Chaos and Entropy of a Lattice Gas Cellular Automaton

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Foundations of statistical physics

... the essential features of the evolution do not depend on specific dynamical properties such as positivity of the Lyapunov exponents, ergodicity or mixing...

J. Lebowitz, Boltzmann's entropy and time's arrow, Phys. Today 1973

A simple stochastic model

- M *macroscopic* configurations $x_1, \ldots, x_M$.
- $P(x) = 1/M$ (microcanonical distribution). $S = \log(M)$.
- Coarse-grained stochastic dynamics:

$$W(x'|x) = \begin{cases} 1/\alpha & \text{for } \alpha M \text{ entries;} \\ 0 & \text{otherwise.} \end{cases}$$

- W is irreducible.

Entropy and Lyapunov exponents

The Kolmogorov-Sinay entropy (information production in the coarse-grained dynamics) is

$$K = -\sum_{x} P(x) \sum_{x'} W(x'|x) \log \left(W(x'|x) \right) = \log(\alpha) + \log(M).$$

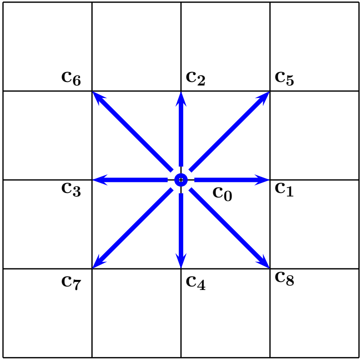
- K is the sum of positive Lyapunov exponents.
- We can assume $K \propto \lambda_0$.
- Since $\log(M) = S$ we get

$$\lambda_0 \propto \log(\alpha) + S.$$

A multiparticle model: LGCA

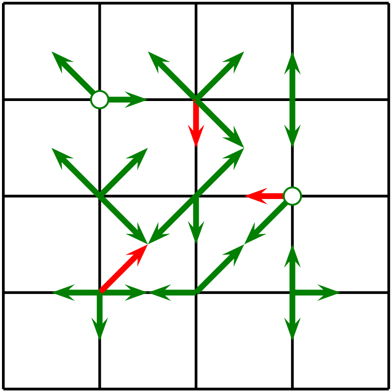
- Lattice gas cellular automata (LGCA) are discrete, deterministic dynamical models.
- Hydrodynamical behavior.
- Multispeed LGCA have equilibrium thermodynamics.
- It is possible to define the largest Lyapunov exponent λ_0.

The $D2Q9$ LGCA: Discrete space and velocities

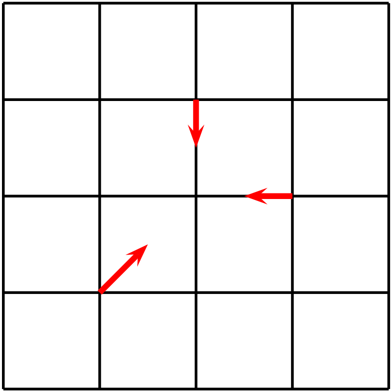


$$c_i = \begin{cases} 0 & i = 0, \\ 1 & i = 1, 2, 3, 4, \\ \sqrt{2} & i = 5, 6, 7, 8. \end{cases}$$

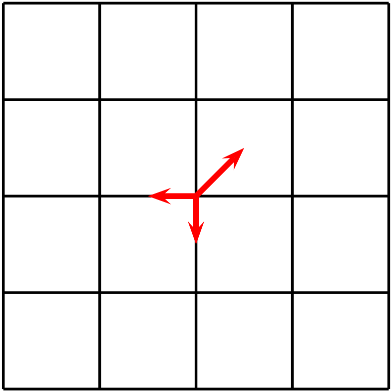
Streaming and collision



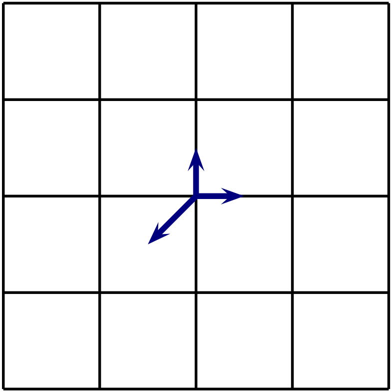
Streaming and collision



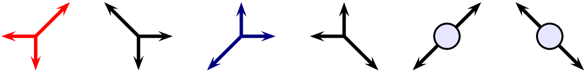
Streaming and collision



Streaming and collision



Multiple collisions



Exclusion principle

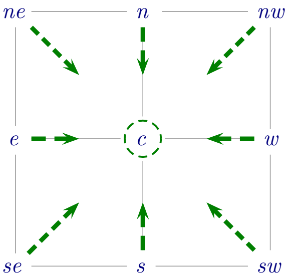
$$s(\mathbf{r},t) = (s_8, s_7, \ldots, s_0), \quad s_k = 0, 1.$$

b states cellular automaton

$$s(\mathbf{r},t) = \sum_{k=0}^{8} s_k 2^k, \quad 0 \leq s(\mathbf{r},t) < 2^9 = b,$$

$$s(\mathbf{r},t+1) = \mathbf{CS}(\{s(\mathbf{r}',t)\}_{r' \in \mathcal{V}(\mathbf{r})}).$$

Streaming and collision

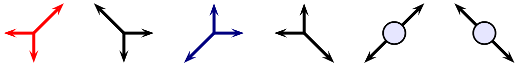


$$s_k(\mathbf{r}, t+1) = C_k(s_0(c,t), s_8(ne,t), s_4(n,t), s_7(nw,t),$$
$$s_3(w,t), s_6(sw,t), s_2(s,t), s_5(se,t), s_1(s,t))$$

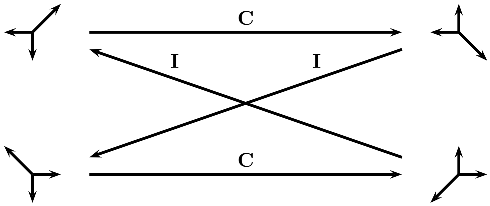
$$k = 0, \ldots, 8$$

The $D2Q9$ LGCA

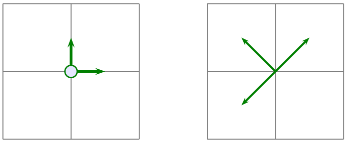
- Deterministic $D2Q9$ LGCA.

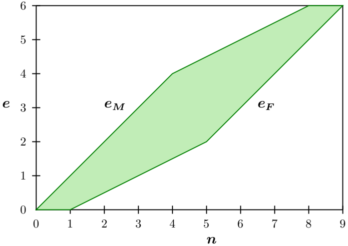


- Reversible $D2Q9$ LGCA.



Fermi energy e_F and maximum energy e_M





$$e_F = \begin{cases} 0 & 0 \le n < 1, \\ (n-1)/2 & 1 \le n < 5, \\ n-3 & 5 \le n \le 9, \end{cases}$$

$$e_M = \begin{cases} n & 0 \le n < 4, \\ (n+4)/2 & 4 \le n < 8, \\ 6 & 8 \le n \le 9. \end{cases}$$

Boolean cellular automaton

$$s(\mathbf{r}) = (s_8(\mathbf{r}), \ldots, s_0(\mathbf{r})), \quad s_k = 0, 1, \quad k = 0, \ldots, 8,$$

$$\mathbf{s} = (s(\mathbf{r}_0), \ldots, s(\mathbf{r}_{L-1}))\,,$$

$$\mathbf{r}_m \in \Lambda, m = 0, \ldots, L, \quad L = |\Lambda|$$

$$\mathbf{s} = (s_0, s_1, \ldots, s_{\mathcal{L}-1})\,, \quad s_n = 0, 1,$$

$$n = 0, \ldots, \mathcal{L} - 1, \quad \mathcal{L} = 9L, \qquad \mathbf{s} \in B^{\mathcal{L}}, \quad B = \{0, 1\}$$

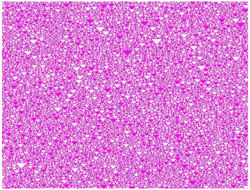
$$s_n(t+1) = F(\mathbf{s}(t)).$$

Boolean derivatives

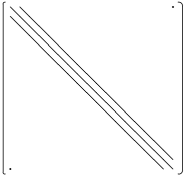
$$
\begin{aligned}
J_{np} = \frac{\partial s_n(t+1)}{\partial s_p(t)} &= \left| F(\dots, s_p, \dots) - F(\dots, 1 - s_p, \dots) \right|, \\
n, p &= 0, \dots, \mathcal{L} - 1, \\
\mathbf{v}(t+1) &= J\left(\mathbf{s}(t)\right) \mathbf{v}(t), \quad \mathbf{v} \in \mathbb{R}^{\mathcal{L}}, \\
|\mathbf{v}(T)| &\sim |\mathbf{v}(0)| e^{\lambda T}, \\
\lambda = \frac{1}{T} \log &\left[\frac{|\mathbf{v}(T)|}{|\mathbf{v}(T-1)|} \frac{|\mathbf{v}(T-1)|}{|\mathbf{v}(T-2)|} \cdots \frac{|\mathbf{v}(1)|}{|\mathbf{v}(0)|} \right] \\
&= \frac{1}{T} \sum_{t=1}^{T} \log \mathbf{u}(t) = \left\langle \log \mathbf{u}(t) \right\rangle_T, \\
u(t) &= |\mathbf{v}(t)| / |\mathbf{v}(t-1)|.
\end{aligned}
$$

F. Bagnoli, R. Rechtman, S. Ruffo, Phys. Lett. A **172** (1992) 34.

Example: elementary cellular automaton rule 150



$J =$



$$s_i(t+1) = s_{i-1} \oplus s_i \oplus s_{i+1}$$

$$\frac{\partial s_i(t+1)}{\partial s_{i+k}} = s_{i+k} \oplus \overline{s_{i+k}} = 1, \qquad k = 0, \pm 1$$

$$\lambda = \log 3$$

Kinetic theory

Evolution equation of a LGCA

$$s_k(\mathbf{r} + \mathbf{c}_k, t+1) = s_k(\mathbf{r}, t) + \delta(s(\mathbf{r}, t)),$$
$$\delta = 0, \pm 1.$$

Boltzmann's transport equation

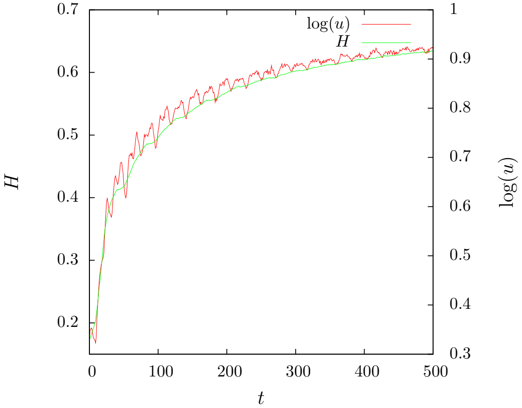
$$f_k(\mathbf{r}, t) = \langle s_k(\mathbf{r}, t) \rangle \, ,$$
$$f_k(\mathbf{r} + \mathbf{c}_k, t+1) = f_k(\mathbf{r}, t) + \Delta_k(s(\mathbf{r}, t)).$$

Boltzmann's H theorem

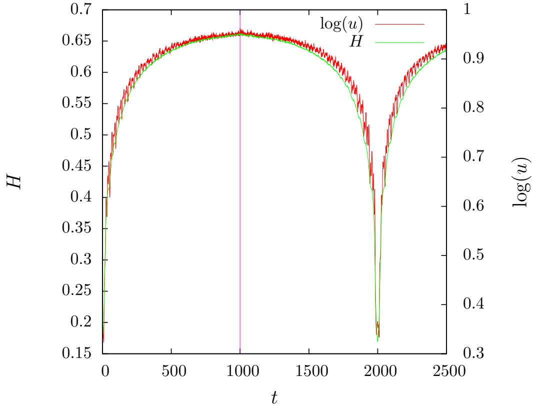
$$H(t) = -\sum_{\mathbf{r}} \sum_k \left[f_k \log f_k + (1 - f_k) \log(1 - f_k) \right],$$
$$\frac{dH}{dt} \geq 0.$$

U. Frisch, D. d'Humierés, B. Hasslacher, Y. Pomeau, J-P. Rivet, Complex Systems **1** 649 (1987).

Boltzmann's H function and maximum Lyapunov exponent



Time reversal



Thermodynamic equilibrium

$$N = \sum_{\mathbf{r}} \sum_{k} f_k(\mathbf{r}), \qquad E = \sum_{\mathbf{r}} \sum_{k} \epsilon_k f_k(\mathbf{r})$$

$$f_1 = f_2 = f_3 = f_4, \quad f_5 = f_6 = f_7 = f_8,$$

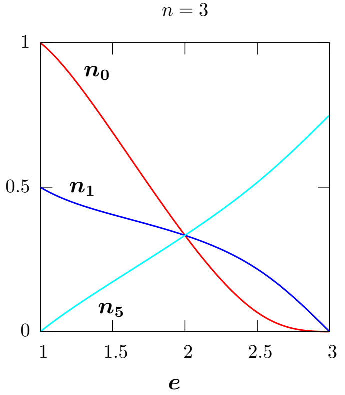
$$N_k = \sum_{\mathbf{r}} f_k(\mathbf{r}),$$

$$n_k = N_k/L, \qquad n = N/L, \qquad e = E/L$$

$$0 \leq n \leq 9, \qquad 0 \leq e \leq 6$$

A. Salcido, R. Rechtman, in P. Cordero, B. Nachtergaele eds., *Nonlinear Phenomena in Fluids, Solids and Other Complex Systems*, Elsevier, 1991.

Entropy density and equilibrium distribution functions



$$S(E, N, L) = \log \Omega(E, N, L) = Ls$$

$$s(e, n) = -\sum_{k=0}^{8} [\hat{n}_k \log \hat{n}_k + (1 - \hat{n}_k) \log(1 - \hat{n}_k)] ,$$

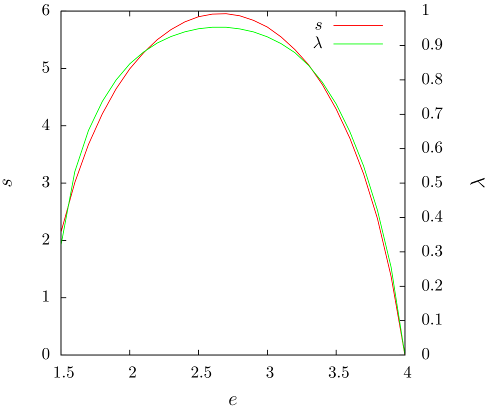
$$\hat{n}_k = [\exp(\beta\epsilon_k - \beta\mu) + 1]^{-1} .$$

$$\beta = \frac{\partial s}{\partial e}, \qquad \mu = \frac{\partial s}{\partial n},$$

$$n = \sum_k \hat{n}_k = \hat{n}_0 + 4\hat{n}_1 + \hat{n}_5$$

$$e = \sum_k \epsilon_k \hat{n}_k = 2\hat{n}_1 + 4\hat{n}_5$$

Equilibrium entropy and maximum Lyapunov exponent



Conclusions

- LGCA are "minimal" models with a hydrodynamic limit. The $D2Q9$ model includes thermal effects.
- Our version of $D2Q9$ is a discrete, deterministic and reversible dynamical system.
- The Jacobian matrix, defined with Boolean derivatives, can be used to measure the sensitivity to a (finite) initial difference.
- Confirm the stochastic toy model:
  - For the relaxation towards equilibrium,

$$\log u(t) = A + BH(t)$$

  - In equilibrium,

$$\lambda = A + Bs$$

- Work is in progress on other systems.