

Entropy and chaos in a discrete hydrodynamical system

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Contents

- 1 Introduction
- 2 The *D2Q9* LGCA
- 3 Maximum Lyapunov exponent of the *D2Q9* LGCA
- 4 Boltzmann's *H* function
- 5 Gibbs entropy of the *D2Q9* LGCA
- 6 Final remarks



Introduction

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...*

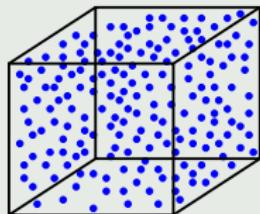
J. Lebowitz, Boltzmann's entropy and time's arrow, *Phys. Today* 1973

*The foundation of statistical laws, as understood by the modern physics community encompasses three principal aspects: the origin of statistical laws from deterministic dynamical equations, the conditions of applicability of different statistical approximations, and criteria for the transition from deterministic to statistical behavior. The discovery of **chaos** in dynamical systems makes it necessary to reconsider our views on each of these aspects, with potentially significant consequences.*

G. M. Zaslavsky, Origin of Statistical Laws, *Phys. Today*, August, 1999

Introduction

Statistical physics, mechanics



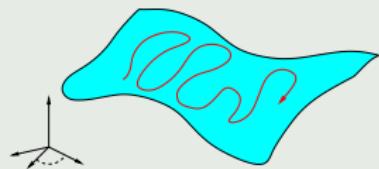
$$(\mathbf{q}, \mathbf{p}) = (q_1, q_2, q_3, \dots, q_{3n}, p_1, p_2, p_3, \dots, p_{3n})$$

$$H(\mathbf{q}, \mathbf{p}) = \sum_{i=1}^{3n} \frac{p_i^2}{2m} + U(\mathbf{q}) = E$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$

Introduction

Statistical physics, ergodic hypothesis



$$\langle f \rangle = \frac{1}{T} \lim_{T \rightarrow \infty} \int_0^T f(\mathbf{q}(t), \mathbf{p}(t)) dt = \int_{\Gamma} \rho(\mathbf{q}, \mathbf{p}) f(\mathbf{q}, \mathbf{p}) d\mathbf{q} d\mathbf{p}$$

$$\rho(\mathbf{q}, \mathbf{p}) = \frac{1}{\Omega(E, V, n)} \delta(E - H(\mathbf{q}, \mathbf{p}))$$

$$\Omega(E, V, n) = \frac{1}{h^{3n}} \int_{\Sigma(E)} d\mathbf{q} d\mathbf{p}$$

$$\Sigma(E, V, n) = \{(\mathbf{q}, \mathbf{p}) \mid H(\mathbf{q}, \mathbf{p}) = E\}$$

Introduction

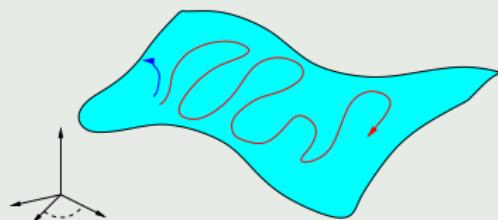
Statistical physics, thermodynamics

$$S(E, V, n) = k \log \Omega(E, V, n)$$

$$\frac{1}{T} = \frac{\partial S(E, V, N)}{\partial E}$$

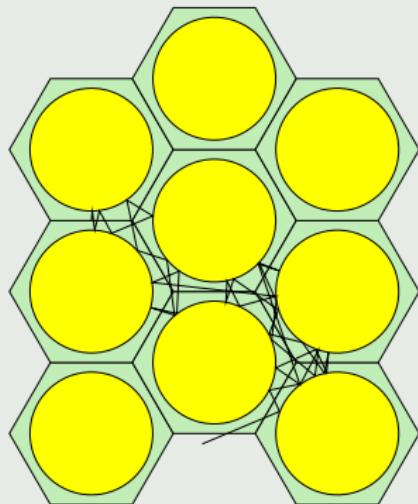
$$\frac{P}{T} = \frac{\partial S(E, V, N)}{\partial V}$$

$$\frac{\mu}{T} = -\frac{\partial S(E, V, N)}{\partial N}$$



Introduction

Lorentz gas



Escape rate formalism

$$D \sim \frac{L^2}{a} \sum_{\lambda_i > 0} \lambda_i - h_{KS}$$

P. Gaspard, G. Nicolis, PRL **65**, 1693, (1990). P. Gaspard, J. R. Dorfman, PRE **52** 3525 (1995). J. R. Dorfman, H. van Beijeren, Physica A **240**, 12, (1997).

Introduction

Entropy vs. Kolmogorov–Sinai entropy

- Molecular dynamics for simple liquids (LJ), 500 particles, 10-20 collision times

$$\frac{h_{KS}}{\Gamma_{coll}} = A + BS_{ex}$$

- h_{KS} Kolmogorov–Sinai entropy
- Γ_{coll} average collision frequency
- $S_{ex} = S - S_{ideal}$

M. Dzugutov, E. Aurell, A. Vulpiani, PRL **81** 1762 (1998)

Introduction

Largest Lyapunov exponent and entropy of the *D2Q9 LGCA*

- Lattice gas cellular automata **LGCA** have fluid dynamics behavior.
- Multispeed **LGCA** have equilibrium thermodynamics.
- The largest Lyapunov **LLE** exponent of deterministic CA can be defined.
- Results
 - Deterministic and reversible *D2Q9 LGCA*.
 - Relation between the **LLE** and thermodynamic entropy density **s**.
 - Relation between the expansion rate of the **LLE** and Boltzmann's **H function**.

Contents

1 Introduction

2 The *D2Q9* LGCA

3 Maximum Lyapunov exponent of the *D2Q9* LGCA

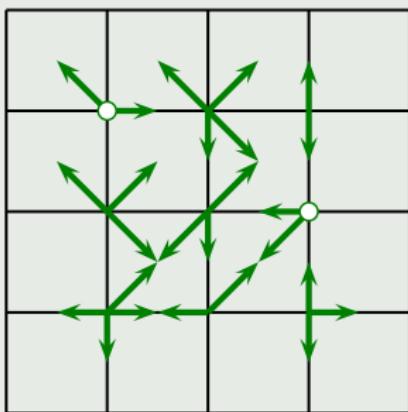
4 Boltzmann's *H* function

5 Gibbs entropy of the *D2Q9* LGCA

6 Final remarks

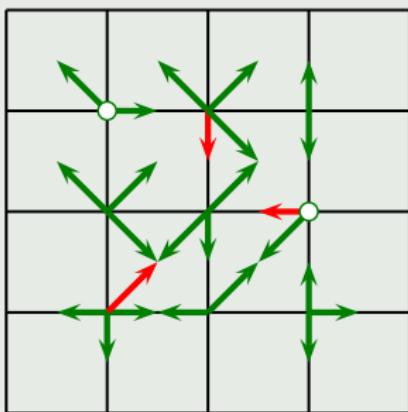
The *D*2Q9 LGCA

Streaming and collision



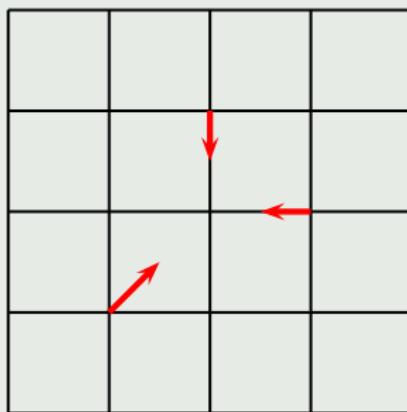
The *D*2Q9 LGCA

Streaming and collision



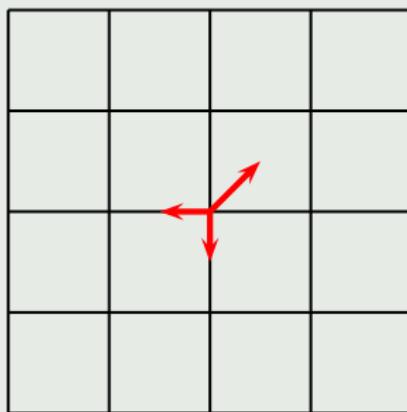
The *D2Q9* LGCA

Streaming and collision

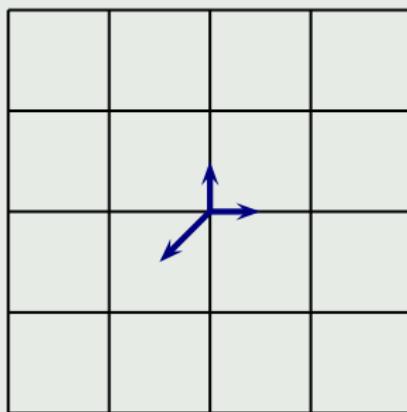


The *D2Q9* LGCA

Streaming and collision



Streaming and collision



The D2Q9 LGCA

Streaming and collision

Mass and momentum conservation



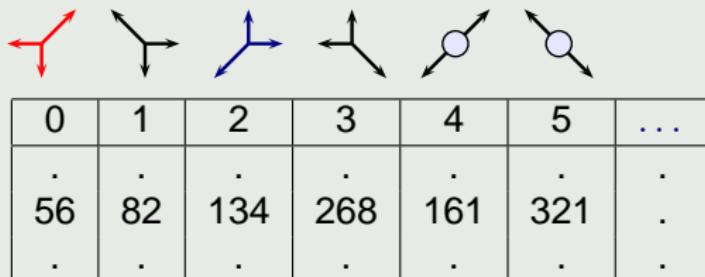
$$s(\mathbf{r}, t) = (s_8, s_7, \dots, s_0), \quad s_k = 0, 1, \quad \text{exclusion principle}$$

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

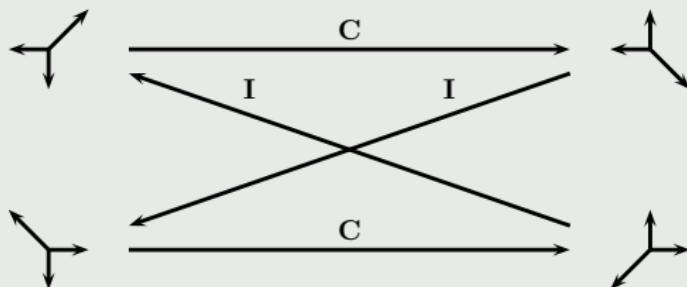
$$s(\mathbf{r}, t+1) = \mathbf{CS}(\{s(\mathbf{r}', t)\}_{\mathbf{r}' \in \mathcal{V}(\mathbf{r})})$$

The *D2Q9* LGCA

Deterministic *D2Q9* LGCA

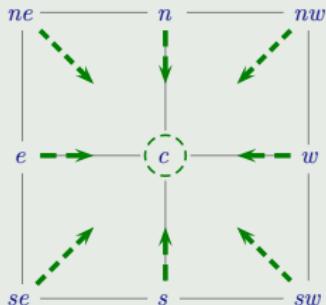


Reversible *D2Q9* LGCA



The D2Q9 LGCA

Deterministic Streaming and collision



$$s_k(\mathbf{r}, t+1) = C_k(s_8(ne, t), s_7(nw, t), s_6(sw, t), s_5(se, t), s_4(n, t), s_3(w, t), s_2(s, t), s_1(e, t), s_0(c, t), \eta(\mathbf{r}))$$
$$k = 0, \dots, 8$$

Contents

- 1 Introduction
- 2 The *D2Q9* LGCA
- 3 Maximum Lyapunov exponent of the *D2Q9* LGCA
- 4 Boltzmann's *H* function
- 5 Gibbs entropy of the *D2Q9* LGCA
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Maximum Lyapunov exponent of the D2Q9 LGCA

2^9 CA \rightarrow Boolean CA

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

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

$$\mathbf{r}_m \in \Lambda, m = 0, \dots, L-1, \quad L = |\Lambda|$$

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

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

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

F_n depends on k and $\eta(\mathbf{r})$.

Maximum Lyapunov exponent of the D2Q9 LGCA

Boolean derivatives

$$J_{np} = \frac{\partial F_n(\mathbf{s})}{\partial s_p} = |F_n(\dots, s_p, \dots) - F_n(\dots, 1 - s_p, \dots)|$$

$$n, p = 0, \dots, \mathcal{L} - 1$$

$$\mathbf{v}(0) = \mathbf{s}(0) \oplus \mathbf{x}(0), \quad |\mathbf{v}(0)| = 1, \quad \text{initial damage}$$

$$\mathbf{v}(t+1) = J(\mathbf{s}(t)) \mathbf{v}(t), \quad \mathbf{v} \in \mathbb{R}^{\mathcal{L}}$$

$$|\mathbf{v}(T)| \sim |\mathbf{v}(0)| e^{\lambda T}$$

$$\lambda = \frac{1}{T} \log \left[\frac{|\mathbf{v}(T)|}{|\mathbf{v}(T-1)|} \frac{|\mathbf{v}(T-1)|}{|\mathbf{v}(T-2)|} \dots \frac{|\mathbf{v}(1)|}{|\mathbf{v}(0)|} \right]$$

$$= \frac{1}{T} \sum_{t=1}^T \log \mathbf{u}(t) = \langle \log \mathbf{u}(t) \rangle_T$$

$$u(t) = |\mathbf{v}(t)| / |\mathbf{v}(t-1)|$$

Contents

- 1 Introduction
- 2 The *D2Q9* LGCA
- 3 Maximum Lyapunov exponent of the *D2Q9* LGCA
- 4 Boltzmann's *H* function
- 5 Gibbs entropy of the *D2Q9* LGCA
- 6 Final remarks



Boltzmann's H function

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

$$H(t) = - \sum_{\mathbf{r}} \sum_k [f_k \log f_k + (1 - f_k) \log(1 - f_k)]$$

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

Fluid dynamics

Fluid dynamics equations



Chapman–Enskog expansion



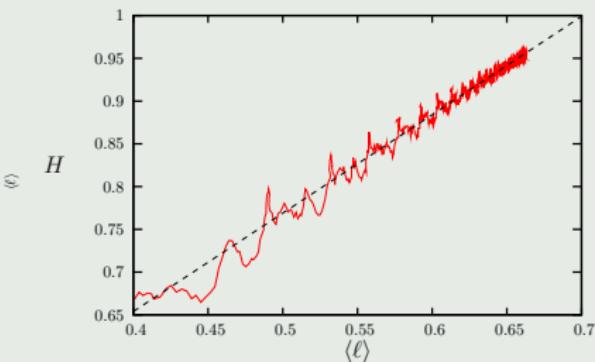
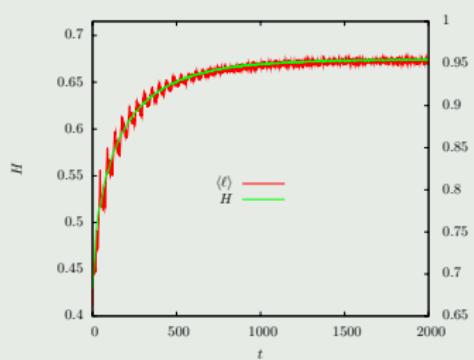
Conservation theorems



Boltzmann's transport equation

Boltzmann's H function

H and $\log u$



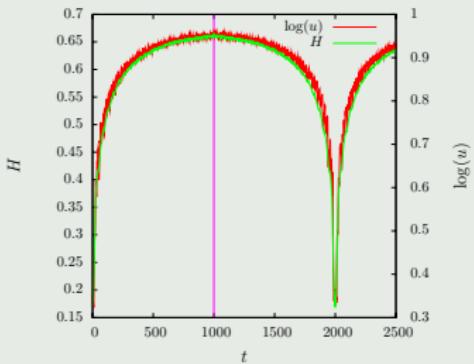
$$f_k(\mathbf{r}, t) = (1/R) \sum_i^R s_k^{(i)}(\mathbf{r}, t)$$

$$u(t) = |\mathbf{v}(t)| / |\mathbf{v}(t-1)|$$

$$\begin{aligned} H(t) &= - \sum_{\mathbf{r}, k} [f_k(\mathbf{r}, t) \log f_k(\mathbf{r}, t) \\ &\quad + (1 - f_k(\mathbf{r}, t)) \log(1 - f_k(\mathbf{r}, t))] \end{aligned}$$
$$\langle \ell(t) \rangle = (1/R) \sum_i^R \log u^{(i)}(t)$$

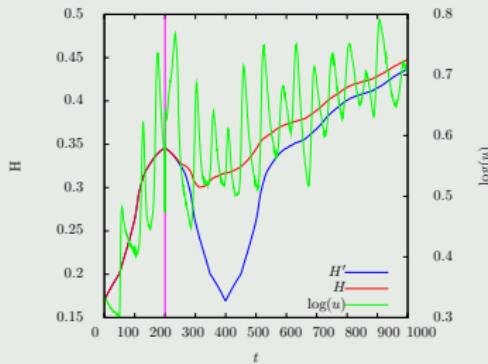
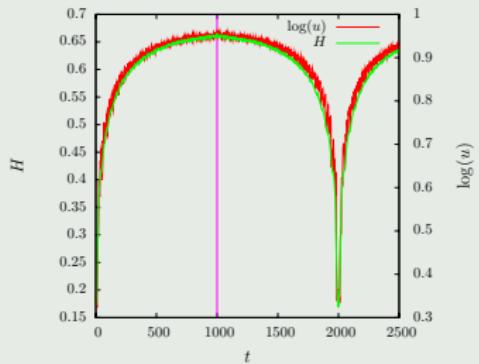
Boltzmann's H function

Time reversal



Boltzmann's H function

Time reversal



Contents

1 Introduction

2 The *D2Q9* LGCA

3 Maximum Lyapunov exponent of the *D2Q9* LGCA

4 Boltzmann's *H* function

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6 Final remarks



Gibbs entropy of the D2Q9 LGCA

Entropy

$$S = - \sum_{\mathbf{s}} p(\mathbf{s}) \log p(\mathbf{s})$$

$$p(\mathbf{s}) \sim \prod_{\mathbf{r}, k} f_k(\mathbf{r})^{s_k(\mathbf{r})} (1 - f_k(\mathbf{r}))^{1-s_k(\mathbf{r})}$$

$$S = - \sum_{\mathbf{r}, k} f_k(\mathbf{r}) \log f_k(\mathbf{r}) + (1 - f_k(\mathbf{r})) \log(1 - f_k(\mathbf{r}))$$

Gibbs entropy of the D2Q9 LGCA

Thermodynamic equilibrium

$$S = S/L = - \sum_k f_k \log f_k + (1 - f_k) \log(1 - f_k)$$

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

$$\epsilon_0 = 0, \quad \epsilon_{1,2,3,4} = 1/2, \quad \epsilon_{5,6,7,8} = 1$$

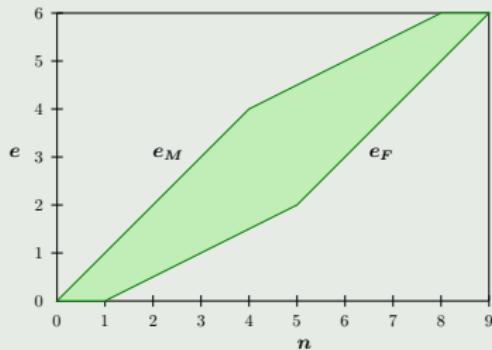
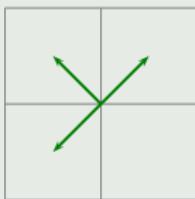
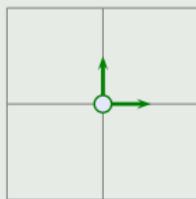
$$n = N/L, \quad e = E/L$$

$$n = f_0 + 4f_1 + 4f_5, \quad e = 2f_1 + 4f_5$$

$$S = - [f_0 \log(f_0) + (1 - f_0) \log(1 - f_0) + \\ 4(f_1 \log(f_1) + (1 - f_1) \log(1 - f_1)) + \\ 4(f_5 \log(f_5) + (1 - f_5) \log(1 - f_5))]$$

Gibbs entropy of the D2Q9 LGCA

Fermi energy e_F and maximum energy e_M

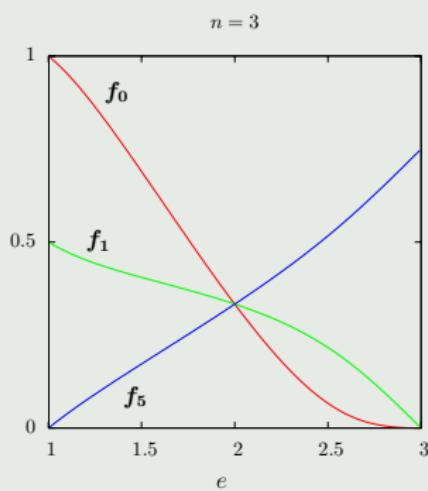


$$e_F = \begin{cases} 0 & 0 \leq n < 1 \\ (n-1)/2 & 1 \leq n < 5 \\ n-3 & 5 \leq n \leq 9 \end{cases}$$

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

Gibbs entropy of the D2Q9 LGCA

Entropy density and equilibrium distribution functions



$$n = \sum_k f_k, \quad e = \sum_k \epsilon_k f_k$$

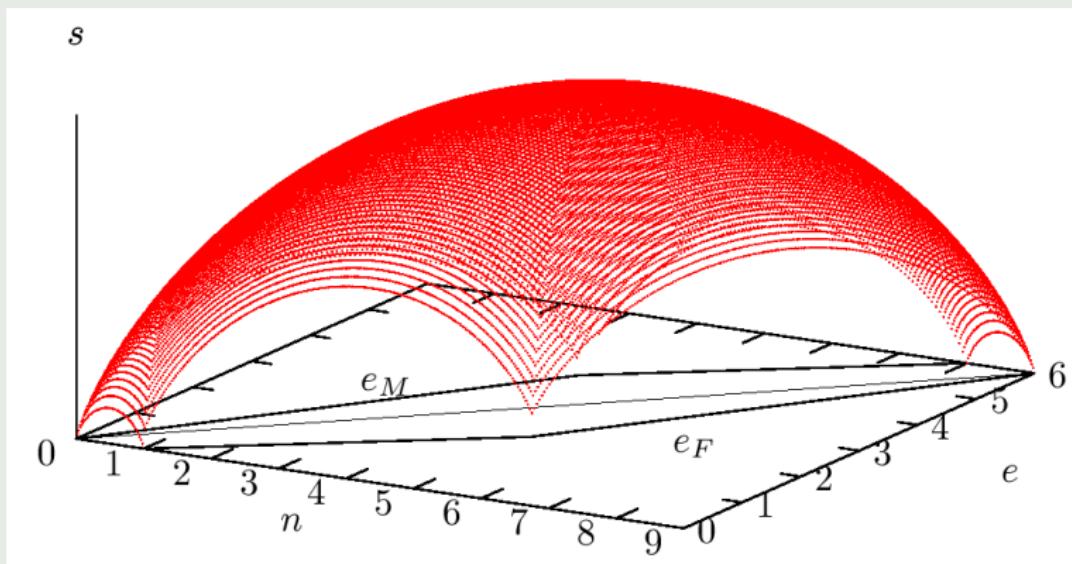
$$s = - \sum_k [f_k \log(f_k) + (1 - f_k) \log(1 - f_k)]$$

$$f_k = [\exp(\beta \epsilon_k - \beta \mu) + 1]^{-1}$$

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

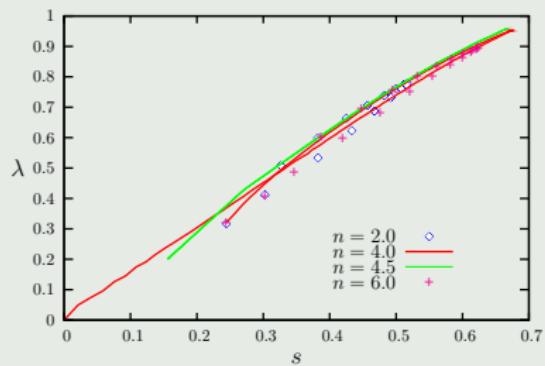
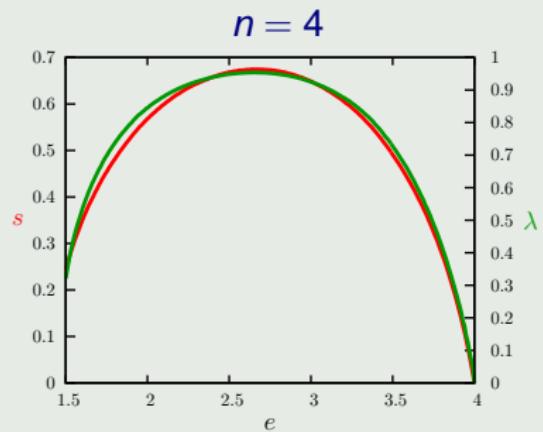
Gibbs entropy of the D2Q9 LGCA

Entropy density



Gibbs entropy of the $D2Q9$ LGCA

s and λ



Contents

- 1 Introduction
- 2 The *D2Q9* LGCA
- 3 Maximum Lyapunov exponent of the *D2Q9* LGCA
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- 5 Gibbs entropy of the *D2Q9* LGCA
- 6 Final remarks



Final remarks

Markov chain

$P(x) = 1/M$, microcanonical distribution

$$W(x'|x) = \begin{cases} 1/\alpha M & \alpha M \text{ entries in a row (column)} \\ 0 & (1 - \alpha)M \text{ entries in a row (column)} \end{cases}$$

$$S = - \sum_x P(x) \log P(x) = \log M$$

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



Final remarks

- LGCA are **minimal** models with a hydrodynamic limit. The *D2Q9* model includes thermal effects.
- The *D2Q9* evolution can be **deterministic** and **reversible**.
- The Jacobian matrix, defined with Boolean derivatives, can be used to measure the sensitivity to a (finite) initial difference.
- In an irreversible process
 $\log u(t) = BH(t)$.
- In equilibrium
 $\lambda = A + Bs$.
- The value of λ is related to the number of 1's in the Jacobian matrix J , the value of s is related to the number of available states.

Thank you

