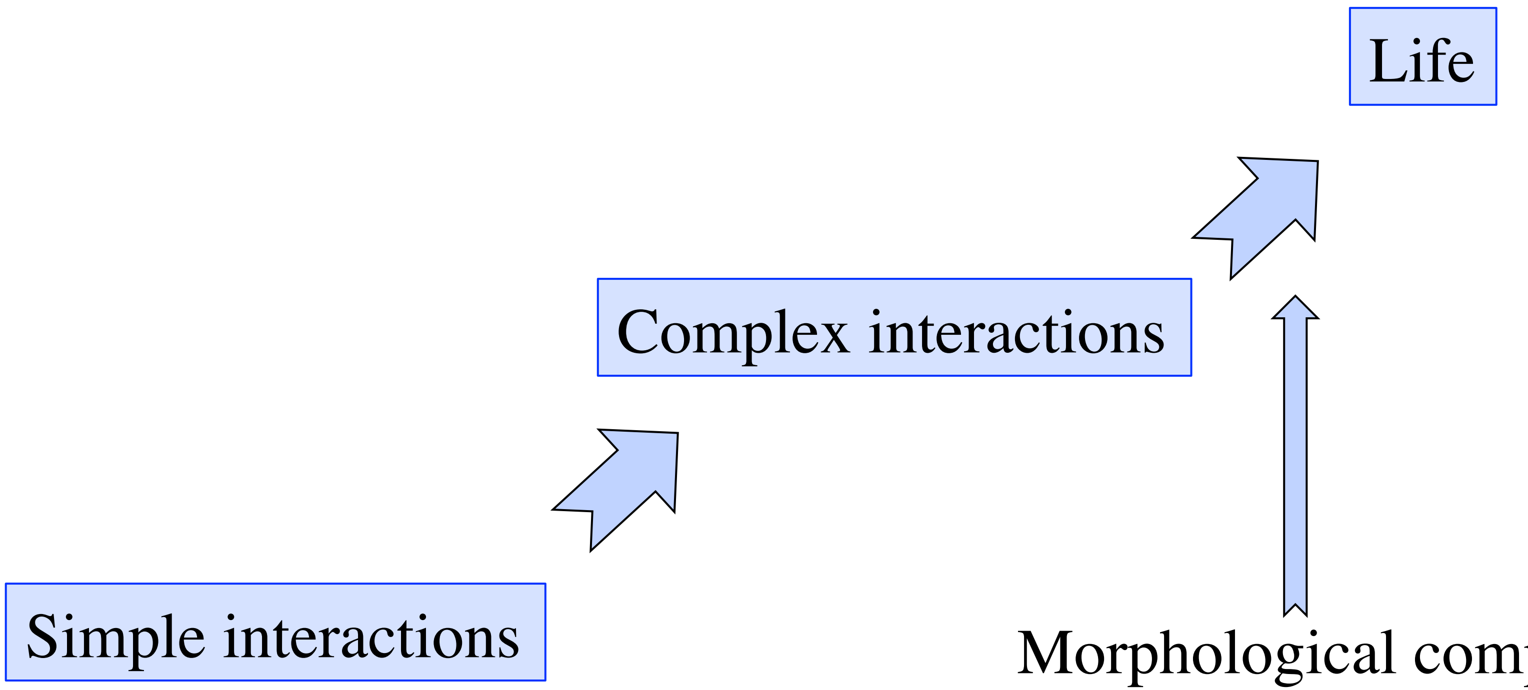
# Non-equilibrium pattern formation with extended particles
# or
# Microscopic models for morphological computation

Norman Packard
European Center for Living Technology
ProtoLife Inc.

(work with Rob Shaw)

# Morphological computation and the origin of life

- Morphological computation on a molecular scale coincides with the origin of life:




Morphological computation:
where life gives purpose
to complex dynamics

# Concentrate on programmability for now…

Morphological computation requires a physical instantiation with…

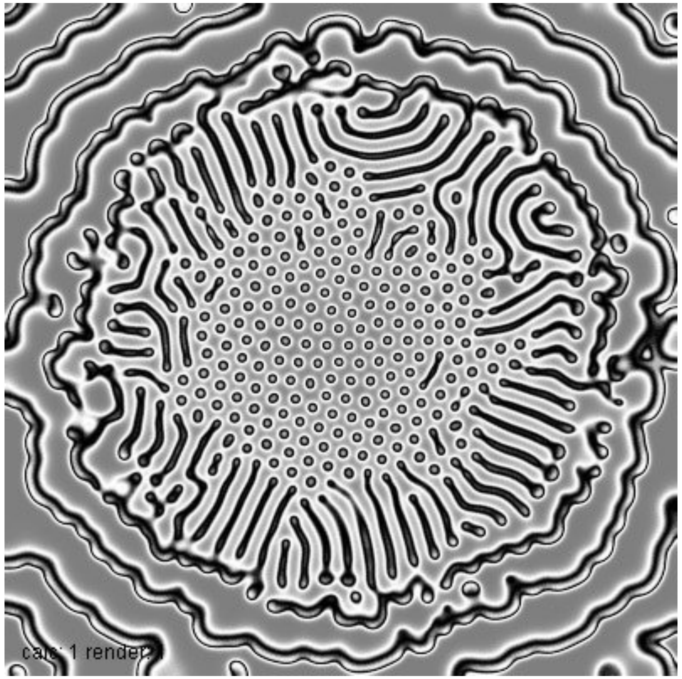
- I/O
- Programmability
- Function, purpose

Through design of complex dynamics

<u>How do you control Macro by designing Micro??</u>

- Decorations on vescicles
- Embedded magnets
- …

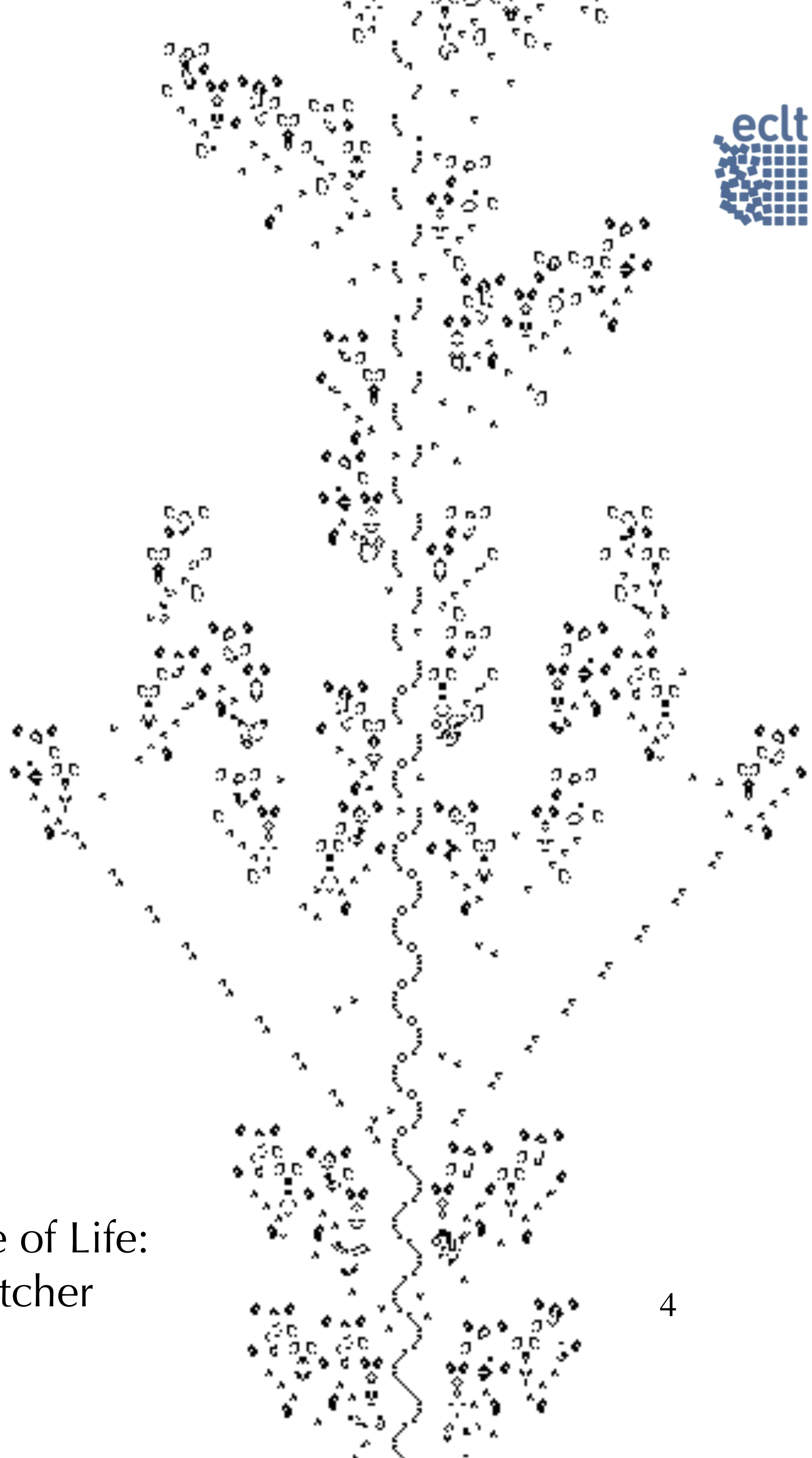
Goal: engineer micro
to get desired emergent macro



Reaction diffusion

**How do you make local rules**
**that can create complexity? Computation???**

Conway's game of Life:
Zigzag wikistretcher



# Want the “Ising model” for morphological computation

- For phase transitions, the Ising magnet:  lattice of ones and zeros with nearest neighbor interactions (tending to align).

- For morphological computation:  consider lattice gas of particles with hard core exclusion
  - Hard sphere gas (3d) / hard disk gas (2d)
  - Simple exclusion processes (SEP), Asymmetric SEP (ASEP)
  - Hard square gas
  - Kob – Anderson
  - Domino gas

# Domino gas

- Model diffusion through membranes
- Simple particles: Fickian diffusion across a membrane

$$J = -D\nabla\rho \qquad\qquad \frac{d\rho}{dt} = D\nabla^2\rho$$

- Spatially extended particles:
  - Nonlinear diffusion properties.
  - Blocking reduces exploration of microstates
- For lattice models, use Kawasaki update
  - Choose a particle at random
  - Choose a possible move at random
  - Execute the move if possible (not blocked)

# Macroscopic states of nonequilibrium systems are typically attractors

- Consider two types of departure from equilibrium:
  - Concentration gradient (chemical potential)
  - Applied field = bias in probability of moving in different directions

- Simplest example (?)
  Dominos falling against a semi-permeable membrane.

Fixed point attractor in the clogged state, with fluctuations caused by leaks.

# Membranes with structure can rectify

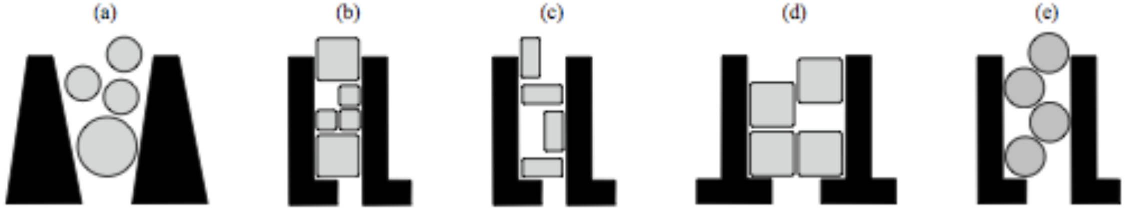



FIG. 1: Blocking of membrane pores with different pore geometries and different particle types. (a) Large and small disks moving in continuous space. (b) Large and small squares moving on a lattice, with a spacing of the size of the small squares. (c) Dominos moving on a lattice; while in a pore, a domino cannot rotate. (d) Single species of square, moving on a lattice with spacing one-half the size of the square. (e) Single species of disk, in the continuum. In all cases, blockers must move upward to re-establish flow. In model simulations, particles in (a) and (e) move in continuous two-dimensional space, governed by Hamiltonian dynamics. Particles in (b-d) move on a lattice, with Monte Carlo updates.

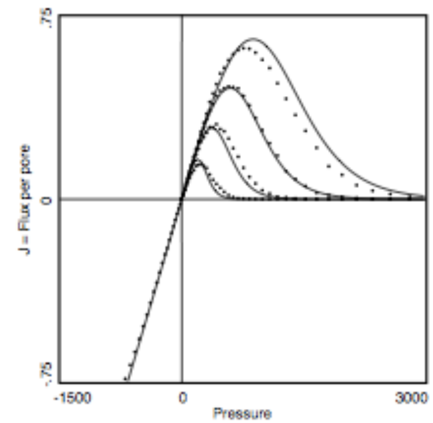
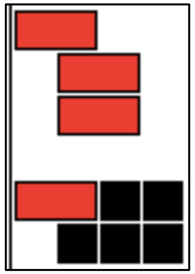
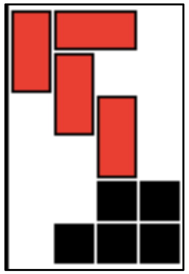



FIG. 4: Steady-state flow of small disks through a membrane pore with the geometry of Fig. 1(a), as a function of pressure in the chamber. The dots are data points from a simulation, and the curves are generated by the steady-state equation above. The relative pore lengths are 2, 3, 5, and 10 (from the top curve down). Flows through the reversed pore geometry are plotted as negative values.

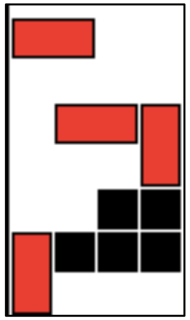
# Study the microstates



Blocked



Unblocked



Flow

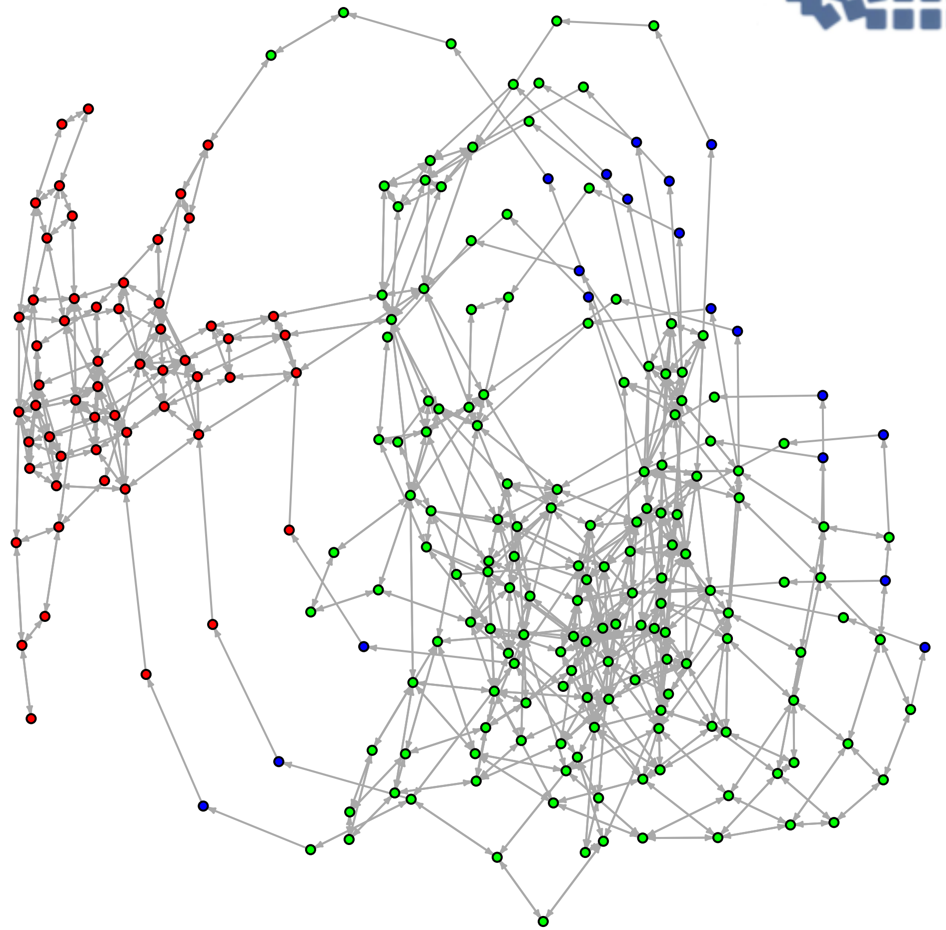
Construct states $x_i$, with $i$ ranging over all cells in the chamber

$$x_i = \begin{cases} 0 \text{ if empty} \\ 1 \text{ if bottom V} \\ 2 \text{ if top V} \\ 3 \text{ if right H} \\ 4 \text{ if left H} \end{cases}$$

## Microstate structure

- Keystone states: states that must be traversed to move from blocking state to nonblocking state.
- Backing up required to unblock

- Full state space ~ product structure
- Membrane clogging ~ critical probability of clogging.



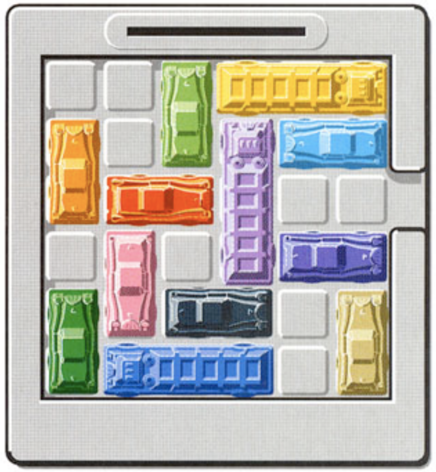
Lesson: keystone states cause complex macrostates



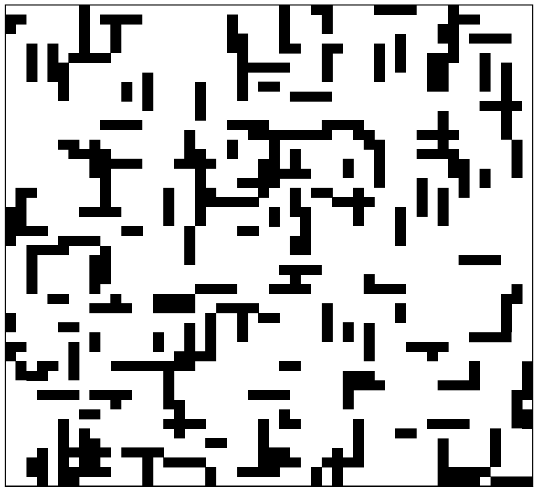
MTHICK=5 diam= 22

# Rush hour gas

- Children's game
- Can be difficult!
- PSPACE hard
- Logic gates may be constructed.

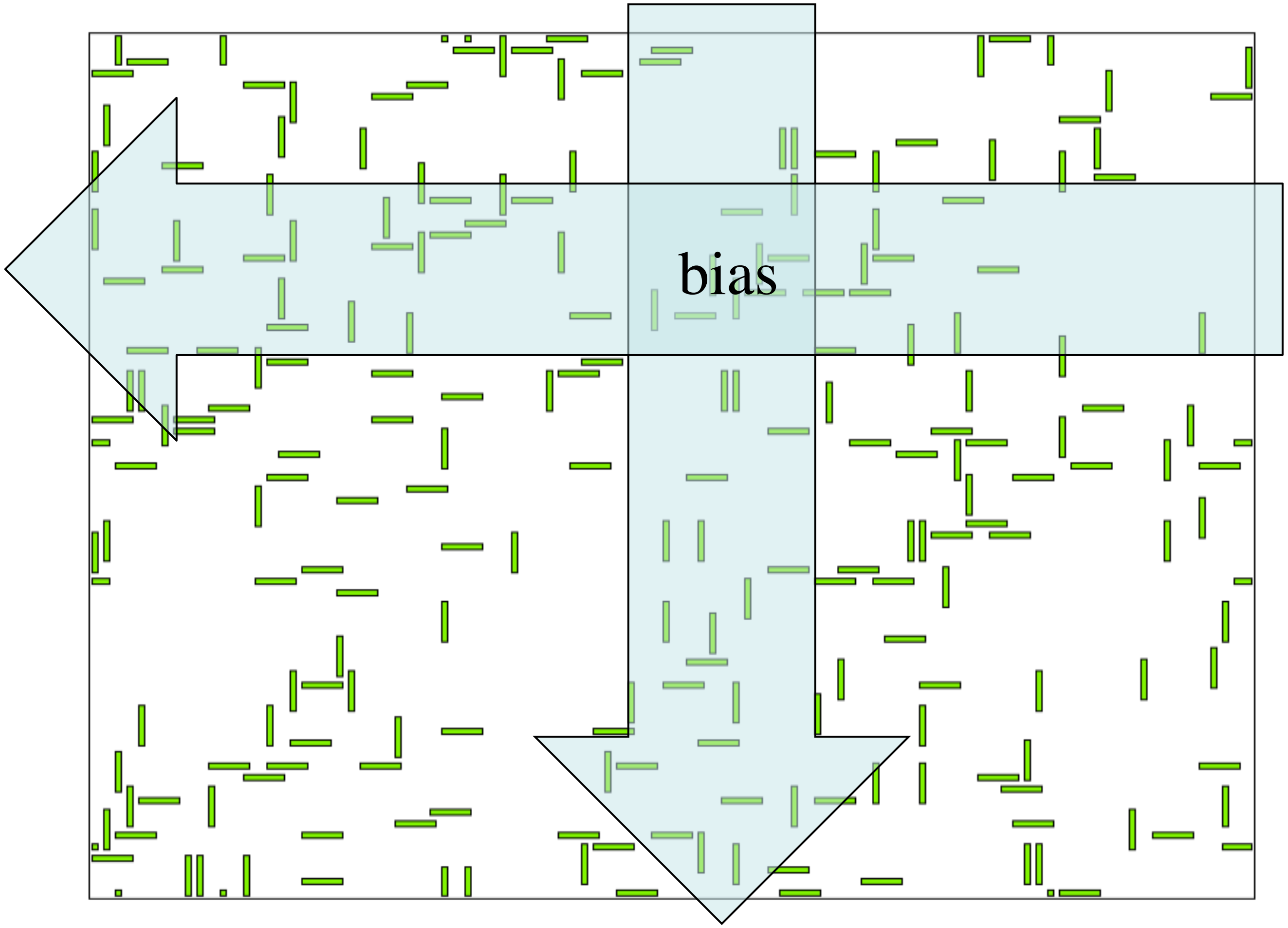


Form a "rush hour gas" by enlarging lattice, applying Kawasaki dynamics.



# Add a field

- Downward and to the left
- Physics literature:  2-d asymmetric exclusion process
  - Cf. also traffic models



# Phase diagram

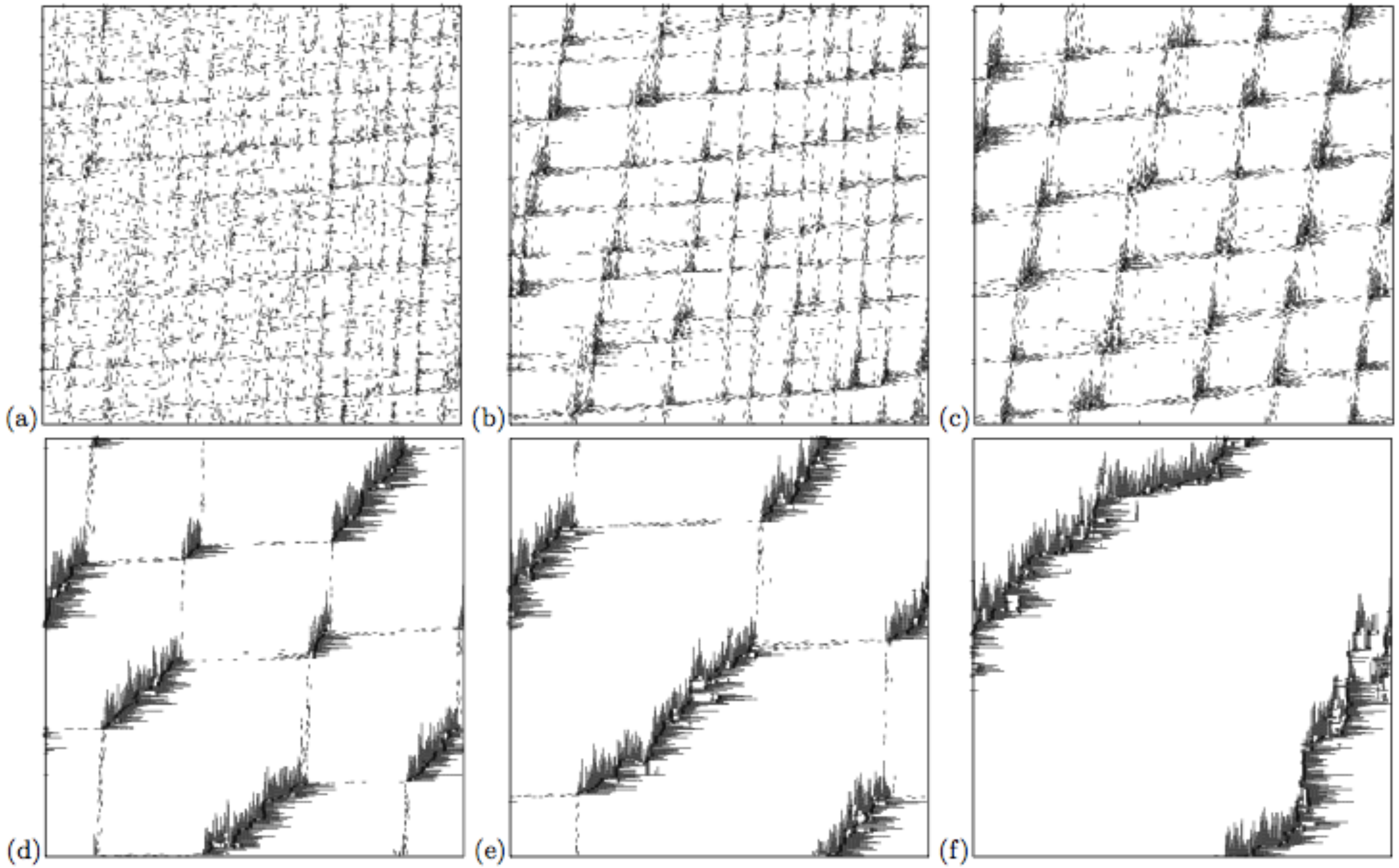
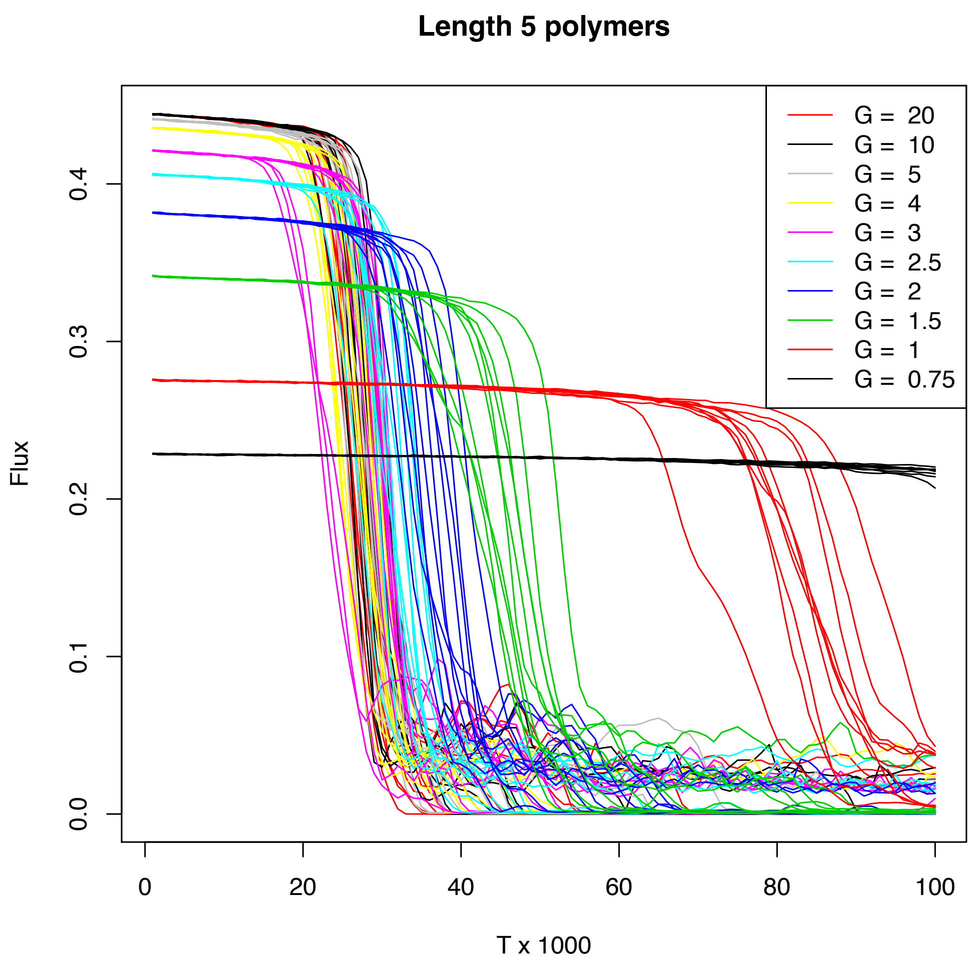


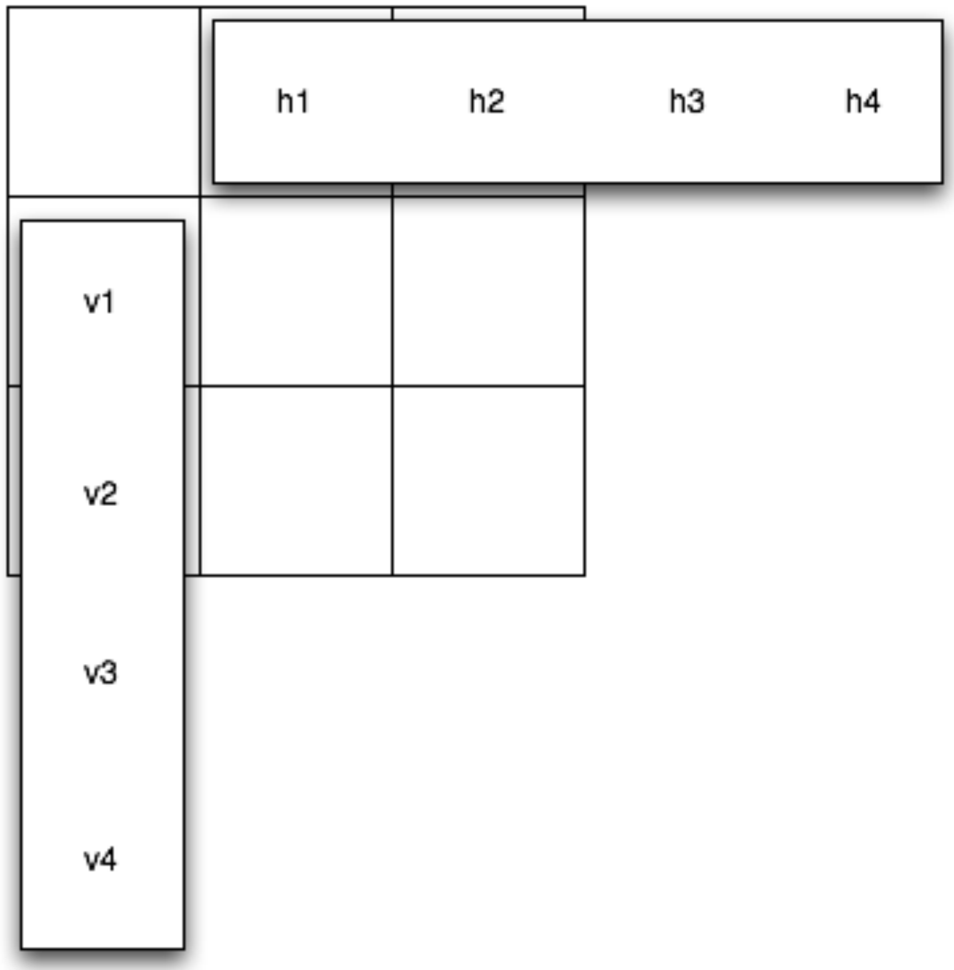
FIG. 2: A sequence of macroscopic states obtained for a gas of 5-mers after a transient from a random initial condition, as density is varied from 0.1 to 0.125, with G=3. The 5-mers are biased to move preferentially downward and to the left. The grid-like structures translate in the opposite direction (upward and to the right); i.e. they have a wave velocity in the opposite direction to the direction of the flux. Note that if 5-mers are added gradually, the intermediate translating grid states persist to much higher densities.

# Long transient to traveling wave



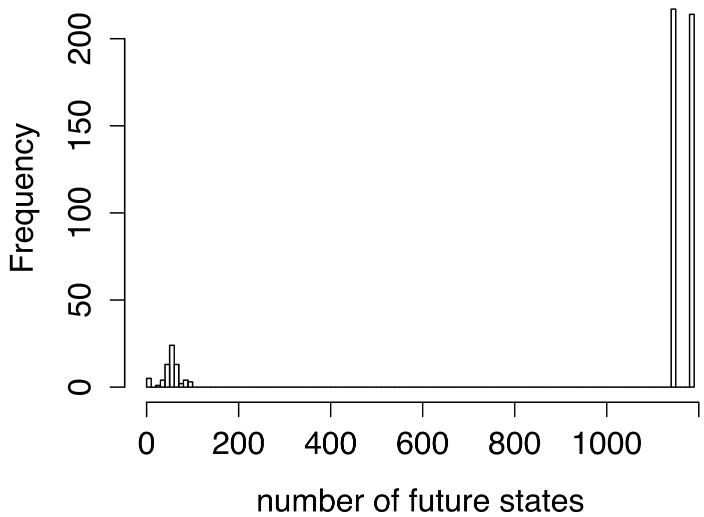
## Counting local states

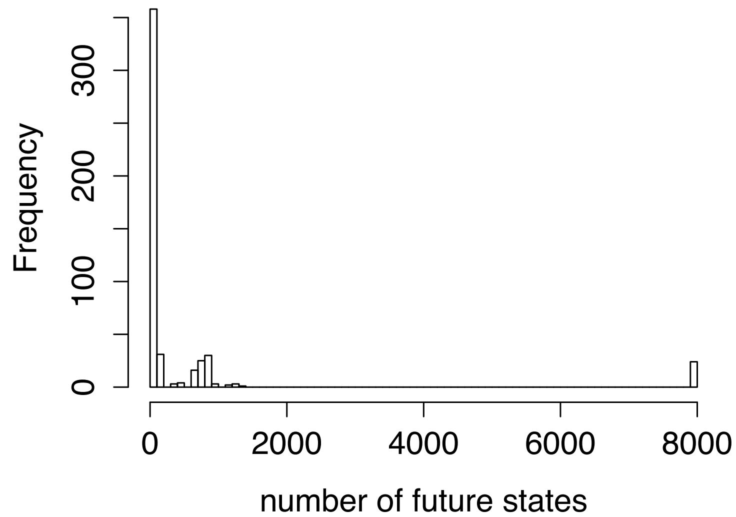
$$(x_1, \ldots , x_9) = (0,1,2,5,0,0,6,0,0)$$




$$x_i = \begin{cases} 0 \ \text{if empty} \\ 1 \ \text{if h1} \\ 2 \ \text{if h2} \\ 3 \ \text{if h3} \\ 4 \ \text{if h4} \\ 5 \ \text{if v1} \\ \ldots \\ 8 \ \text{if v4} \end{cases}$$

# Future state distributions



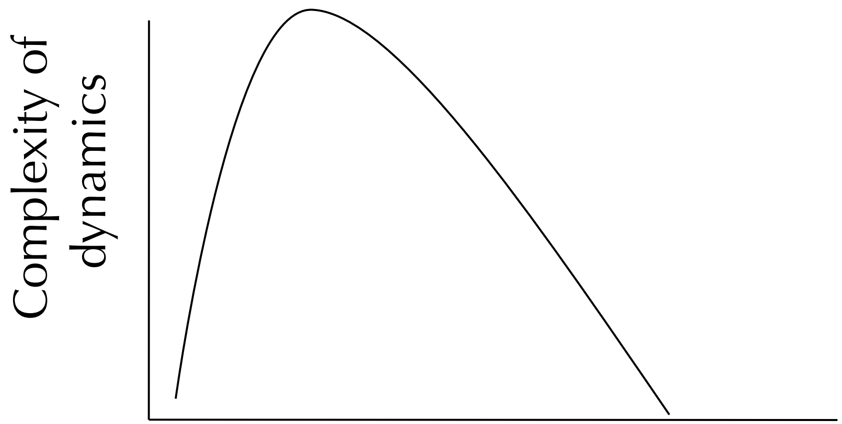




Dilute system,
simple diffusive dynamics

Traveling waves,
complex dynamics

# Lesson

- As parameter variation changes the number of future local states, complexity of dynamics goes through a maximum

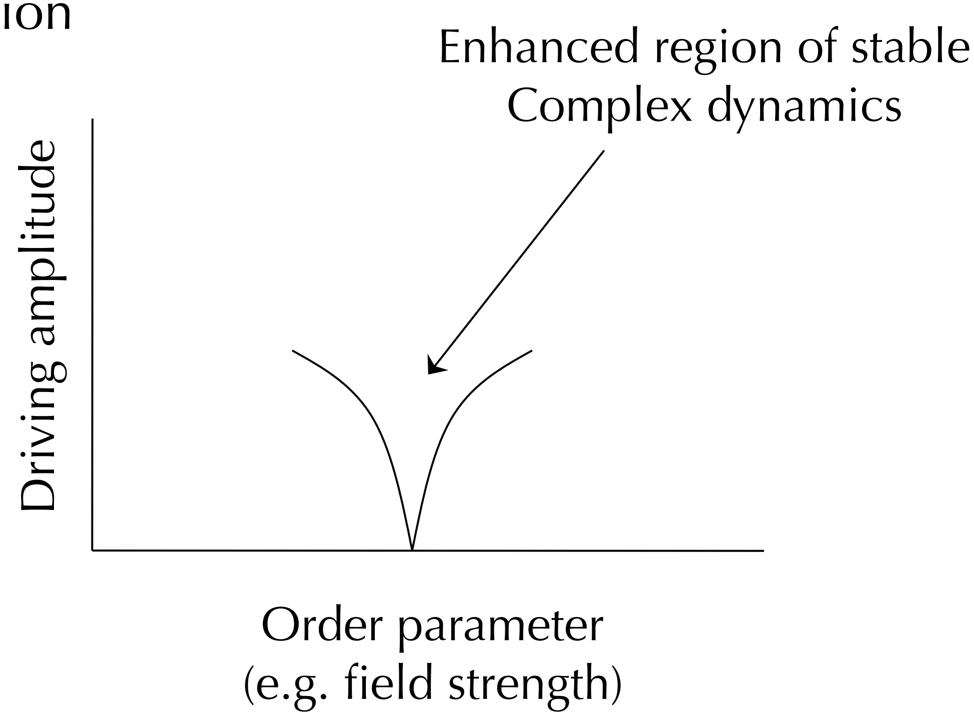



Small number of future states; overconstrained

Large number of future states; unconstrained

## Ways to stabilize, robustify structures

- Add (small) periodic driving
- Annealed preparation
- Modulating mixtures



# Future directions

- Further engineering guidelines
- Quantify dynamics with information theory (topological version?)
- Connections with thermodynamics (should be simple!)
  - Chemical potential
  - Field strength
- Make contact with physical systems.