

Microscopic Shock Structure in Model Particle Systems: The Boghosian-Levermore Cellular Automaton Revisited

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This paper is dedicated to Natascha A. Brunswick.

Abstract

We carried out new computer simulations of the Boghosian-Levermore stochastic cellular automaton for the Burgers equation. The existence of an extra "conservation law" in the dynamics—even and odd lattice sites exchange their contents at every time step—implies that the automaton decomposes into two independent subsystems; the simulations show that the density from each subsystem exhibits a "shock front" which does not broaden with time. The location of the shock in a particular microscopic realization differs from that predicted by the Burgers equation by an amount which depends only on the initial microscopic density of the particle system, that is, fluctuations in the stochastic dynamics do not affect the shock profile on the time scale considered. This is in complete accord with theoretical expectations. The apparent broadening of the shock in the original Boghosian-Levermore simulations is shown to result from averaging the two subsystem densities.

1. Introduction

The time evolution of hydrodynamic variables, such as the macroscopic density and velocity profiles of a fluid, is described by suitable autonomous hydrodynamic equations—Euler, Navier-Stokes, etc. The hydrodynamic variables themselves correspond to certain collective aspects of the positions and velocities of fluid molecules whose evolution is governed by microscopic laws, and the hydrodynamical equations ought therefore to be derivable from the more fundamental microscopic dynamics. Such a derivation would, in addition to its intrinsic interest, also clarify the domain of validity of the macroscopic laws and yield corrections to them. While these corrections can be expected to be unimportant, for most practical purposes, when the solution of the hydrodynamic equations is smooth, they might become significant in the case of strong instabilities or discontinuities, such as shocks.

Unfortunately, a precise derivation of macroscopic behavior from microscopic dynamics is a difficult mathematical problem and there are few rigorous results along these lines for systems with realistic (Hamiltonian) dynamics. There has, however, been considerable progress in recent years in deriving hydrodynamical laws for model systems with stochastic microscopic dynamics; see [14] for a review. These simple models contain many of the essential ingredients responsible for the hydrodynamic behavior of real systems. In particular, the hydrodynamic laws are seen to be a consequence of general features of the microscopic dynamics, particularly of the conservation laws. They become exact in suitable scaling limits, i.e., when the ratio of micro to macro length and time scales goes to zero. When this ratio is small but not zero (say, Angstroms to centimeters) the corrections to the hydrodynamic description will also be small. Exceptions can occur, however, when

the macroscopic flows are unstable; the hydrodynamic equations may then cease to describe the actual behavior of the particle system after a long time.

An interesting question that has been recently studied in this context is what happens to the system when the hydrodynamic equations predict the formation of shocks. For example, it is known that the Burgers equation

$$(1.1) \quad \frac{\partial}{\partial t} u + c \frac{\partial}{\partial x} u[1 - u] = 0, \quad 0 \leq u(x, t) \leq 1, \quad c > 0,$$

gives rise to discontinuities in $u(x, t)$ even if the initial profile $u(x, 0)$ is smooth. There are several types of microscopic particle models for which (1.1) is the appropriate equation for the macroscopic density profile, in particular: (a) a continuous time process known as the asymmetric simple exclusion process (ASEP), studied in [16], [15], and [2], and (b) a discrete time cellular automaton invented by Boghosian and Levermore (BLCA); see [3]. The question is: will the discontinuity in the density profile for the solution of (1.1) be visible on the microscopic scale in the particle model or will there be some smoothing on an intermediate scale?

The theory developed for the ASEP predicts that the former alternative holds: the shock profile will form in the microscopic particle system and, despite the inevitable microscopic fluctuations, will be present without substantial broadening even after a long macroscopic time. Instead, these fluctuations will manifest themselves as random deviations between the location of the "microscopic shock" and the shock predicted by (1.1). The square of this difference, averaged over different microscopic realizations, will grow linearly in time, with a diffusion constant determined by microscopic density fluctuations in the initial macroscopic state. Fluctuations due to the stochasticity of the dynamics will produce broadenings of smaller magnitude; they are expected to scale as $t^{1/3}$ rather than $t^{1/2}$ (see [18]).

There seems to be little doubt that this theoretical analysis applies to the BLCA as well as to the ASEP, once an extra conservation law in the former is taken into account. Our computer simulations were carried out mostly for the BLCA, which serves as a prototype of CA's used for modeling higher dimensional flows (see [11]), or more precisely of a stochastic version of these CA's developed in [5]. The extra conservation law in the BLCA is similar to that found by Zanetti for FHP models; see [20]. We present both models briefly, and describe the theoretical results for the ASEP, in Section 2. The results of computer simulations are given in Section 3. Concluding remarks are presented in Section 4.

2. The Models

The Asymmetric Exclusion Process (ASEP)

The ASEP represents a system of particles moving in the one-dimensional lattice \mathbb{Z} ; each site of the lattice \mathbb{Z} is empty or is occupied by one particle. A configuration is specified by a collection of occupation numbers $\underline{\eta} = \{\eta(x)\}_{x \in \mathbb{Z}}$, with $\eta(x) = 0, 1$. The process takes place in continuous time: particles attempt to jump to the

adjacent site on the right or left at a constant but asymmetric rate, succeeding when that site is unoccupied. The hydrodynamic equation for the density profile is then (1.1), with c the difference in left and right jump rates. We will not give a detailed description of the ASEP, but rather summarize the results of a theoretical analysis.

Suppose that the initial occupation numbers $\eta_0(x)$ are independent and distributed according to an initial shock between densities u_{\pm} , with $u_+ > u_-$:

$$(2.1) \quad \text{Prob}(\eta_0(x) = 1) = \begin{cases} u_+, & \text{if } x \geq 0; \\ u_-, & \text{if } x < 0. \end{cases}$$

The physically appropriate (entropic) solution of (1.1) for the corresponding macroscopic initial condition $u(x, 0) = u_{\pm}$ for $x \gtrless 0$ is $u(x, t) = u(x - vt, 0)$, with $v = c(1 - u_+ - u_-)$. At the microscopic level, there is a well-defined shock position X_t such that:

- (i) The shock is microscopically sharp (see [7], [6], [10], [8]). Specifically, if $\hat{\eta}_t$ denotes the configuration obtained by translating η_t by X_t , then $\hat{\eta}_t(x)$ approaches its asymptotic density as $x \rightarrow \pm\infty$ at a rate uniform in time: for $\epsilon > 0$ there is a $y_\epsilon > 0$ such that if $|x| \geq y_\epsilon$ then

$$|E\hat{\eta}_t(x) - u_{\pm}| < \epsilon,$$

where the sign in u_{\pm} is the same as the sign of x . (The result actually proved is stronger: as $x \rightarrow \pm\infty$, the local statistical state near x approaches a Bernoulli state, of density u_{\pm} , at a rate uniform in time.)

- (ii) The average position of the microscopic shock moves as the shock of the entropic solution of the Burgers equation: $EX_t = c(1 - u_+ - u_-)t$.
- (iii) Overall fluctuations in the shock position are of order $t^{1/2}$ (see [6]): there exists a diffusion constant D such that

$$(2.2) \quad \lim_{t \rightarrow \infty} t^{-1} E[X_t - EX_t]^2 = D.$$

In fact, this result is established rigorously only for $u_- = 0$, but is believed to hold generally.

- (iv) The fluctuations described by (2.2) are due principally to fluctuations in the initial configuration; randomness during the evolution has a lower order effect (see [12], [8]). Specifically, if for each initial configuration η_0 we let E_{η_0} denote the expectation conditioned on this initial configuration, then

$$\lim_{t \rightarrow \infty} t^{-1} E[X_t - E_{\eta_0} X_t]^2 = 0.$$

Again, the result has been proven only for $u_- = 0$.

The Boghosian-Levermore Cellular Automata (BLCA)

The BLCA also represents particles moving in \mathbb{Z} ; each particle now has a velocity ± 1 and an exclusion rule prevents two particles of the same velocity from occupying the same site. A configuration of the system is specified by occupation variables $\{\eta(x; \sigma)\}_{x \in \mathbb{Z}, \sigma = \pm 1}$, where $\eta(x; \sigma) = 1$ if there is a particle at x with velocity σ and $\eta(x; \sigma) = 0$ otherwise. At each integral time t the automaton undergoes a two-step updating which depends on an asymmetry parameter p , $0 \leq p \leq 1$:

Step 1—Velocity flips. Particle positions are fixed, but if there is a single particle at x then its velocity changes stochastically, so that after the updating the velocity is $+1$ with probability p and -1 with probability $1 - p$. All of the choices of new velocities for different space-time points are independent.

Step 2—Advection. Particle velocities are fixed, but each particle moves deterministically one lattice unit in the direction of its velocity.

It is clear from this description that the variables $\eta_t(x; \sigma)$ with $t + x$ odd evolve independently from those with $t + x$ even, and that the system thus decomposes into two independent automata.

Let ρ be the macroscopic density for this automaton; note that $0 \leq \rho \leq 2$. It was shown formally by Boghosian and Levermore in [3] that, for lattice spacing a and time step τ in macroscopic units, the Burgers equation (1.1), with $u = \rho/2$ and $c = (2p - 1)a/\tau$, is the appropriate macroscopic equation. Related rigorous results are contained in [13]. It is believed, although as yet unproved, that a microscopic shock position X_t exists and satisfies the properties (i)–(iv) discussed above for the ASEP; moreover, it appears that at least some of these properties may be derived by techniques similar to those used for the ASEP; see [9].

3. Simulations

Boghosian and Levermore (see [3]) simulated the BLCA using periodic boundary conditions on an automata of 2^{16} sites; a density profile was obtained at different times by counting the number of particles in spatial “bins” of 2^7 or 2^9 consecutive sites. Under these conditions, the extra conservation law noted above implies that the experiment is really a simulation of two independent automata, each with 2^{15} sites. The theoretical results suggest that to see the microscopically sharp shock it is necessary to separate the results from the two sublattices; otherwise, the process of counting in bins superimposes two shocks which (due to fluctuations in the initial configuration) may be located at different positions. The result will appear to be a shock smeared in space or, if the two shocks are separated sufficiently, a shock profile with an intermediate step.

To investigate the effect we have rerun the simulations on both the Cyber 205 at the John von Neumann Center (using a 2^{15} -site lattice and a dynamics which mimics the original sub-lattice dynamics) and the Cellular Automata Machine (using a 2^{16} -site lattice and the original dynamics). In the first case, and after sub-lattice separation in the second, we see a shock which is sharp on the micro-scale of the experiment; the latter is determined by a spatial averaging of the results over bins of 2^6 sites. This result is as expected from property (i) above.

In our simulations, as in [3], the scaling is chosen so that $a = 2^{-16}$ and $\tau = 2^{-18}$ (the system then has macroscopic length $L = 1$), the macroscopic initial density is

$$(3.1) \quad \rho(x, 0) = 2u(x, 0) = 1 + 0.4 \cos 2\pi x,$$

and the asymmetry parameter p is 0.625; the resulting Burgers equation (1.1) has $c = 1$. The exact solution of (1.1) with periodic boundary condition and initial condition (3.1) is known (see [3]): a shock forms at position $x = 0.75$ and time $t = 5/4\pi \approx 0.398$ and thereafter remains stationary, reaching a maximum amplitude $(\Delta\rho)_{\max} = 0.8$ at time $t = 0.625$ and then decaying in amplitude. A rigorous analysis of microscopic behavior in this periodic geometry has not been carried out in either the ASEP or the BLCA, but the general behavior discussed in Section 2 is expected to persist.

The results from typical Cyber runs are shown in Figures 1 and 2. Figure 1 gives the time history of a single simulation. To facilitate comparison with similar

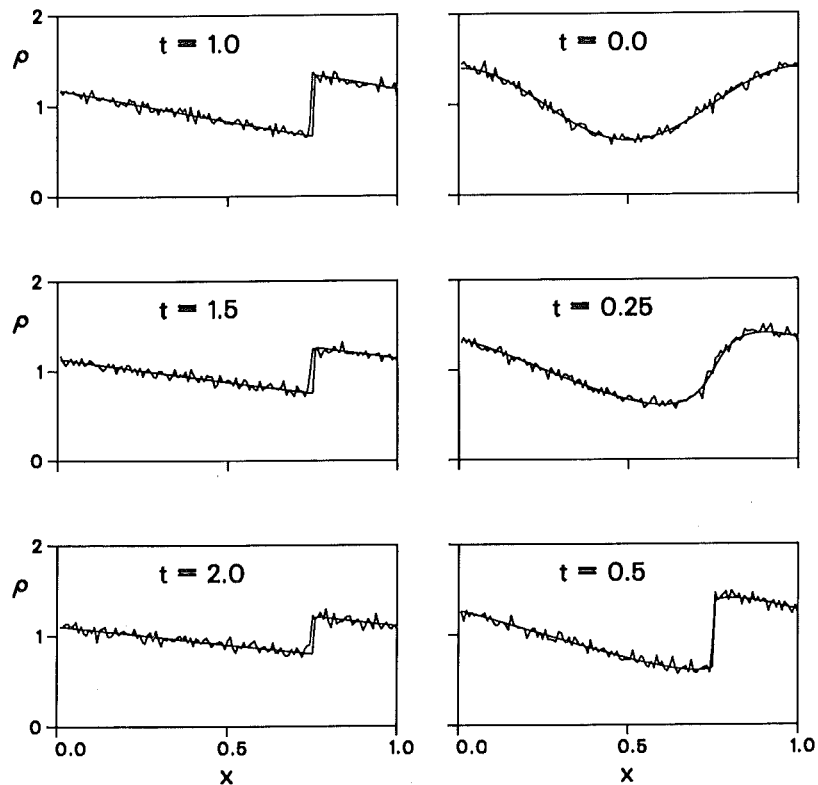


Figure 1. Shock profiles for BLCA simulation and for exact solution of the Burgers equation.

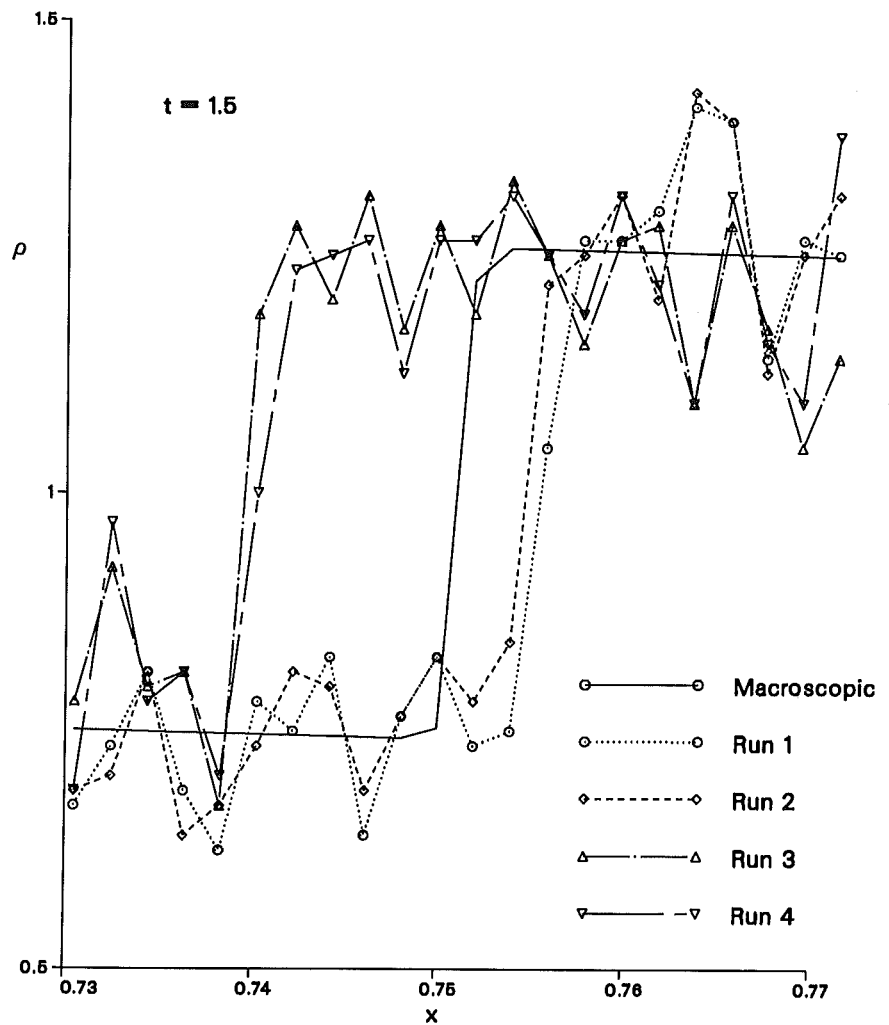


Figure 2. Detail of shock profiles for exact solution of the Burgers equation and for four BLCA simulations. Runs 1 and 2 had identical (microscopic) initial conditions, as did runs 3 and 4.

figures in [3], data is averaged into 2^7 bins of 2^8 sites each (this is the number of bins used for most figures in [3], although there each bin contains data from both subsystems). The exact solution of the Burgers equation is also plotted.

Figure 2 shows an expanded view of the region near the shock at time $t = 1.5$. Results from four simulations are shown; runs 1 and 2 are generated with the same (microscopic) initial configuration but with different stochastic choices for the dynamics, as are runs 3 and 4. Data are averaged in bins of size 2^6 ; the macroscopic solution is plotted at this same resolution. Note that for each run the shock shows

no broadening at this resolution (the presence of a data point in the middle of a rise signals only that a bin overlaps the shock front). Note also that the microscopic shock position depends primarily on the initial configuration rather than on the particular realization of the dynamics, in accordance with properties (iii) and (iv) above. In fact, even density fluctuations on the scale of bins appear to be relatively independent of the dynamics.

As mentioned above, it is expected (see [14], [6], [8]) that, in the infinite system, the microscopic shock position is determined primarily by density fluctuations in the initial configuration. The periodic geometry will complicate the specifics of this effect, but we can isolate two simple elements in the initial configuration which will affect shock motion. The first is a net excess or deficit of particles: if there are N_0 particles at the 2^{15} sites, and $\bar{\rho} = 2^{-15}N_0$, then the shock should move with average velocity $1 - \bar{\rho}$ (if $u(x, t)$ is a solution of (1.1), so is $b + u(x - 2cbt, t)$, where the argument $x - 2cbt$ is interpreted modulo 1). The second is an effective translation of the initial condition, detectable by the presence of a $\sin 2\pi x$ Fourier component in the initial data: the result will be (roughly) a corresponding constant shock displacement. Estimation of these effects for the data presented in Figure 2 yield predicted shock positions of 0.754 for runs 1 and 2 and 0.742 for runs 3 and 4, in rough accord with the data. We also did simulations in which the initial configuration was chosen randomly, according to (3.1), on part of the lattice, then extended to the entire lattice to preserve on a microscopic level the macroscopic symmetry $\rho(\hat{x}) = 2 - \rho(x)$, where $\hat{x} = 1.5 - x \bmod 1$. As expected, in these simulations the microscopic shock coincided with the macroscopic shock at all times.

We have also carried out simulations of the ASEP on the Cyber, using the same periodic geometry and sinusoidal initial condition as discussed above; the results are similar to those for the BLCA and will not be reported in detail. Note that ASEP simulations for a shock between two constant densities on an infinite line, which confirm in greater detail the theoretical predictions (i)–(iv), have been reported in [4].

4. Concluding Remarks

Generalizations

It is natural to ask whether the shock behavior found here also occurs in one-dimensional systems with Hamiltonian dynamics, or in stochastic or Hamiltonian particle systems in higher dimensions. In particular, do density shocks in real fluids correspond to discontinuities in the density on a microscopic scale? The property of our models illustrated in Figure 2, that the evolution is relatively independent of the particular realization of the dynamics, suggests that similar behavior may occur in deterministic systems. Note that, if so, then we would not expect local equilibrium to hold at the macroscopic shock position; rather, the state there would be superposition of the phases in front of and behind the shock. (This is similar to the situation at a first-order transition in equilibrium; e.g., the Gibbs state of an Ising spin system at zero field and low temperature is a superposition of the plus

and minus magnetization states.) The corresponding result for the ASEP has been derived in [6], [1], [19].

Simulations

The original simulations of the BLCA were carried out by Boghosian and Levermore (see [3]) on a Connection Machine. The Cellular Automata Machine (see [17]) is also well suited to the problem; we use a spiral geometry for the automaton on the master CAM and generate random numbers by a kicked lattice gas on a slave. A full run to $t = 2.5$ takes about three hours. On the other hand, the large number of random numbers needed tends to make simulation on a conventional supercomputer rather slow. To speed up the simulation on the Cyber we modified the idea used on the CAM: we generated a vector of 2^{15} random bits with density p and used random shifts of this vector for updating, with a new random vector generated periodically—for most runs, about every thousand updates. Time for a run was then comparable to the time on the CAM.

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Note Added in Proof

Actually (1.1) is the correct macroscopic equation only for $(2p - 1)$ small. In general the term $u(1 - u)$ in (1.1) should be replaced by $J/2c$, where J is the current in equilibrium at density $2u$, $J = \{1 - [1 - 4u(1 - u)(2p - 1)^2]^{1/2}\}/(2p - 1)$. For the parameters and initial conditions (3.1) considered in [3] and here, the change in the solution produced by this modification is too small to be relevant.

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