b_-} = (\overline{\beta} - \overline{\alpha})\overline{b_2} + \overline{\alpha} \end{array} \quad \Rightarrow \overline{b_\pm} \in [\overline{\beta}, \overline{\alpha}] \tag{3.11}$$

Again, closed equations for these averages are obtained by making the Stoßzahlansatz.

Consider the time-independent case. For the subsystem defined on even sites, introduce the notation

$$(k) = \begin{cases} (k,l) & \text{for } k+l \text{ even} \\ (k,l+1) & \text{for } k+l \text{ odd} \end{cases} \tag{3.12}$$

This corresponds to a structure as shown in figure 2. Introduce the variables

$$\begin{array}{l} f(k) = \frac{1}{2}(b_+(k+1) - b_+(k)) \\ g(k) = \frac{1}{2}(b_+(k+1) + b_-(k)) \end{array} \tag{3.13}$$

then their averages $\overline{f}(k)$ and $\overline{g}(k)$ obey the difference equations

$$\overline{g}(k) = \overline{g}(k-1) \quad \Rightarrow \quad \overline{g}(k) \equiv \overline{g_0} \tag{3.14}$$

and

$$\overline{f}(k+1) - \overline{f}(k) = \frac{1}{1-\overline{g_0}}(\overline{f}(k+1)\overline{f}(k) - \overline{g_0}^2 + \overline{\alpha}\overline{\beta}) \tag{3.15}$$

which can be found from equations (3.10) and (3.13). These equations have homogeneous equilibria:

$$\overline{f}(k) = \overline{f_0} \text{ with } \overline{g_0}^2 - \overline{f_0}^2 = \overline{\alpha}\overline{\beta} \tag{3.16}$$

which correspond to nonnegative averages $\overline{b}_1^e$ and $\overline{b}_2^e$ for the range

$$|\overline{f_0}| \leq \tfrac{1}{2}(\overline{\alpha} - \overline{\beta}) \tag{3.17}$$

There are also inhomogeneous equilibria. Let

$$\overline{f_0} = \sqrt{\overline{g_0}^2 - \overline{\alpha}\overline{\beta}} \quad \text{and} \quad z(k) = -\frac{\overline{f}(k)}{\overline{f_0}}$$

then $z(k)$ obeys the explicit difference equation

$$z(k+1) = \frac{z(k) + \frac{\overline{f_0}}{1-\overline{g_0}}}{1 + \frac{\overline{f_0}}{1-\overline{g_0}} z(k)} \tag{3.18}$$

Further let

$$\overline{f_0'} = \tanh^{-1}\left(\frac{\overline{f_0}}{1 - \overline{g_0}}\right)$$

then using the addition formula

$$\tanh(x_1 + x_2) = \frac{\tanh x_1 + \tanh x_2}{1 + \tanh x_1 \tanh x_2}$$

the solution for (3.18) is given by

$$z(k) = \tanh(\overline{f_0'}(k - k_0)), \text{ where } k_0 \in \Re \tag{3.19}$$

For $\overline{b_+}$ and $\overline{b_-}$ these equilibria read:

$$\begin{array}{rcl} \overline{b_+}(k) & = & \overline{g_0} - \overline{f_0}\tanh(\overline{f_0'}(k - k_0 - \frac{1}{2})) \\ \overline{b_-}(k) & = & \overline{g_0} + \overline{f_0}\tanh(\overline{f_0'}(k - k_0 + \frac{1}{2})) \end{array} \tag{3.20}$$

Next consider a transition (or shock wave) between two homogeneous equilibria, $(\overline{f_0}, \overline{g_0}) = (\overline{f}_1, \overline{g}_1)$ for $k \to \infty$ and $(\overline{f}_2, \overline{g}_2)$ for $k \to -\infty$, moving with a rational velocity $v = p/q$. Assume that this transition relaxes to some stable shape, so

$$\overline{b}_{1,2}(k, l+q) = \overline{b}_{1,2}(k-p, l) \tag{3.21}$$

Define

$$\begin{array}{rcl} \overline{f}(k,l) & = & \frac{1}{2}(\overline{b_+}(k,l) - \overline{b_-}(k,l)) \\ \overline{g}(k,l) & = & \frac{1}{2}(\overline{b_+}(k+1,l) + \overline{b_-}(k,l)) \end{array} \tag{3.22}$$

then by subtracting the equations of (3.10) one finds the continuity equation

$$\left\{\overline{f}(k,l+1) - \overline{f}(k,l)\right\} + \left\{\overline{g}(k,l+1) - \overline{g}(k-1,l+1)\right\} = 0 \tag{3.23}$$

Note that for homogeneous equilibria definitions (3.13) and (3.22) coincide. Using relation (3.21) summation of equation (3.21) over k and l yields

$$\left\{ \sum_{k=-(n+1)p+1}^{-np} - \sum_{k=(n-1)p+1}^{np} \right\} \overline{f}(k,0) + \sum_{l=1}^{q} (\overline{g}(np,l) - \overline{g}(-np,l)) = 0 \quad (3.24)$$

In the limit $n \to \infty$ the remaining summations are over regions where the limiting equilibria dominate. This leads to the velocity of the shock wave:

$$p\overline{f}_1 - p\overline{f}_2 + q\overline{g}_2 - q\overline{g}_1 = 0 \Rightarrow v = \frac{\overline{g}_2 - \overline{g}_1}{\overline{f}_2 - \overline{f}_1} \quad (3.25)$$

4. Relationship between the Boltzmann equation and the cellular automaton

Now that the properties of both the Boltzmann equation and the automaton have been studied we can relate the two systems.

First the lattice is fixed in space–time: site (k,l) is associated with the event

$$(x,t) = (k\Delta, l\Delta)$$

Δ is the spatial and temporal lattice spacing.

Next the averaged quantities of the automaton are related to the physical quantities of the Boltzmann equation. In R.W. the probability during a time interval Δ, a + particle flips is $\Delta\alpha + \mathcal{O}(\Delta^2)$. Therefore we choose:

$$\overline{\alpha} = \alpha\Delta \quad \text{and} \quad \overline{\beta} = \beta\Delta \quad (4.1)$$

When $\alpha > \beta$ it was found in section 2.2 that for R.W., as a consequence of nonlinearity, the interval $[0, \alpha - \beta]$ is an invariant of evolution. For the automaton it was found in section 3.2 that, as a consequence of the exclusion principle, the averages $b_{1,2}$ are restricted to $[0,1]$. Bearing this in mind define

$$\hat{f}_{1,2}(x = k\Delta, t = l\Delta) = (\alpha - \beta) b_{1,2}(k,l) \quad (4.2)$$

From equation (3.4) it is found that these $\hat{f}_{1,2}$ obey the relations

$$\begin{aligned} (\frac{\partial}{\partial t} + \frac{\partial}{\partial x})\hat{f}_1(x,t) &= +\Omega(\hat{f}_1(x,t), \hat{f}_2(x,t)) + \mathcal{O}(\Delta) \\ (\frac{\partial}{\partial t} - \frac{\partial}{\partial x})\hat{f}_2(x,t) &= -\Omega(\hat{f}_1(x,t), \hat{f}_2(x,t)) + \mathcal{O}(\Delta) \end{aligned} \quad (4.3)$$

which differs by $\mathcal{O}(\Delta)$ from the Boltzmann equation (2.2) for the distributions f_1 and f_2. Therefore an initial difference of $\mathcal{O}(\Delta)$ between $\hat{f}_{1,2}$ and $f_{1,2}$ will remain $\mathcal{O}(\Delta)$ on a time scale of at least $\mathcal{O}(1)$.

One can test this result by comparing special solutions of both systems, where R.W. is restricted to $\alpha > \beta$, $f_{1,2} \in [0, \alpha - \beta]$. The homogeneous equilibria (2.25) and (3.16) coincide by the identification

$$\overline{g_0} = \Delta g^e \text{ and } \overline{f_0} = \Delta f^e; \quad |f^e| \leq \tfrac{1}{2}(\alpha - \beta) \quad (4.4)$$

Inhomogeneous equilibria (2.31) and (3.20) both have the shape of a tanh. Their difference of $\mathcal{O}(\Delta)$ is completely accounted for by a shift of half a lattice site, and a contraction

$$\overline{f_0'} = \overline{f_0}(1 + \Delta g^e) + \mathcal{O}(\Delta^2) \tag{4.5}$$

in the space variable x. Shock wave velocities (2.30) and (3.25) coincide and are bounded by

$$|v| \leq \frac{\alpha - \beta}{\alpha + \beta} = \frac{\overline{\alpha} - \overline{\beta}}{\overline{\alpha} + \overline{\beta}} \tag{4.6}$$

Assuming that the conjecture made at the end of section 2.4 is correct, it is concluded that differences between $\hat{f}_{1,2}$ and $f_{1,2}$ remain $\mathcal{O}(\Delta)$ for all solutions for all time scales.

5. Simulations

The automaton constructed in section 3 was simulated by a Turbo C program on an Atari 1040ST computer. Two lines of 16 bit-words, each corresponding to an array of + or − particles, were used to represent the microscopic configuration of the system. To represent the state of scatterers, the bits of two additional words were randomly set with a probability $\overline{\alpha}$ or $\overline{\beta}$. Thanks to the homogeneity and locality property, all bits of a word could be updated simultaneously.

A straightforward method of deciding which bits of a word should be set is to apply a (quasi) random number generator to each bit individually. In this way the probability $c(n)$ that n bits within a word will be set is given by the binomial distribution

$$c(n) = \binom{16}{n} p^n (1 - p^{16-n}), \quad p = \overline{\alpha} \text{ or } \overline{\beta}$$

Now recall that $\overline{\alpha}$ and $\overline{\beta}$ are of order Δ, so very small when $\Delta \ll 1$. Therefore the probability that more than two bits will be set is neglected by truncating all powers of p higher than two in the binomial distribution:

$$\begin{array}{lcrcrcl} c'(0) & = & 1 & - & 16p & + & 120p^2 \\ c'(1) & = & & & 16p & - & 240p^2 \\ c'(2) & = & & & & & 120p^2 \\ c'(k) & = & 0 & & & & 2 < k \leq 16 \end{array} \tag{5.1}$$

For $p \in [0, \frac{1}{15}]$ equation (5.1) again defines a distribution, i.e. it is normalized and positive definite. Further single bits are set with a probability p and the products of two bits are uncorrelated, i.e. $\overline{b_i b_j} = p^2$ for $i \neq j$. Products of more than two different bits are zero, so they are completely anticorrelated. This truncation leads to the following procedure. A random number x_i is generated in order to decide whether zero, one, or two bits are to be set. In the case where one bit is to be set, its place (16 alternatives) is determined by

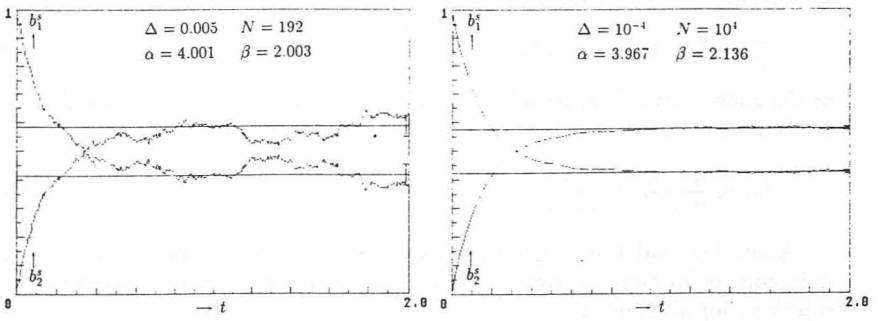

Figure 3: Simulation of relaxation toward equilibrium using homogeneous initial distributions and periodic boundary conditions. The averages b_1^s and b_2^s were taken over the entire spatial lattice (N sites). The horizontal solid lines correspond to the appropriate homogeneous equilibria. Error bars at the right margins indicate the expected fluctuations.

using information from the same random number x_i. When two bits are to be set, a second random number x_{i+1} is generated to determine their places (120 alternatives). In this way no more than two random numbers are needed to fill a word, which is about a factor 10 less than in the straightforward method.

Spatial averaging of a single evolution was used to estimate ensemble averages, instead of averaging over a large set of evolutions all subject to a given initial distribution. Define the spatial average over N sites at site (k, l) by

$$b_{1,2}^s(k,l) \equiv \frac{1}{N}\sum_{i=1}^{N} b_{1,2}(k+i,l) \tag{5.2}$$

It can be shown (see for instance [8]) that if correlations between different $b_{1,2}$'s are of no importance

$$b_i^s(k,l) - \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} \frac{f_{1,2}(x, l\Delta)\,dx}{\alpha - \beta} = \mathcal{O}\left(\sqrt{\frac{1}{4N}}\right) \tag{5.3}$$

where $x_1 = k\Delta$ and $x_2 = (k+N)\Delta$. So this spatial average of a single automaton evolution approximates to the spatial average of the Boltzmann equation, the typical difference being $\sqrt{1/4N}$.

First the system was subject to periodic boundary conditions. All initial distributions were found to relax to the homogeneous equilibrium (3.16) belonging to the conserved total particle number, with fluctuations of the order given by (5.3). In figure 3 the evolution of two homogeneous initial distributions is presented by averaging over all lattice sites. Relaxation times were

indeed found to be of the order of a few collisions. Correlations between + and − particles at the same site were estimated by

$$c(l) = \frac{< b_+ b_- > - < b_+ >< b_- >}{\sqrt{< b_+ > (1 - < b_+ >) < b_- > (1 - < b_- >)}} \tag{5.4}$$

where $< x > \equiv \frac{1}{N} \sum_{k=1}^{k=N} x(k,l)$ and N is the number of lattice sites. These estimates were found to fluctuate around zero, with amplitudes of $\mathcal{O}(\frac{1}{\sqrt{N}})$.

Next fixed boundaries were imposed: at each advection step, a + (−) particle at the site furthest to the most left (right) was created, with a certain probability. Figure 4 shows the evolution of homogeneous initial distributions. The lattice spacing was $\Delta = 2^{-10}$ and the lattice consisted of $N = 6144$ sites, so $x \in [0, 6]$; $\alpha = 40$ and $\beta = 10$. Spatial averages were taken over 400 lattice sites. The observed evolution was in agreement with theory: after an initial relaxation, three shock waves appeared. At $t \approx 10$

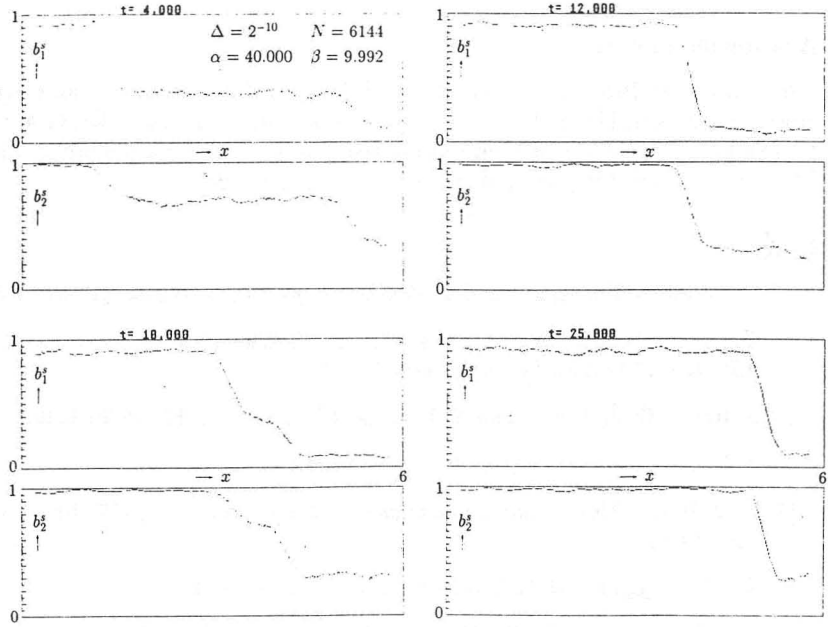

Figure 4: Simulation of shock wave interaction as a function of time, using homogeneous initial distributions and fixed boundaries. The spatial lattice consisted of $N = 6144$ sites. Averages were taken over 400 lattice sites.

both waves interact, resulting in a single wave. The velocities of the waves were in agreement with (3.25).

6. Conclusions

A cellular automaton for the solvable Ruijgrok–Wu model has been constructed, analyzed, and simulated. With the relationship given in section 4 it has been shown that for $\alpha > \beta$ the two systems coincide qualitatively. Quantitatively the automaton is an approximation of R.W. up to the first order of the lattice spacing Δ. These deviations could not be found by simulations for they were obscured by the statistical fluctuations of $\mathcal{O}(\sqrt{\Delta})$. In addition, simulations show that the Stoßzahlansatz, which had to be made for both systems in order to derive closed evolution equations for one-particle distributions, is correct.

Two Boltzmann equations (with different α and β) can be related by a combination of a Lorentz and scaling transformation. Such exact relations cannot be obtained for the automaton due to the discreteness of the lattice. However on the basis of the relations between the two systems as established in section 4 it is concluded that two automata, $(\overline{\alpha}_1, \overline{\beta}_1)$ and $(\overline{\alpha}_2, \overline{\beta}_2)$, for which $\overline{\alpha}_{1,2} > \overline{\beta}_{1,2}$, *can* be related up to terms of order Δ for all time scales.

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