Outils, Modélisation et Simulation en Calcul Numérique

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Programme du cours

- Modélisation par Automates Cellulaires (BC+MD)
- Les Gaz sur réseaux (BC)
- La méthode de Boltzmann sur réseaux (BC)
- Méthodes Monte-Carlo (MD)
- Réseaux de Neurones (MD)
- Dynamique Moléculaire (BC)

Cellular Automata Modeling of Complex systems

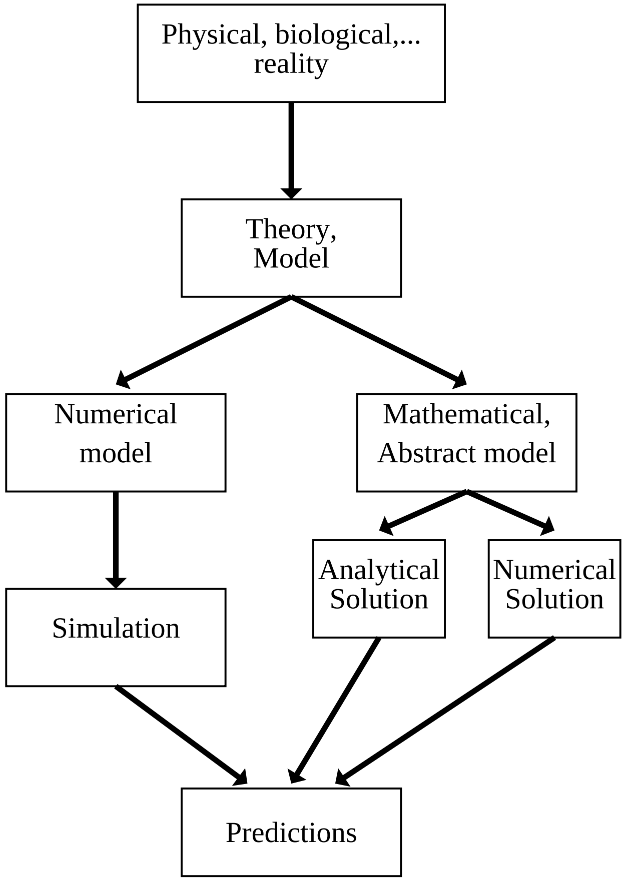
- Concepts and Motivation
- Definition
- Examples
- From microscopic rules to macroscopic equations: reaction-diffusion systems

Why Cellular automata models ?

1. Are PDEs the only (and best) way to describe a physical, biological, social process?

2. Models and computer simulations are often more appropriate

3. Everything should be made as simple as possible but not simpler (A. Einstein).



Cellular Automata

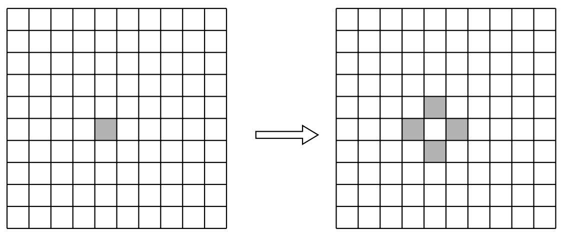
- Mathematical abstraction of the real world
- Mathematical object, new paradigm for computation
- Elucidate some links between **complex systems**, **universal computations**, **algorithmic complexity**, **undecidability**, **irreducibility**, **intractability**.

CA Definition

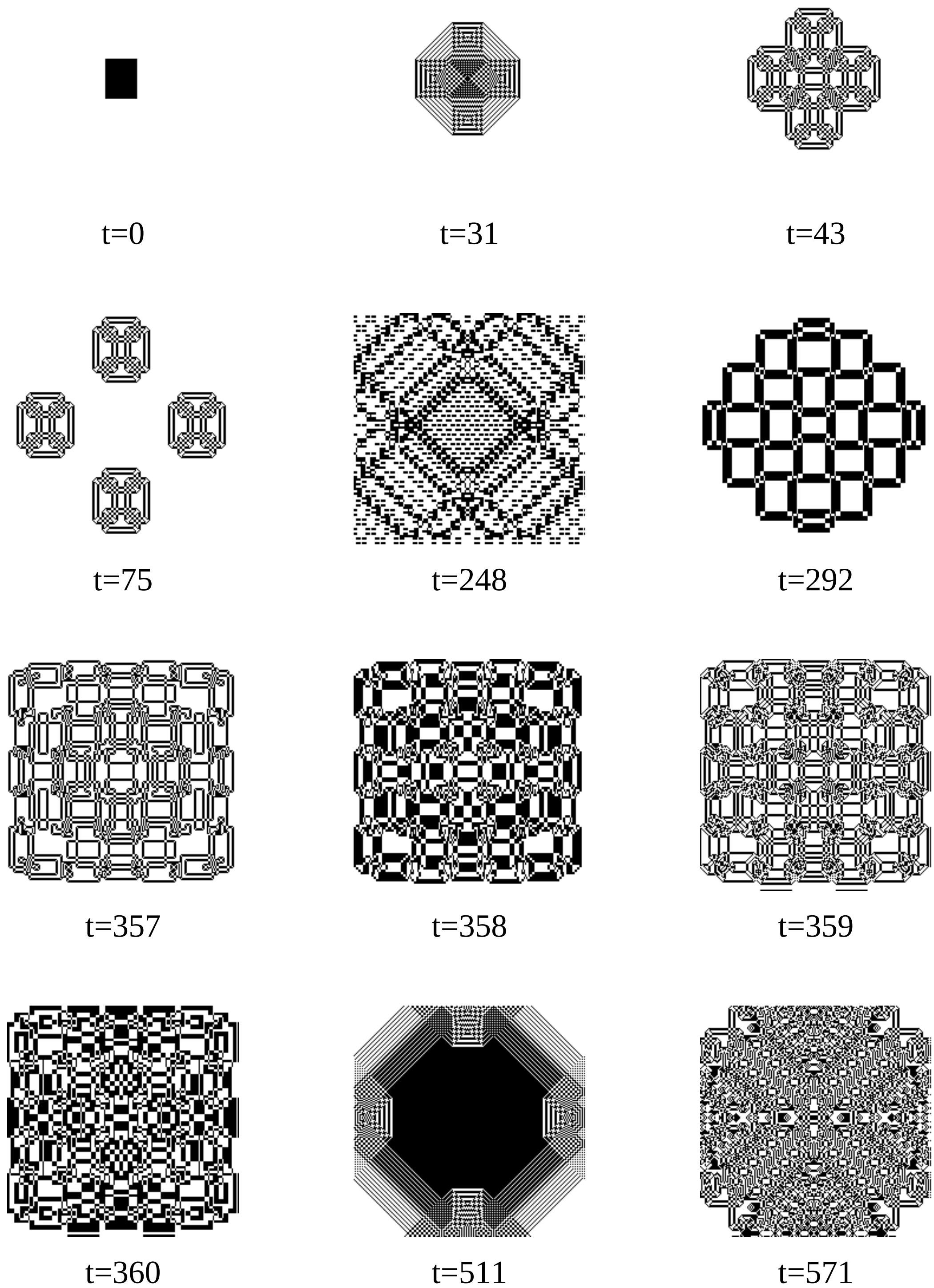
- Fictitious Universe
- Discrete space: regular lattice of cells/sites in d dimensions.
- Discrete time
- Possible states for the cells: discrete set
- Local, homogeneous **evolution rule** (defined for a neighborhood).
- Synchronous (parallel) updating of the cells
- Boundary conditions

Parity Rule

- Square lattice (chessboard)
- Possible states $s_{ij} = 0, 1$
- Rule: each cell sums up the states of its 4 neighbors (north, east, south and west).
- If the sum is even, the new state is $s_{ij} = 0$; otherwise $s_{ij} = 1$



Generate "complex" patterns out of a simple initial condition.


t=0
t=31
t=43
t=75
t=248
t=292
t=357
t=358
t=359
t=360
t=511
t=571

Parity rule (cont'ed)

- One can unravel the way the pattern builds up (be more efficient than running the rule)
- Complexity is due to the superposition of the initial pattern translated of various quantities.
- Pattern is "simple" at some specific time steps.

(a) (b) (c)

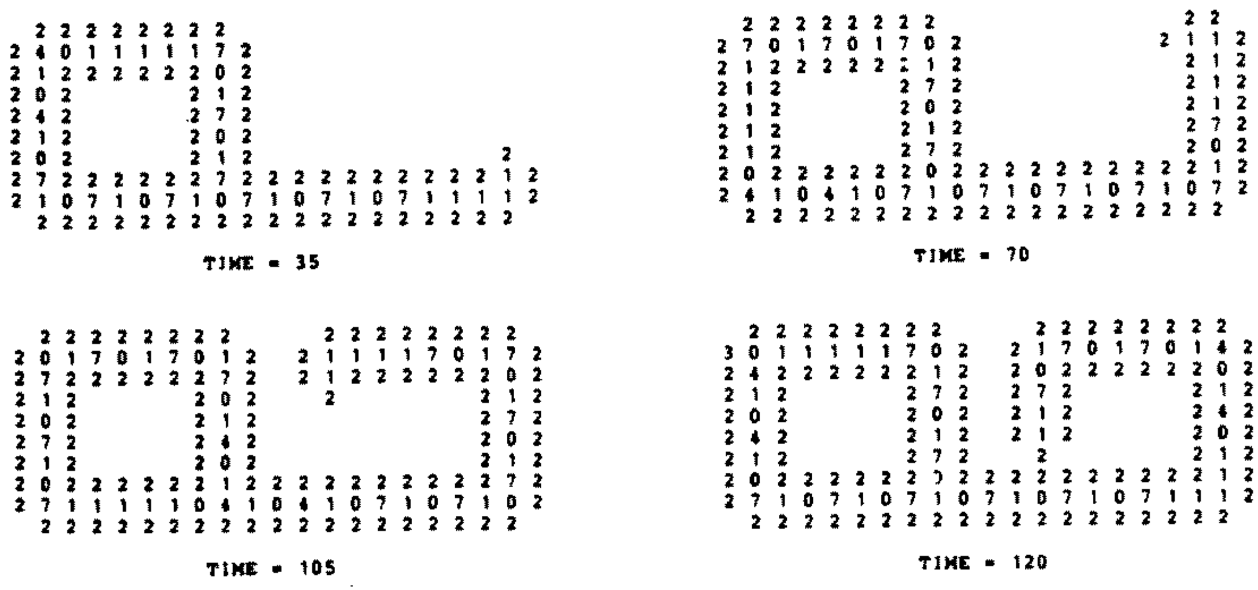
von Neumann's CA

- Origin of the CA's (1940s)
- Design a better computer with self-repair and self-correction mechanisms
- Logical mechanisms for self-reproduction: necessary and sufficient conditions
- Before the discovery of DNA: find and algorithmic way
- Formalization in a fully discrete world
- Automaton with 29 states, arrangement of thousands of cell which can self-reproduce
- Universal computer

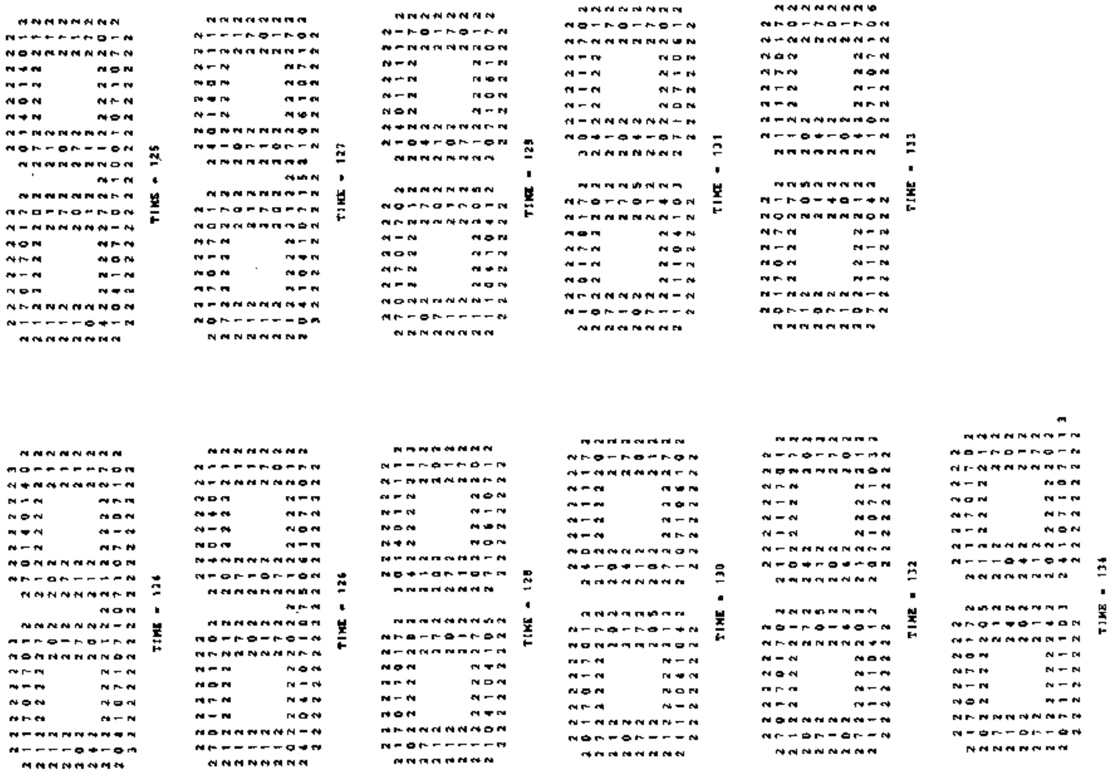
Langton's CA

- Simplified version (8 states).
- Not a universal computer
- Structures with their own fabrication recipe
- Using a reading and transcription mechanism

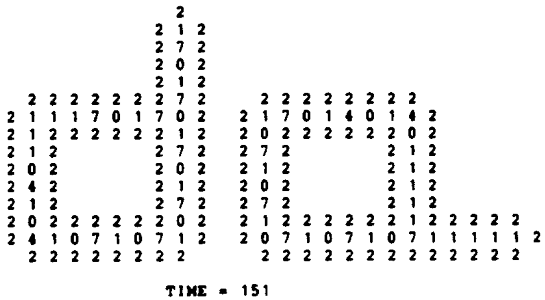
Langton's CA: basic cell replication



Time evolution of Langton's Automaton:



Langton's Automaton : spatial evolution



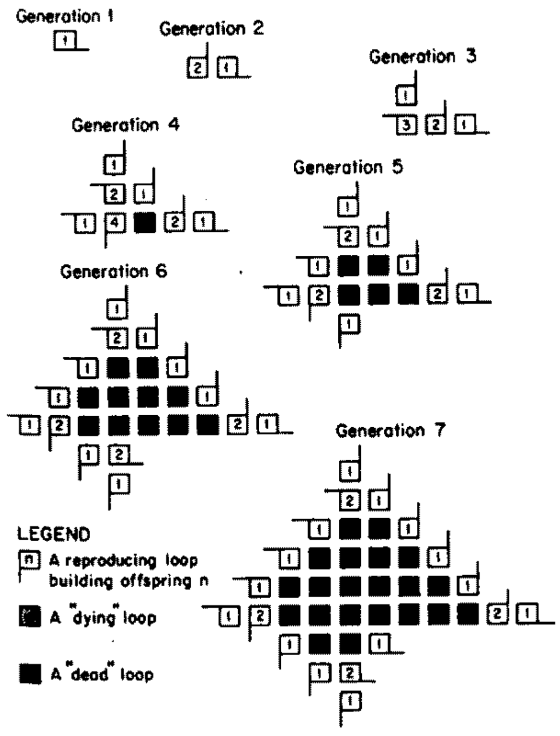


Fig. 10. Growth of loop colony. Seven generations of growth in a colony of loops.

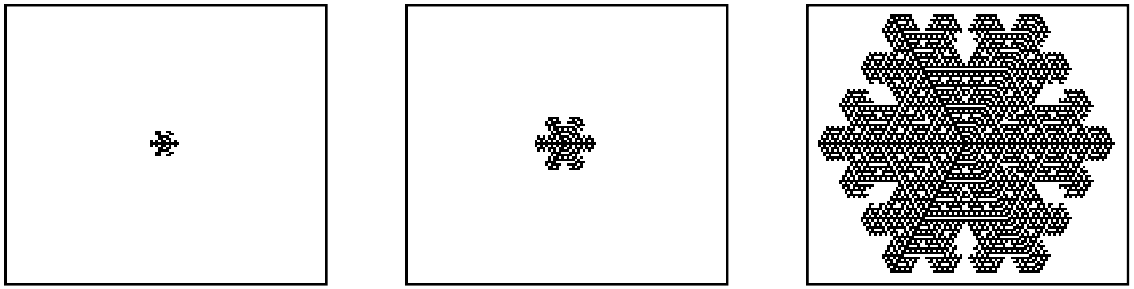
Langton's CA: some conclusions

- Not a biological model, but an algorithmic abstraction
- Reproduction can be seen from a mechanistic point of view (Energy and matter are needed)
- No need of a hierarchical structure in which the more compicated builds the less complicated
- Evolving Hardware.

CA as a mathematical abstraction of reality

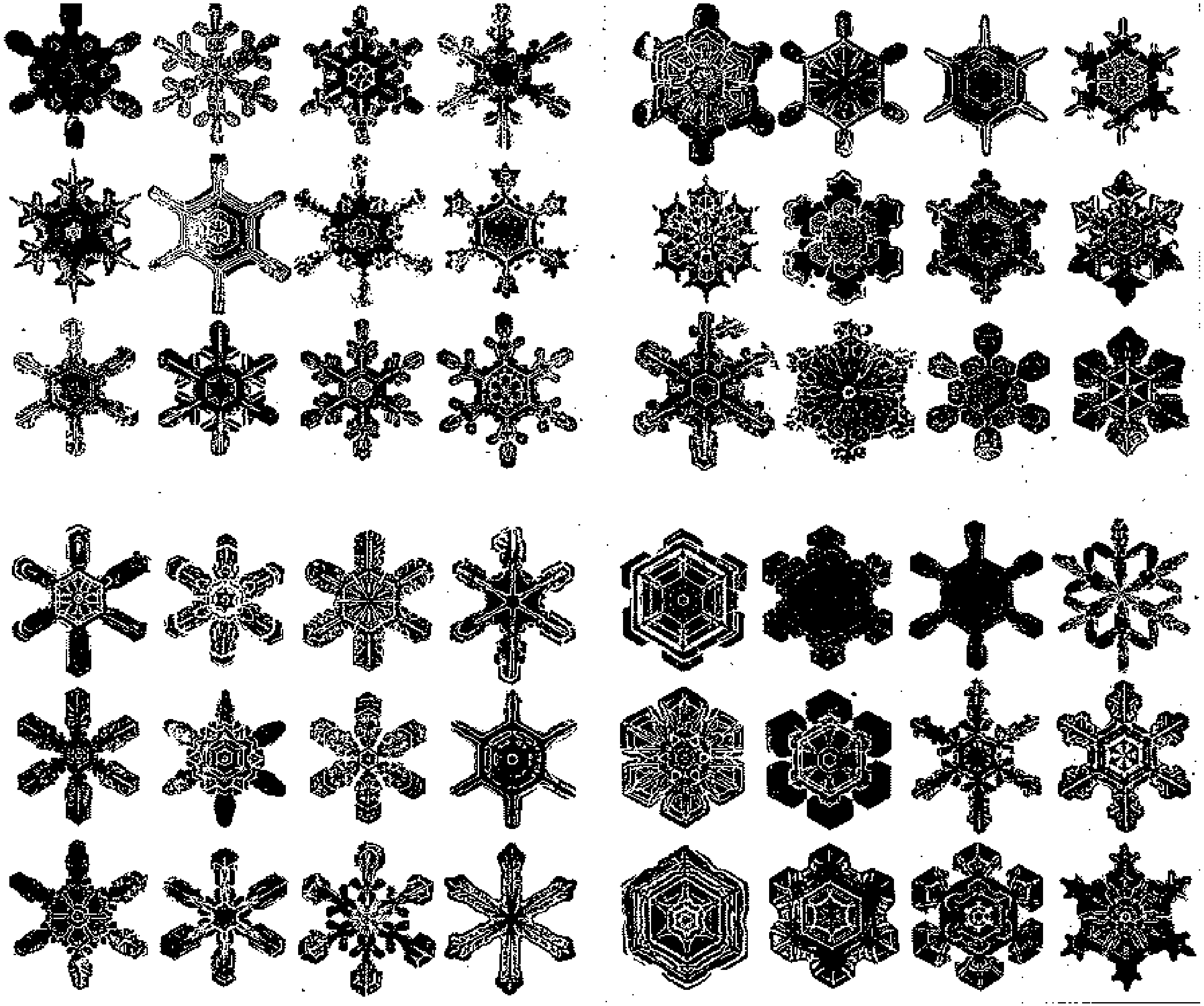
- Several levels of reality: macroscopic, mesoscopic and microscopic.
- The macroscopic behavior depends very little on the details of the microscopic interactions.
- Only "symmetries" or conservation laws survive. The challenge is to find them.
- Consider a fictitious world, particularly easy to simulate on a (parallel) computer with the desired macroscopic behavior.
- Simple, flexible, intuitive, efficient

A Caricature of reality



t=4 t=10 t=54

What is this ?



Snowflakes model

- Very rich reality, many different shapes
- Complicated true microscopic description
- Yet a simple growth mechanism can capture some essential features

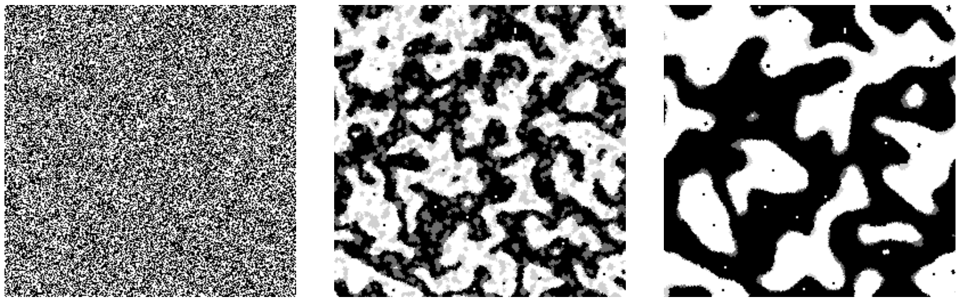
- **A vapor molecule solidifies (→ice) if one and only one already solidified molecule is in its vicinity**
- **Growth is constrained by 60^o angles**

Cooperation models: annealing rule

- Growth model in physics: droplet, interface, etc
- Biased majority rule: (almost copy what the neighbors do)

Rule:

$\text{sum}_{ij}(t)$	0 1 2 3 4 5 6 7 8 9
$s_{ij}(t+1)$	0 0 0 0 1 0 1 1 1 1



(a) (b) (c)

The rule sees the curvature radius of domains

Cells differentiation in drosophila

In the embryo all the cells are identical. Then during evolution they differentiate

- slightly less than 25% become neural cells (neuroblasts)
- the rest becomes body cells (epidermioblasts).

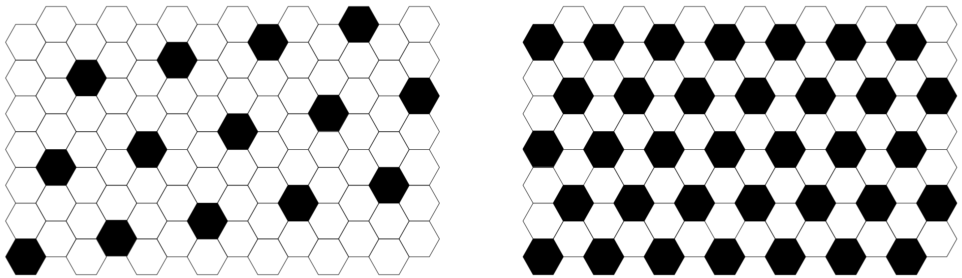
Biological mechanisms:

- Cells produce a substance S (protein) which leads to differentiation when a threshold S_0 is reached.
- Neighboring cells inhibit the local S production.

CA model for a competition/inhibition process

- Hexagonal lattice
- The values of S can be 0 (inhibited) or 1 (active) in each lattice cell.
- A $S = 0$ cell will grow (i.e. turn to $S = 1$) with probability p_{grow} provided that all its neighbors are 0. Otherwise, it stays inhibited.
- A cell in state $S = 1$ will decay (i.e. turn to $S = 0$) with probability p_{decay} if it is surrounded by at least one active cell. If the active cell is isolated (all the neighbors are in state 0) it remains in state 1.

Differentiation: results



The two limit solutions with density 1/3 and 1/7, respectively.

- CA produces situations with about **23%** of active cells, for almost any value of p_{anihil} and p_{growth}.

- Model robust to the lack of details, but need for hexagonal cells

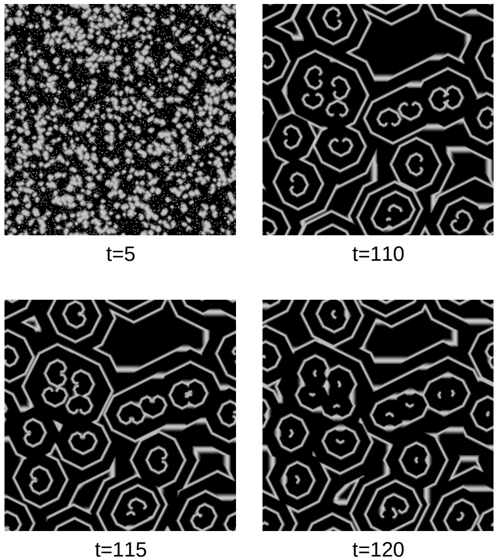
Excitable Media, contagion models

- 3 states: (1) normal (resting), (2) excited (contagious), (3) refractory (immuned)

  1. excited $\rightarrow$ refractory
  2. refractory$\rightarrow$ normal
  3. normal $\rightarrow$ excited, if there exists excited neighbors (otherwise, normal $\rightarrow$ normal).

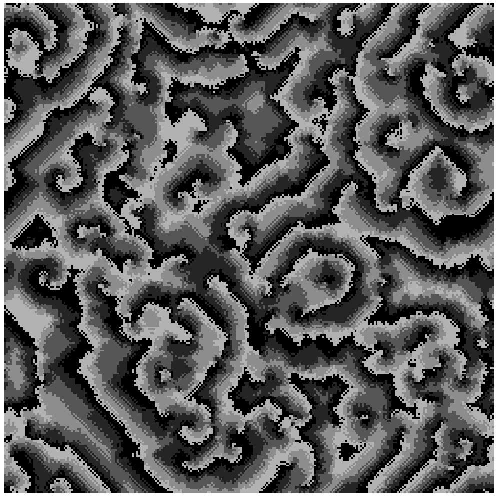
Greenberg-Hastings Model

- $s \in \{0, 1, 2, ..., n-1\}$
- normal: $s = 0$; excited $s = 1, 2, ..., n/2$; the remaining states are refractory
- contamination if at least k contaminated neighbors.



Large Belousov-Zhabotinski (tube worm)

The state of each site is either 0 or 1; a local timer controls the 0 period.



(i) where the timer is zero, the state is excited;

(ii) the timer is decreased by 1 unless it is 0;

(iii) a site becomes refractory whenever the timer is equal to 2;

(iv) the timer is reset to 3 for the excited sites which have two, or more than four, excited sites in their Moore neighborhood.

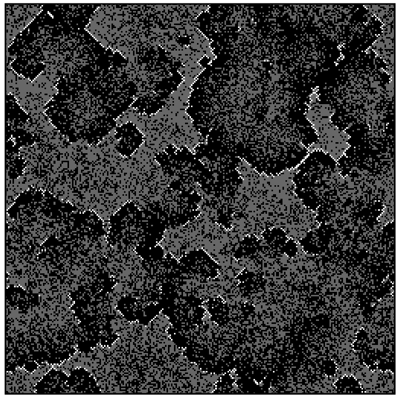
Forest fire

(1) a burning tree becomes an empty site;

(2) a green tree becomes a burning tree if at least one of its nearest neighbors is burning;

(3) at an empty site, a tree grows with probability p;

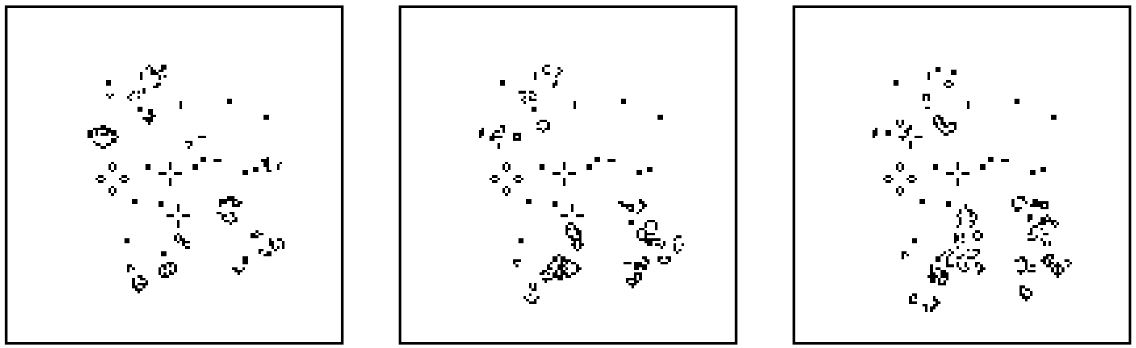
(4) A tree without a burning nearest neighbor becomes a burning tree during one time step with probability f (lightning).



Complexity: The game of life

Rules:

- Square lattice, 8 neighbors
- Cells are dead or alive (0/1)
- Birth if exactly 3 living neighbors
- Death if less than 2 or more than 3 neighbors

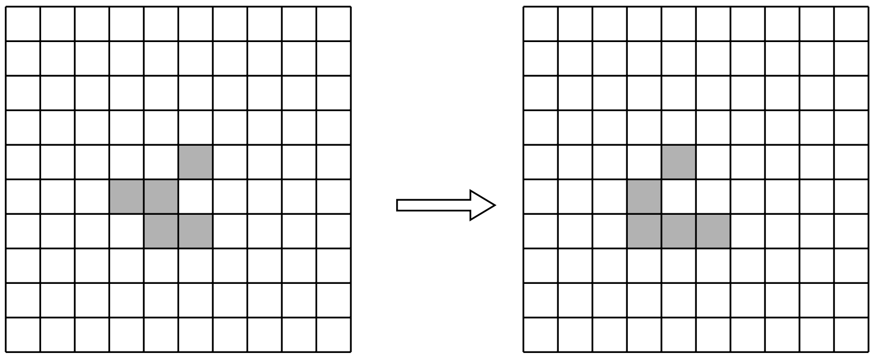


t t+10 t+20

Complex Behavior in the game of life

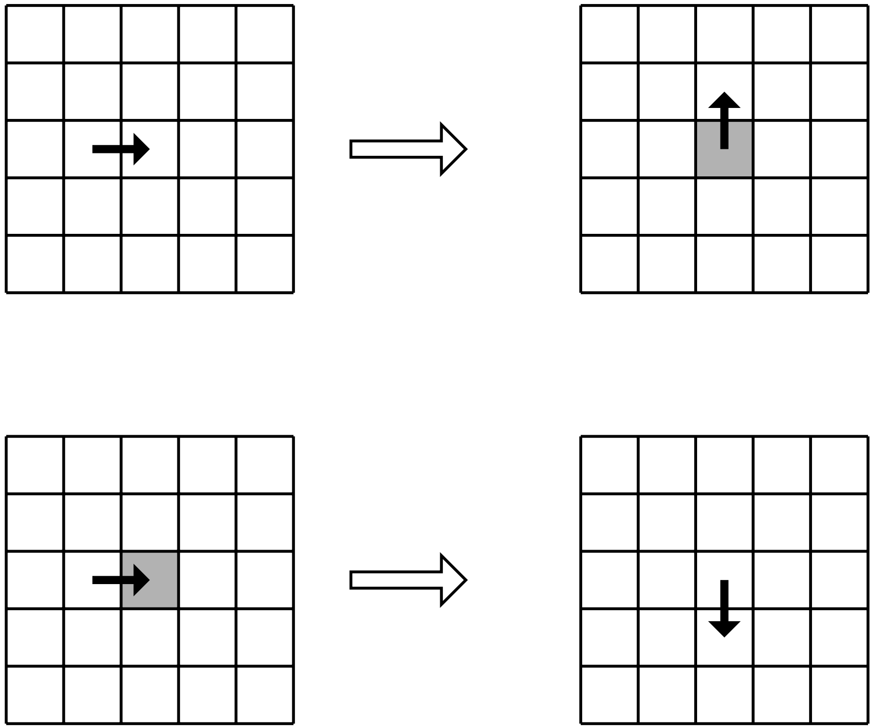
Collective behaviors develop (beyond the local rule)

“Gliders” (organized structures of cell) can emerge and can **move** collectively.



Langton's ant

Artificial animal moving on a square lattice



Question: What is the trajectory of this ant ?

- Macroscopically complicated motion
- Formation of a “highway”

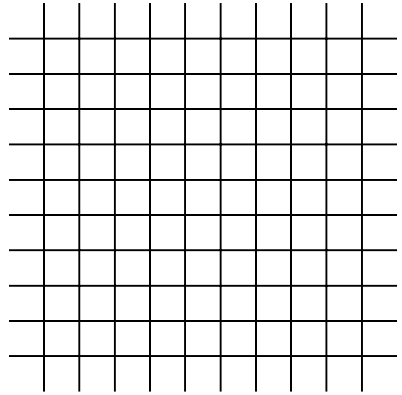
t=6900 t=10431 t=12000

Is the motion always non-bounded ?

Assume it can be confined in a finite region

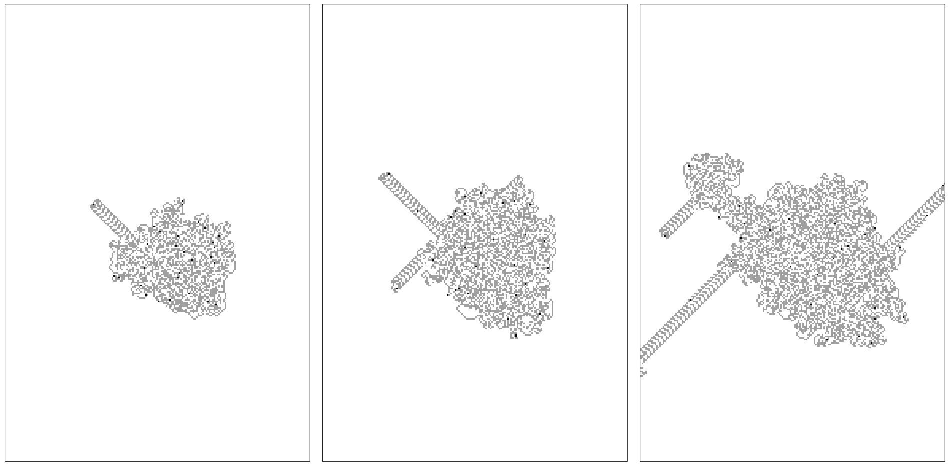
- Note that the rule implies a partition of the space in H and V cells.
- Then some cells are visited infinitely often
- If the upper-left cell is H, it must be black

$\rightarrow$ **Contradiction!**



What about many ants?

- Adapt the "change of color" rule
- Cooperative and destructive effects
- The trajectory can be bounded or not
- Past/futur symmetry explains periodic motion

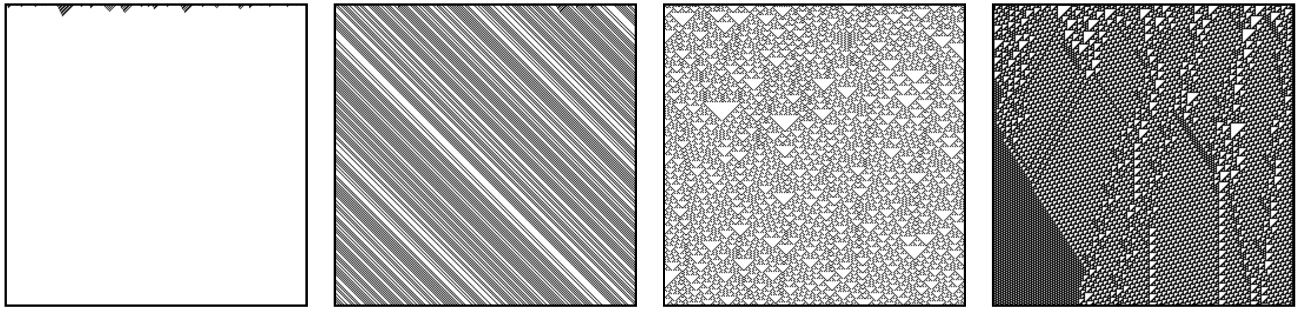


t=2600 t=4900 t=8564

Microscopic versus Macroscopic in Langton's ant model

- One knows everything on the microscopic motion
- But very little on the global motion
- Two distinct realities ?
- One must simulate the micro to get the macro $\rightarrow$ complex system
- The "universal law" is not enough

Wolfram's rules: complexity classes



(a) (b) (c) (d)

- **Class I** Reaches a fixed point
- **Class II** Reaches a limit cycle
- **Class III** self-similar, chaotic attractor
- **Class IV** unpredicable persistent structures, irreducible, universal computer

Note: it is **undecidable** whether a rule belongs or not to a given class.

Other simple rules

- time-tunnel

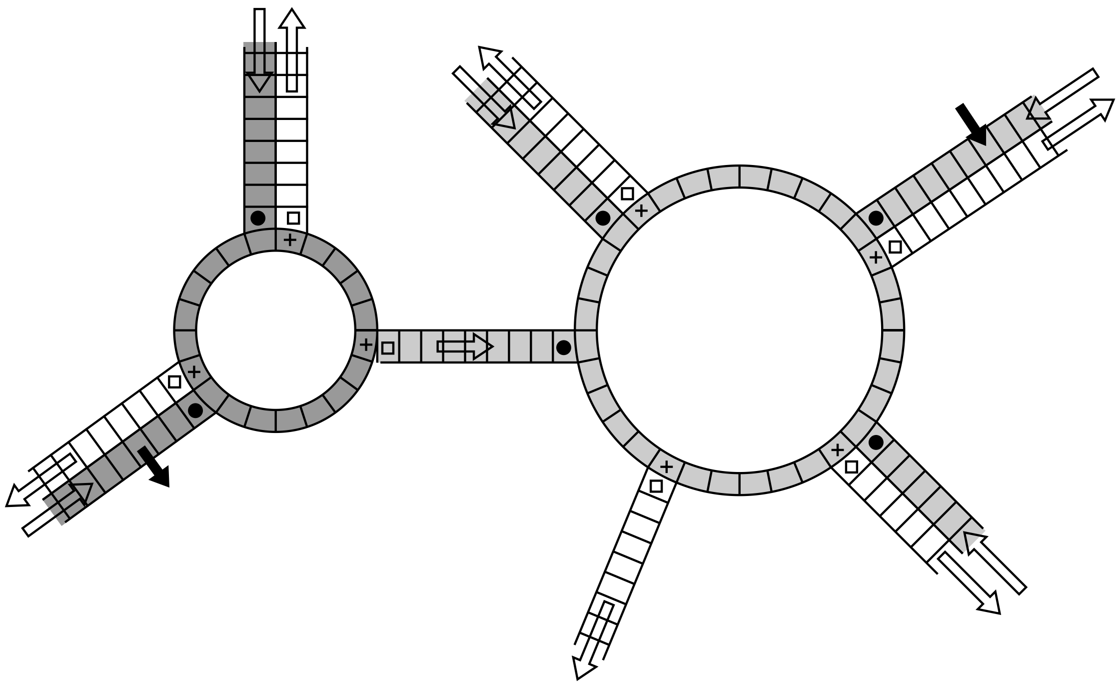
$$
\begin{aligned}
Sum(t) &= C(t) + N(t) + S(t) + E(t) + W(t) \\
C(t+1) &= \begin{cases} C(t-1) & \text{if } Sum(t) \in \{0, 5\} \\ 1 - C(t-1) & \text{if } Sum(t) \in \{1, 2, 3, 4\} \end{cases}
\end{aligned}
$$

- random

$$C(t+1) = (S(t).and.E(t)).xor.W(t).xor.N(t).xor.C(t)$$

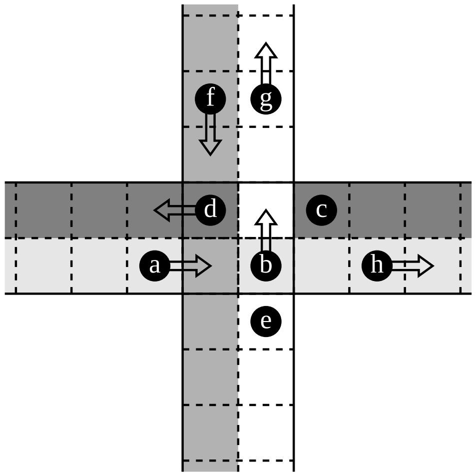
- string: a one-dimensional spring-bead system

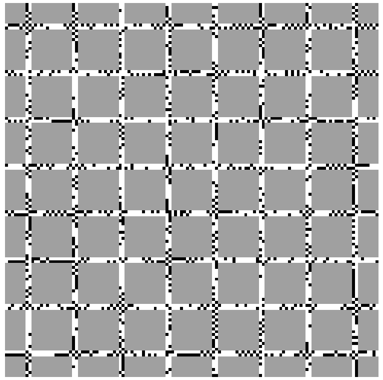
Traffic Models



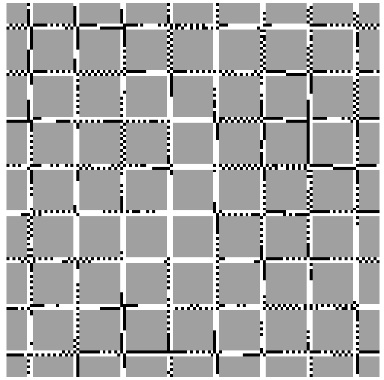
A vehicle can move only when the downstream cell is free.

Traffic in a Manhattan-like city



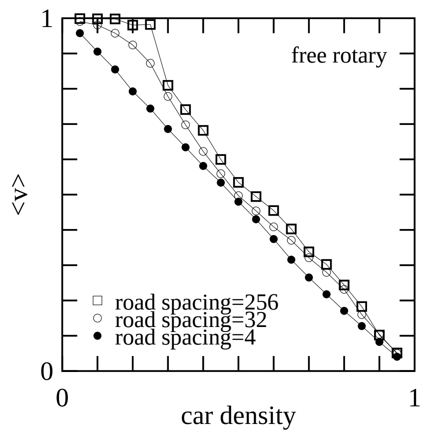


(a)

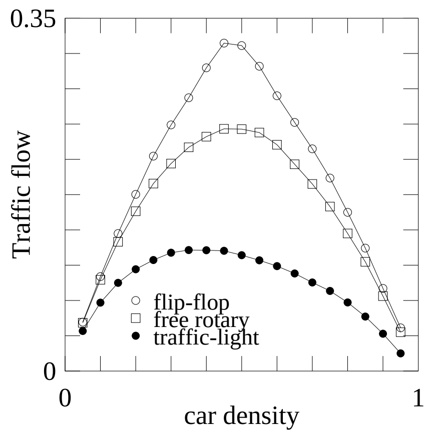


(b)

(a)



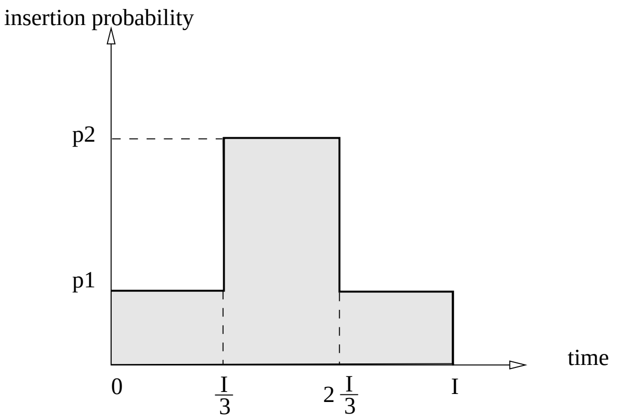
(b)

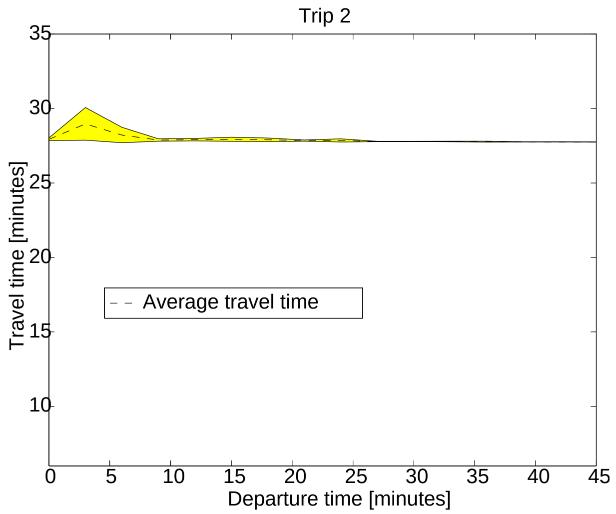


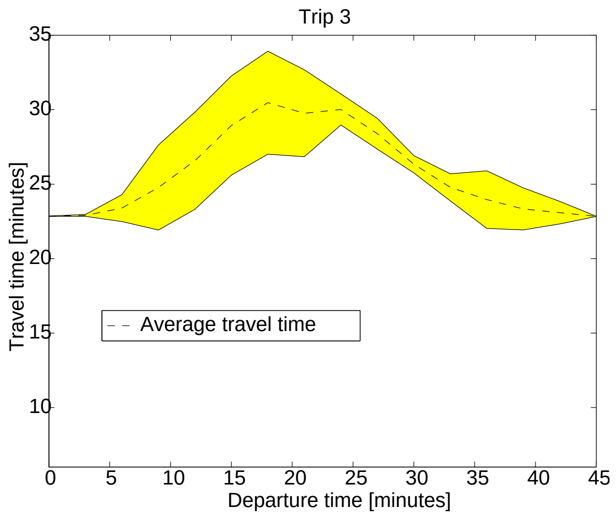
Case of the city of Geneva

- 1066 junctions
- 3145 road segments
- 560886 road cells
- 85055 cars

Travel time during the rush hour







Socio-physics Model: competion of opinion in a society

- Devise a simple model which captures the generic properties of a group of persons having to choose between two options.
- Model in the sense of statistical physics, with simplified agents.
- Spatially extented system with temporal evolution: what is the wining opinion ?
- Define good strategies and explain some features of a social group as an emergent behavior.

A Cellular Automata Model

- The individuals move and interact in a discrete space.
- Two types of individuals: A and B, according to their current opinion.
- Always 4 individuals per site (any mixture of A and B).
- Initial density b_0 de B, random initial configuration.
- Diffusive displacement with diffusion constant D.
- Confrontation takes place with probability k (agressivity) at each cell.

Rule for the competion of opinion CA

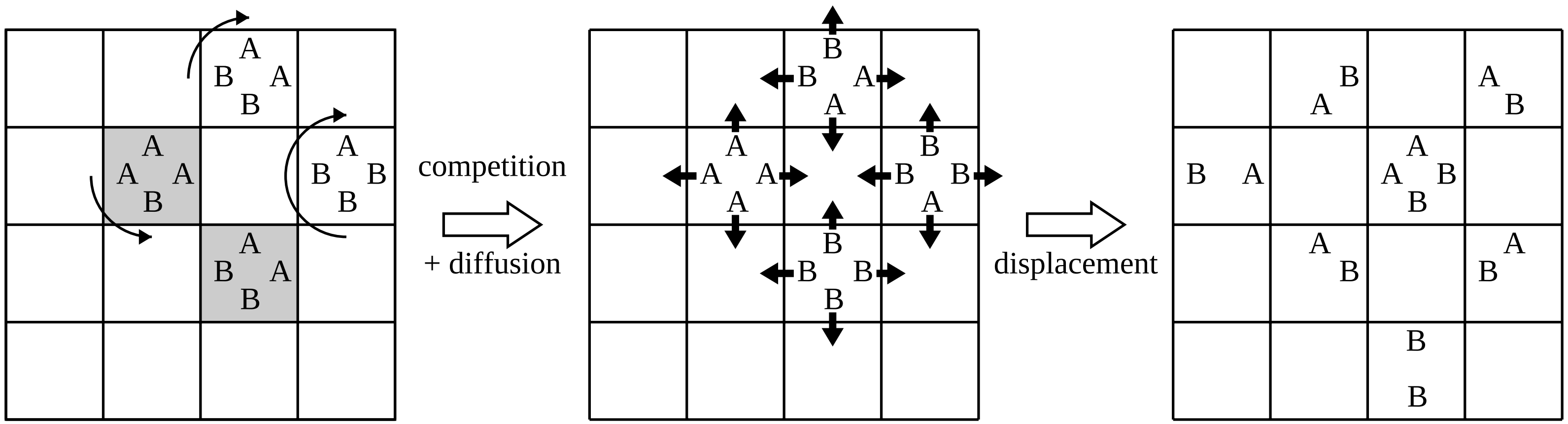


Figure 1: A confrontation take place in gray cell, followed by a random re-direction of the resulting individuals (with a rotation of the configuration by 0, 90, -90 or 180 degrees).

Confrontation rule

The following rule is applied with probability k.

- The local majority species (if any) wins:

$$nA + mB \rightarrow \begin{cases} (n+m)A & \text{if } n > m \\ (n+m)B & \text{if } n < m \end{cases}$$

  where $n + m = 4$.

- When there is an equal number of A and B on a site, B wins with probability $1/2 + \beta/2$. $\beta \in [0, 1]$ is the bias accounting for some advantage (or extra fitness) of species B.

Between fights both population agents perform a random walk on the lattice.

Applications:

- Smoker versus non-smoker: Bias due to social recognition.
- competing standards (Linux vs Windows). Bias due to price, quality.
- epidemic systems.
- Darwinian Evolution (punctuated equilibria).

Evolution of the initial configuration

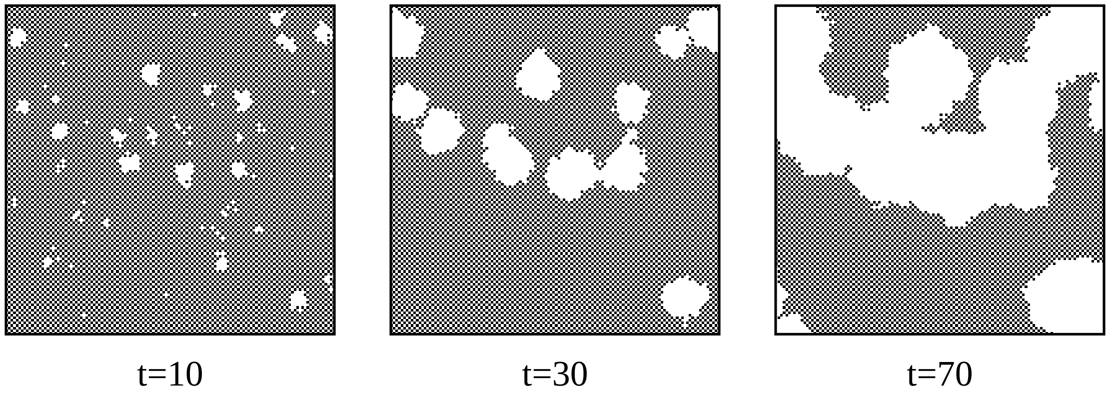


Figure 2: Configurations of the competion CA model, at three different times. The A and B species are represented by the gray and white regions, respectively. The parameters of the simulation are $b_0 = 0.1$, $k = 0.5$ and $\beta = 1$.

Phase diagram

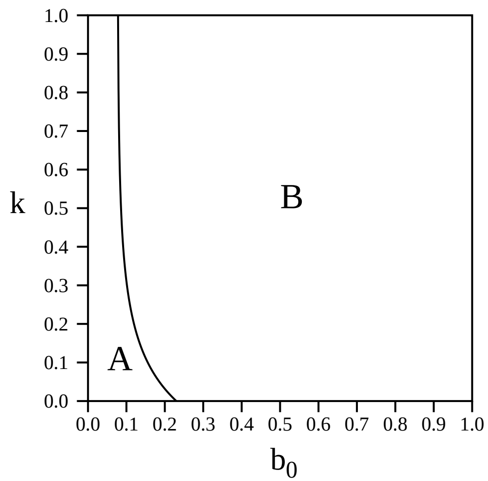


Figure 3: Phase diagram for the socio-physical model with $\beta = 1$. The curve delineates the regions where either A (on the left) or B (on the right) wins depending on b_0, the initial density of B and k, the probability of a confrontation.

Observation

- **Spatial organization is a key ingredient to overcome the less fitted majority.**
- $k = 0$: mean-field case.
- Speed of the annihilation process: a few iterations are sufficient to get rid of the looser, except very near the curve.
- Importance of finite size systems.
- More sophisticated models: evolving agent, shared intelligence, effect of strength versus intelligence.

Conclusion

- complex systems
- Biologial models
- Social models
- Traffic models
- Reaction Diffusion processes
- Hydrodynamics
- Erosion in fluids, snow & sand
- Wave propagation
- Fracture processes