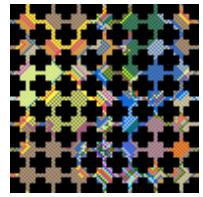


Computer modeling and simulation of natural phenomena

Bastien Chopard

Computer Science Department,
University of Geneva, Switzerland

Lugano, Oct 18, 2016

Examples of models and methods

- N-body systems, molecular dynamics
- Mathematical equations : ODE, PDE
- Monte-Carlo methods (equilibrium, dynamic, kinetic)
- **Cellular Automata and Lattice Boltzmann method**
- multi-agent systems
- Discrete event simulations
- Complex network
- L-systems.....

What is a model ?

Many definitions :

- Simplifying abstraction of reality
- containing only the essential elements with respect to the problem
- A mathematical or rule-based representation of a phenomena
- But a model may also be :
  - A fit of data
  - An animal (medical study)
  - ...

What is a good model ?

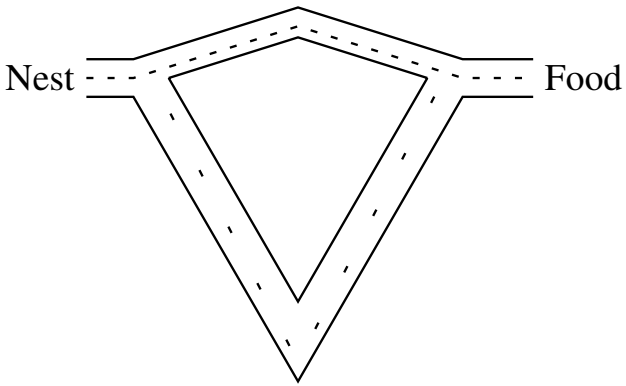
A Einstein :

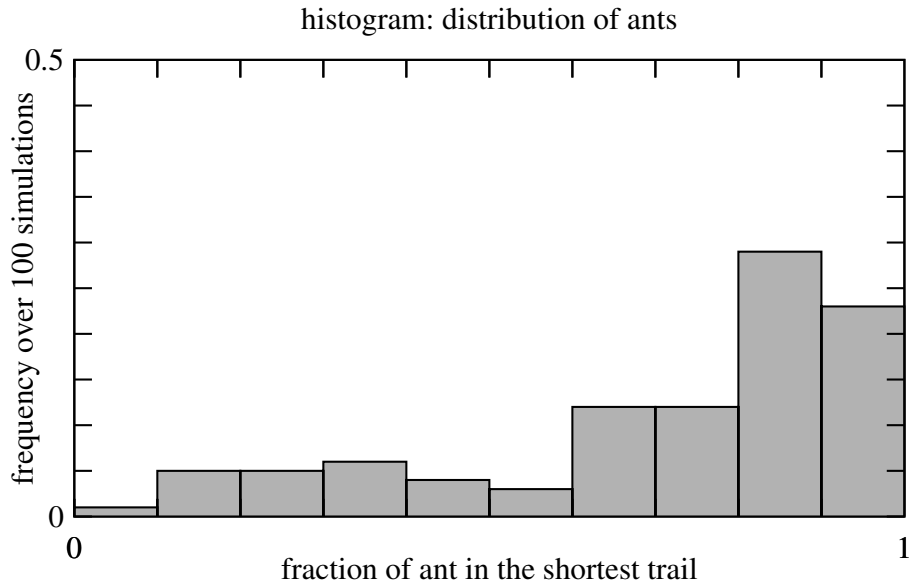
Everything should be made as simple as possible, but not simnpler

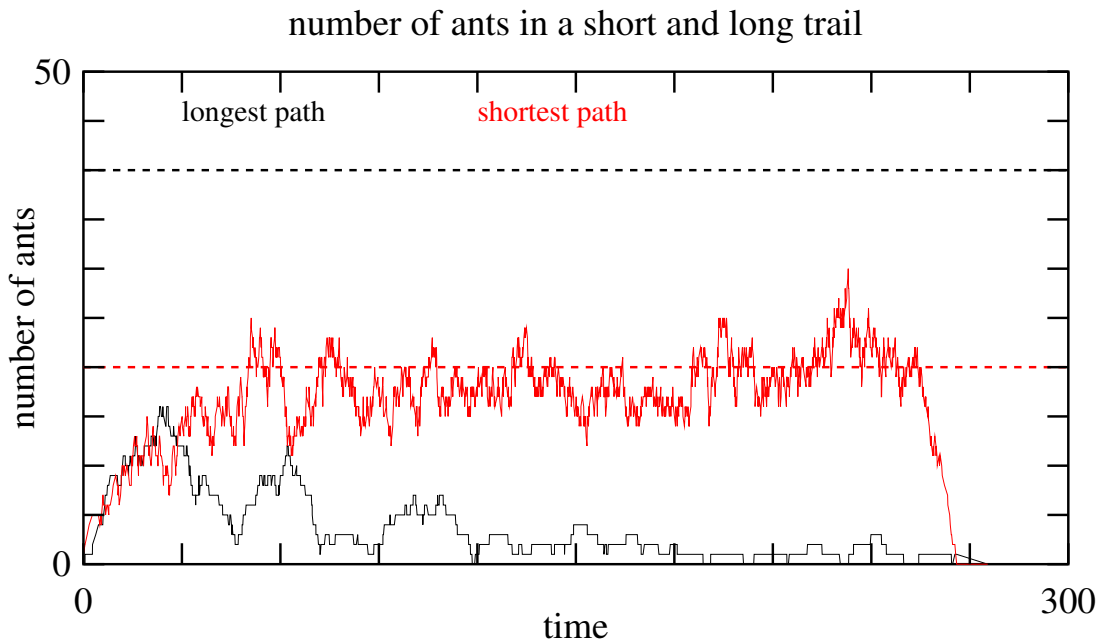
- In silico simulations : understand, predict and control a process
- Allows scientists to formulate new questions that can be addressed experimentally or theoretically
- Adapt the model to the problem

Discrete Event Simulations

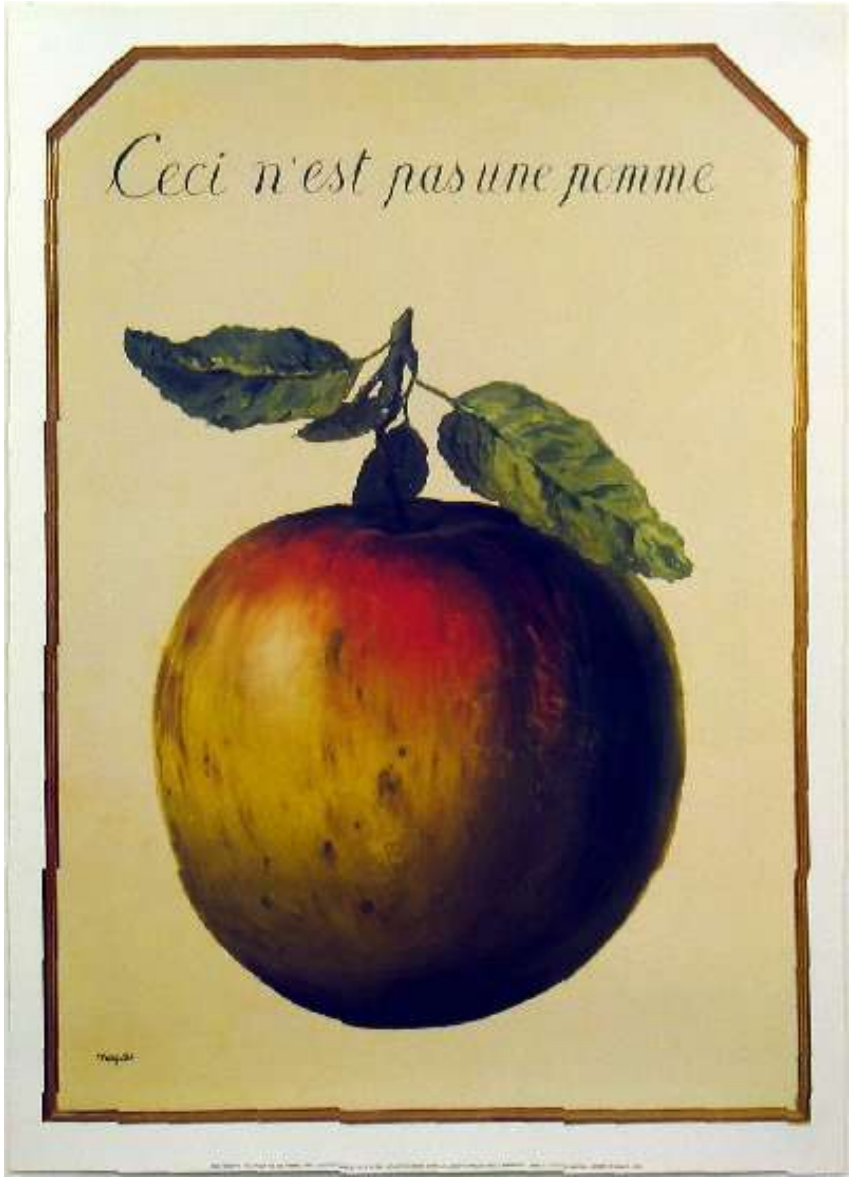
Do ants find the shortest path between nest and food ?



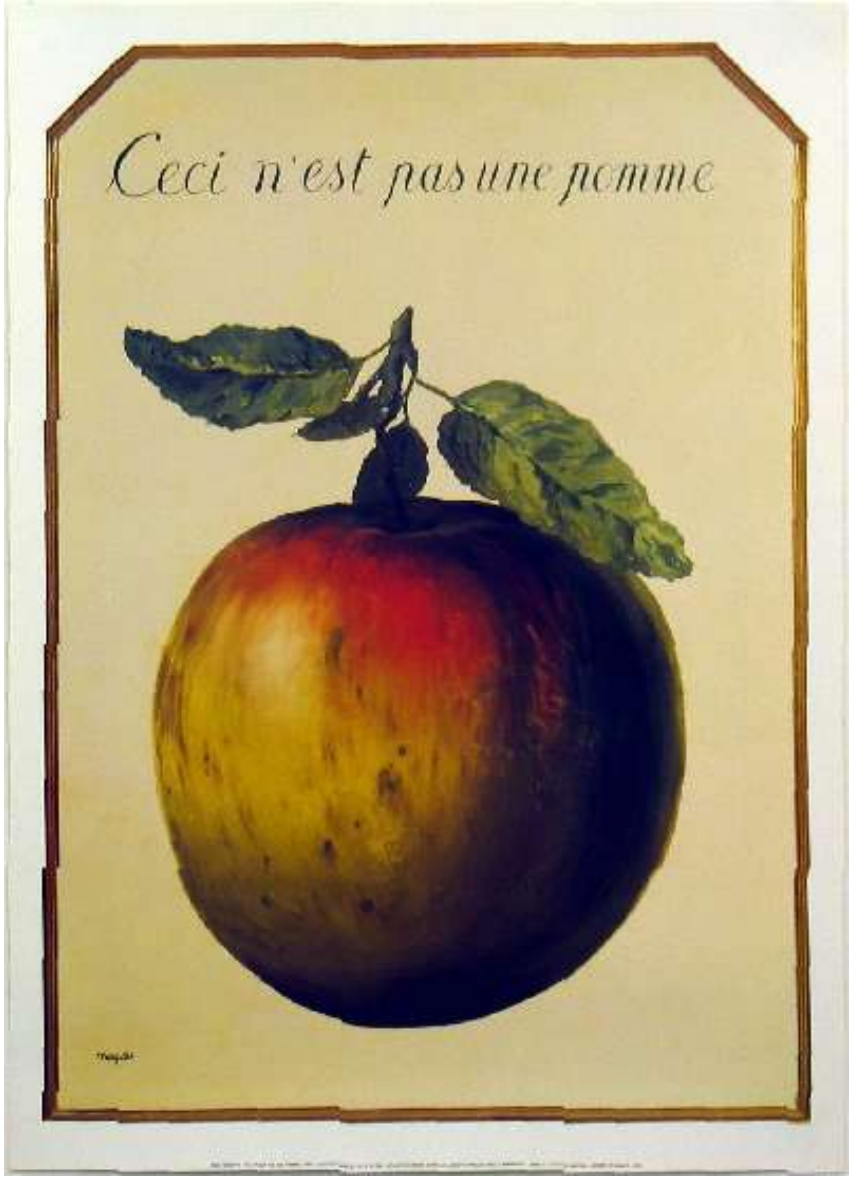




Magritte's apple



Magritte's apple



- A model is only a model, not reality

Same reality, different models, different languages

Hydrodynamics

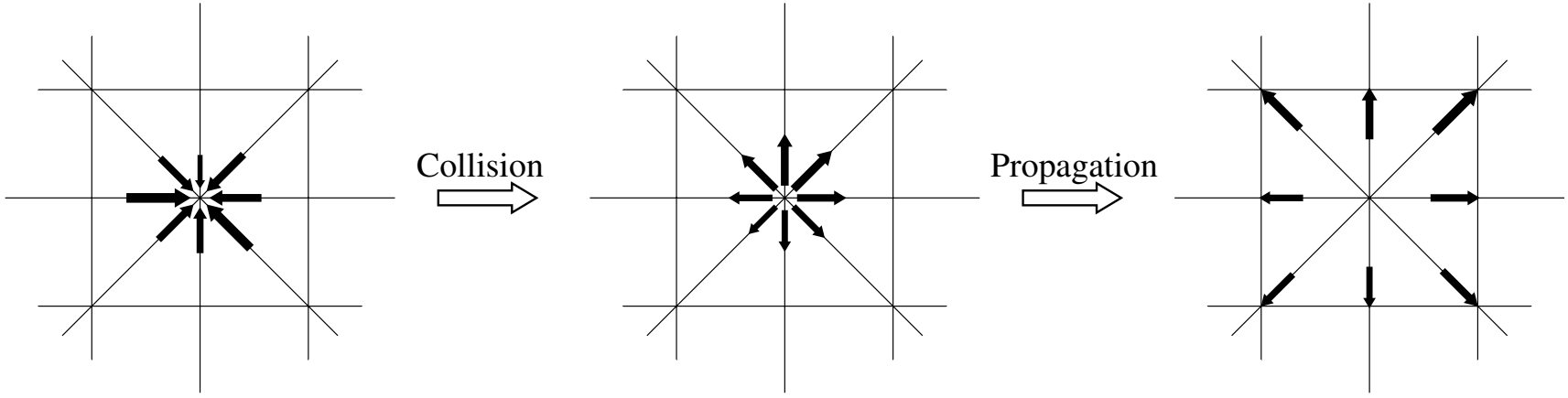
$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u}$$

phenomenon $\rightarrow$ PDE$\rightarrow$ discretization $\rightarrow$ numerical solution

From PDEs to virual universe

One defines a discret universe as an abstraction of the real world

phenomenon $\rightarrow$ computer model

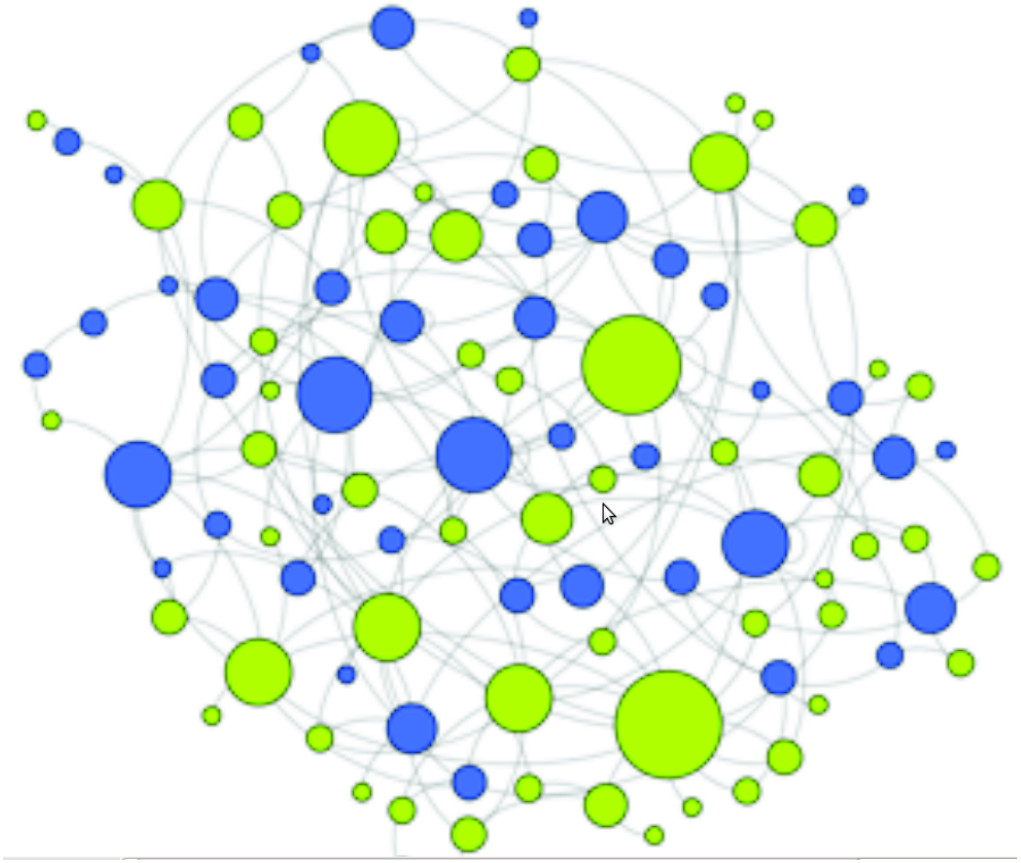


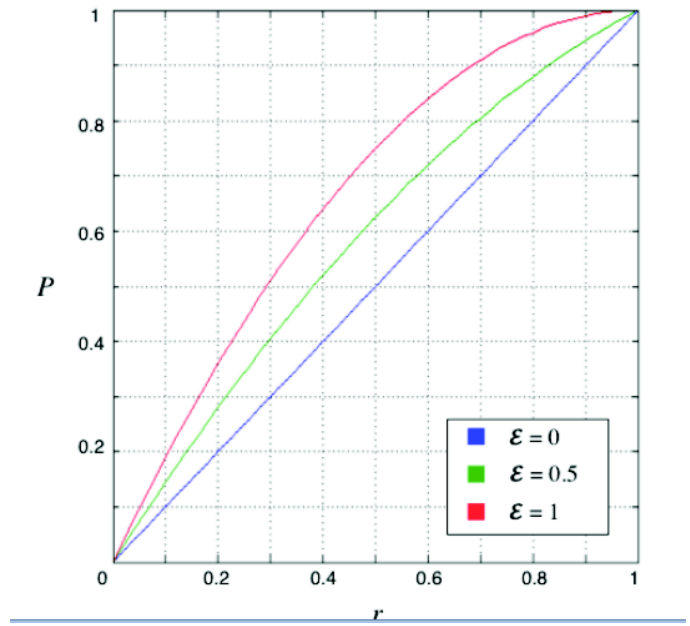
Multi-Agent Model

- Set of bacteria moving in space with concetration $\rho(x, y)$ of nutrient
- Let $\rho_i(t)$ be the concentration seen by bacteria b_i at time t
- if $\rho_i(t) \geq \rho_i(t - \delta t)$, the bacteria move straight with probability 0.9
- if $\rho_i(t) < \rho_i(t - \delta t)$, the bacteria move straight with probability 0.5
- Otherwise it makes a random turn
- Movie

Beyond the physical space : complex network

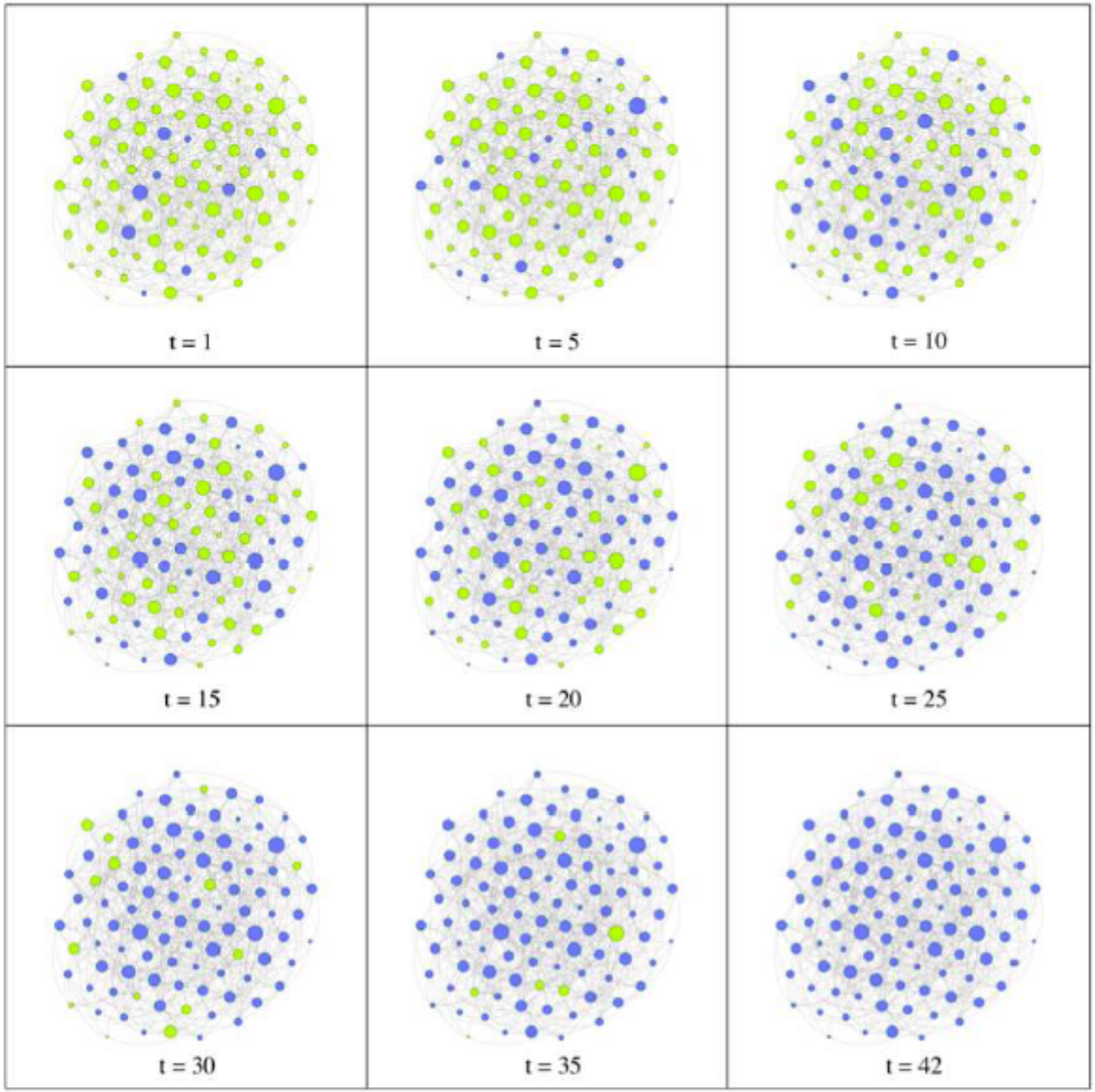
A model of opinion propagation in a social network





(Lino Velasquez, UNIGE)

Voter model : time evolution

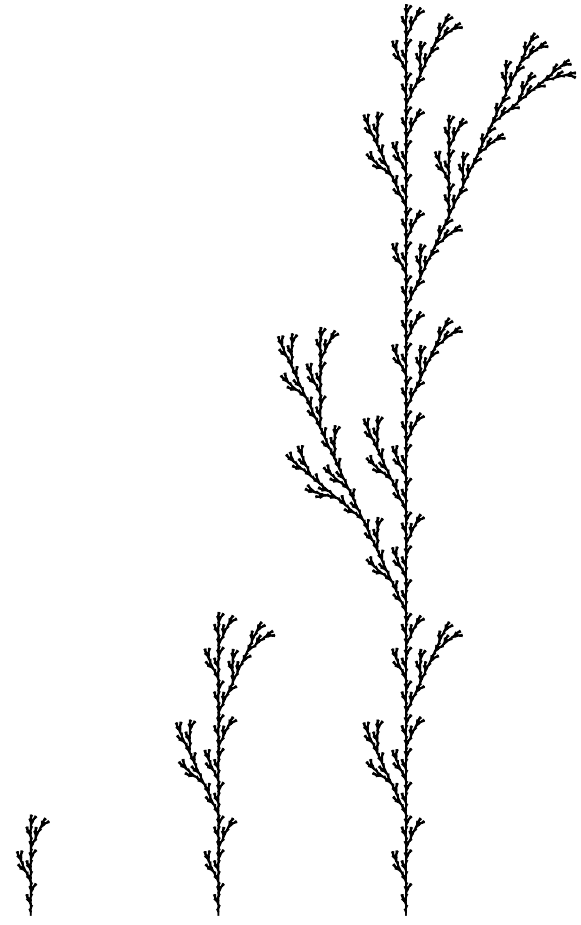


Réseau aléatoire, N = 100, p = 0.05, $\varepsilon = 0.3$

L-systems $F \to F[+F]F[-F]F$, $\beta = 25^o$.

F [+ F] F [- F] F [+ F [+ F] F [-
F] F] F [+ F] F [- F] F [- F [+ F]
F [- F] F] F [+ F] F [- F] F [+ F [
+ F] F [- F] F [+ F [+ F] F [- F]
F] F [+ F] F [- F] F [- F [+ F] F [
- F] F] F [+ F] F [- F] F] F [+ F]
F [- F] F [+ F [+ F] F [- F] F] F [
+ F] F [- F] F [- F [+ F] F [- F]
F] F [+ F] F [- F] F [- F [+ F] F [
- F] F [+ F [+ F] F [- F] F] F [+
F] F [- F] F [- F [+ F] F [- F] F]
F [+ F] F [- F] F] F [+ F] F [- F]
F [+ F [+ F] F [- F] F] F [+ F] F
[- F] F [- F [+ F] F [- F] F] F [+
F] F [- F] F

Code for 3 iterations



Iterations 3,4 and 5

Cellular Automata

B. Chopard et M. Droz : Cellular Automata Modeling of Physical Systems, Cambridge University Press, 1998.

B. Chopard, *Cellular Automata and lattice Boltzmann modeling of physical systems*, Handbook of Natural Computing, Rozenberg, Grzegorz ; Bäck, Thomas ; Kok, Joost N. (Eds.) Springer, pp. 287–331, 2013

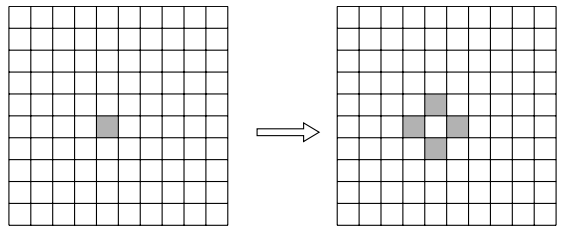
Definition

What is a Cellular Automata ?

- Mathematical abstraction of the real world, modeling framework
- Fictitious Universe in which everything is discrete
- But, it is also a mathematical object, new paradigm for computation
- Elucidate some links between **complex systems**, **universal computations**, **algorithmic complexity**, **intractability**.

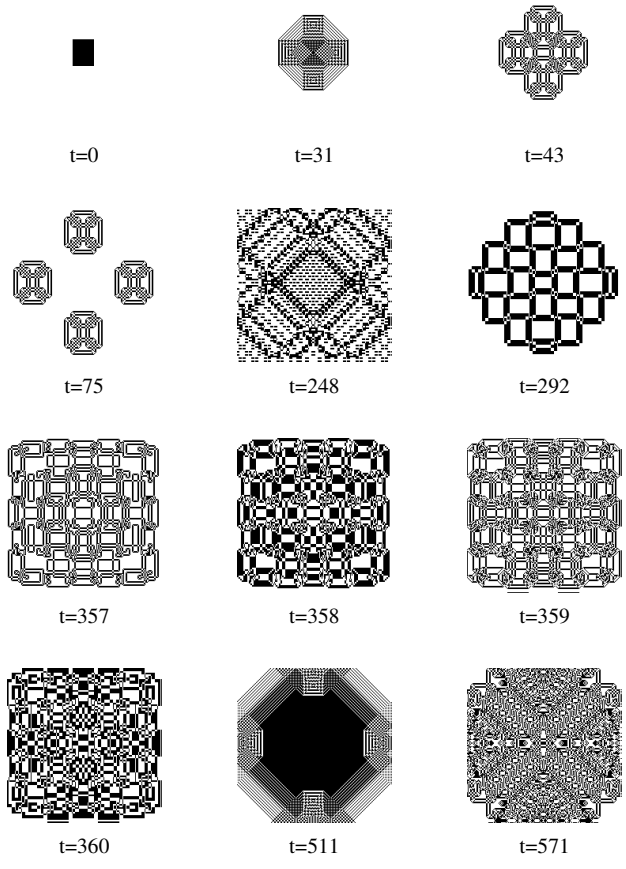
Example : the Parity Rule

- 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.

Pattern generated by the Parity Rule

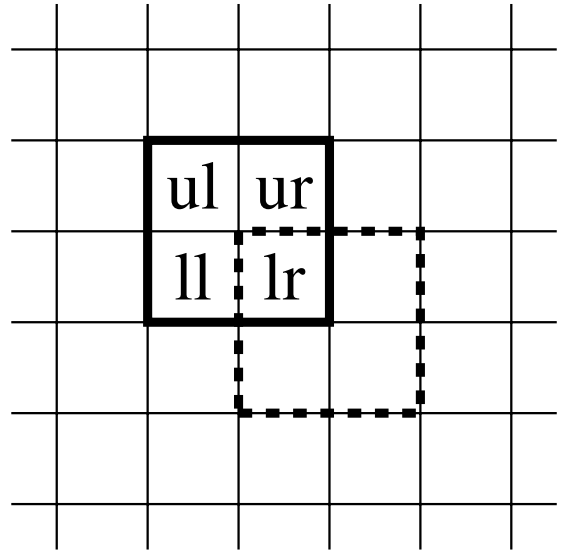


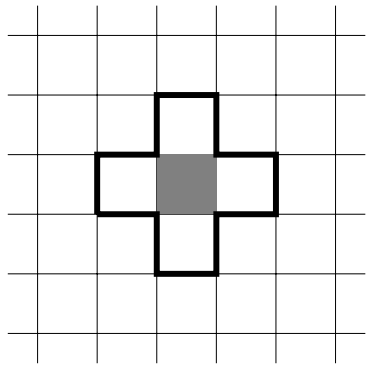
CA Definition

- Discrete space A : regular lattice of cells/sites in d dimensions.
- Discrete time
- Possible states for the cells : discrete set S
- Local, homogeneous **evolution rule** Φ (defined for a neighborhood $\mathcal{N}$).
- Synchronous (parallel) updating of the cells
- Tuple : $< A, S, \mathcal{N}, \Phi >$

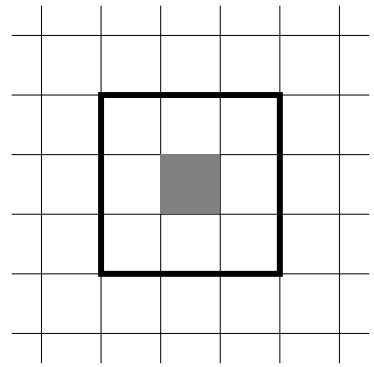
Neighborhood

- von Newmann
- Moore
- Margolus
- ...





(a)



(b)

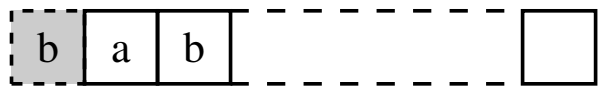
Boundary conditions

- periodic
- fixed
- reflexive
- ....

periodic

fixed

adiabatic



reflection

Generalization

- Stochastic CA
- Asynchronous update : loss of parallelism, but avoid oscillations
- Non-uniform CA

Implementation of the evolution rule

m states per cells, k neighbors.

- On-the-fly calculation
- Lookup table
- Finite number of possible universes : m^{m^k} possible rules where m is the number of states per cell and k the number of neighbors.

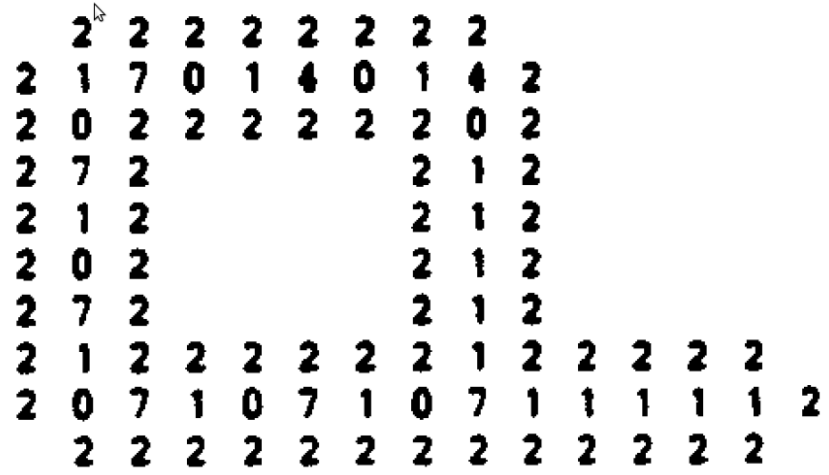
Historical notes

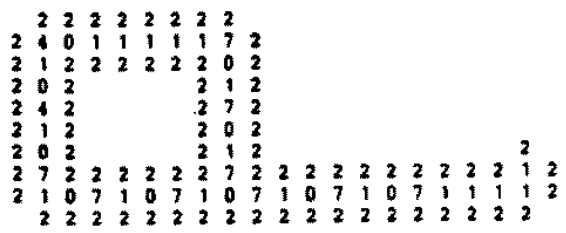
- Origin of the CA's (1940s) : John von Neumann and S. Ulam
- Design a better computer with self-repair and self-correction mechanisms
- Simpler problem : find the logical mechanisms for self-reproduction :
- Before the discovery of DNA : find an algorithmic way (transcription and translation)
- Formalization in a fully discrete world
- Automaton with 29 states, arrangement of thousands of cells which can self-reproduce
- Universal computer

Langton's CA

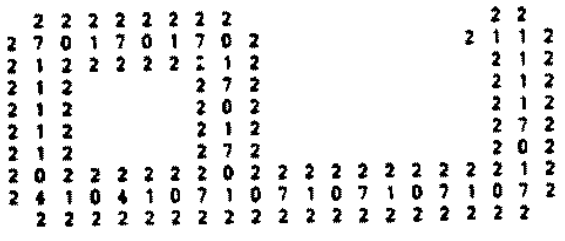
- Simplified version (8 states).
- Not a universal computer
- Structures with their own fabrication recipe
- Using a reading and transformation mechanism

Langton's CA : basic cell replication

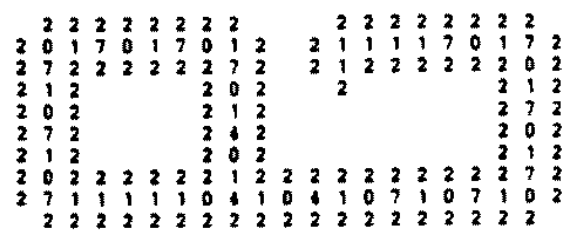




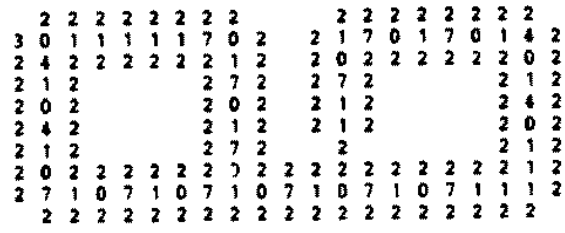
TIME = 35



TIME = 70

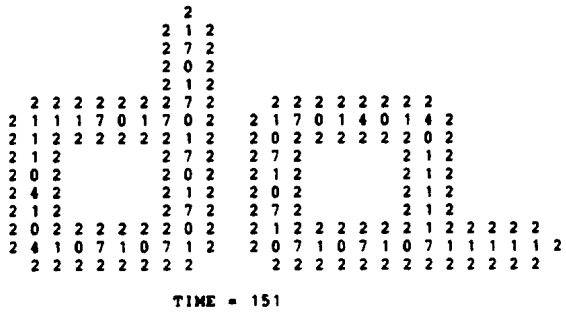


TIME = 105



TIME = 120

Langton's Automaton : spatial and temporal evolution



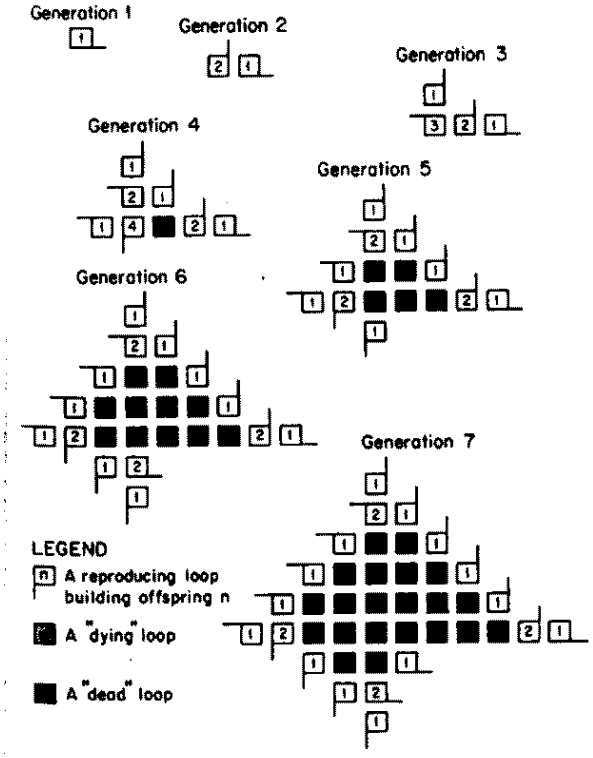


Fig. 10. Growth of loop colony. Seven generations of growth in a colony of loops.

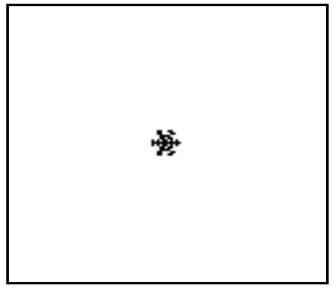
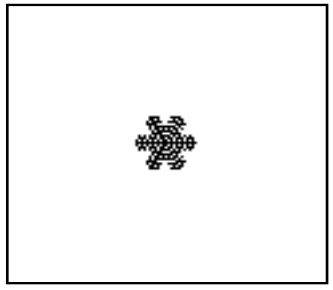
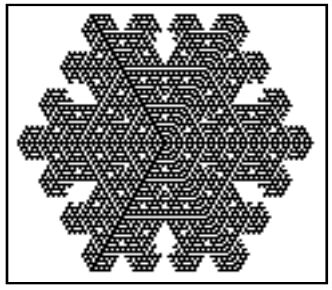
Langton's CA : some conclusions

- 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

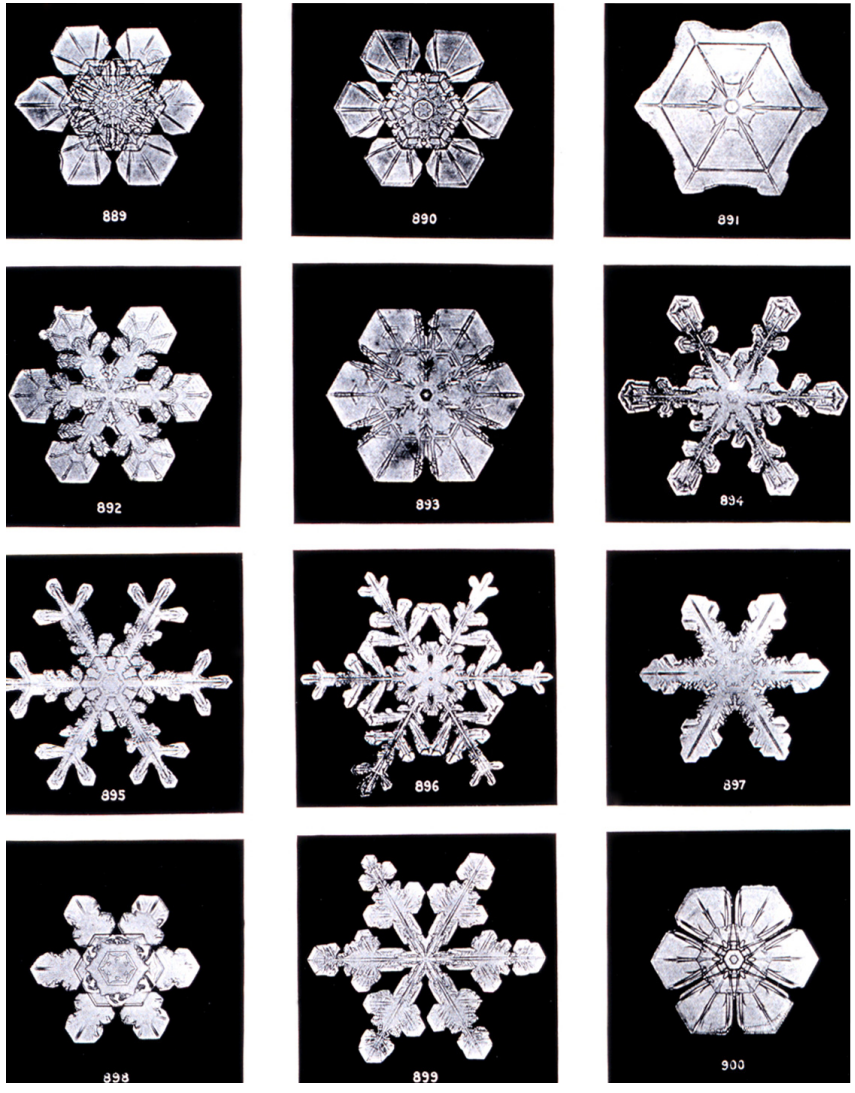
- Several levels of reality : macroscopic, mesoscopic and microscopic.
- The macroscopic behavior depends very little on the details of the microscopic interactions.
- Only “symmetries” or conservation laws survive. The challenge is to find them.
- Consider a fictitious world, particularly easy to simulate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

A Caricature of reality

What is this ?

The real thing



Wilson Bentley, 1902

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 ($\rightarrow$ice) if one and only one already solidified molecule is in its vicinity**
• **Growth is constrained by 60^o angles**

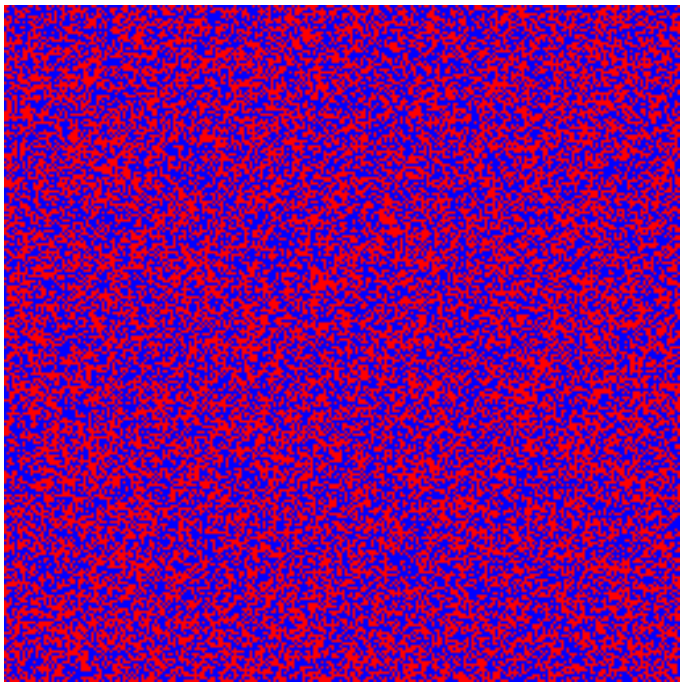
Examples of CA rules

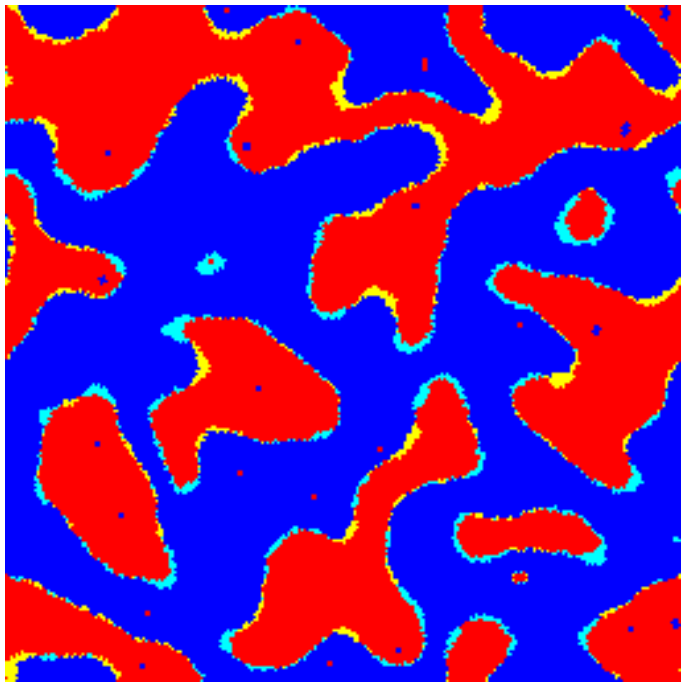
Cooperation models : annealing rule

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

Rule :

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





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).

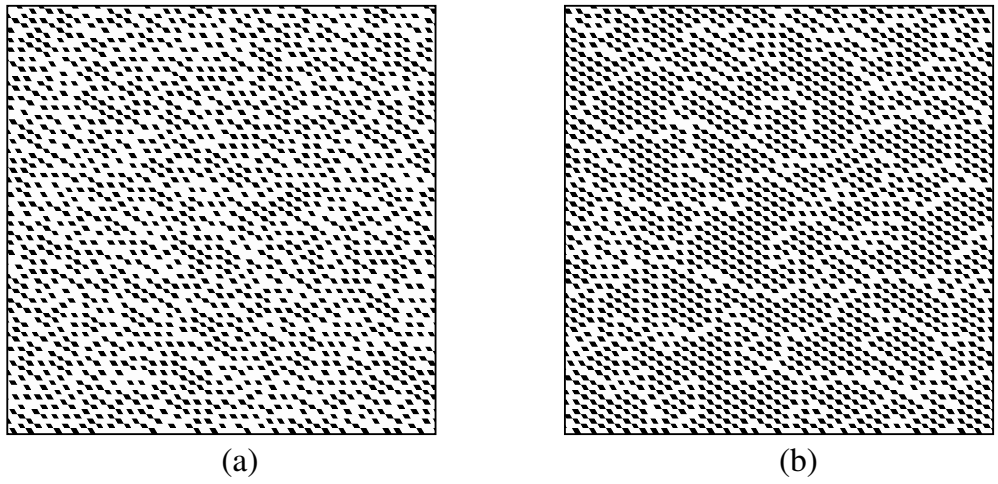
Biological mechanisms :

- 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.

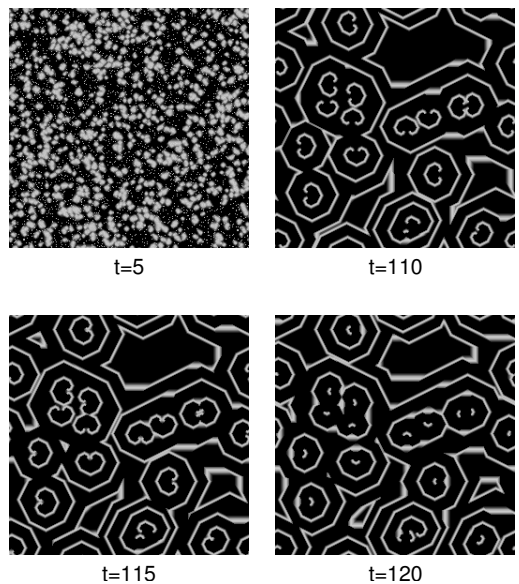
- CA produces situations with about **23%** of active cells, for almost any value of p_{anihil} and p_{growth}.
- Model robust to the lack of details, but need for hexagonal cells

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).

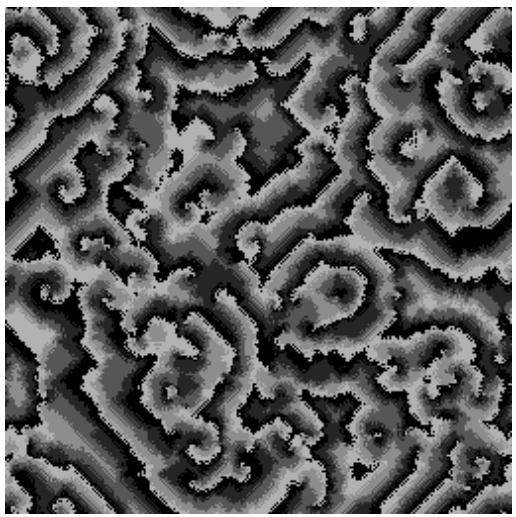
Greenberg-Hastings Model

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



Belousov-Zhabotinski (tube worm)

The state of each site is either 0 or 1 ; a local timer with values 0, 1, 2 or 3 controls the 0 period.



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

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

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

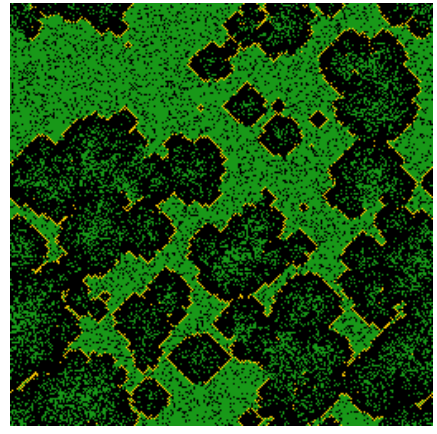
Forest fire

(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 ;

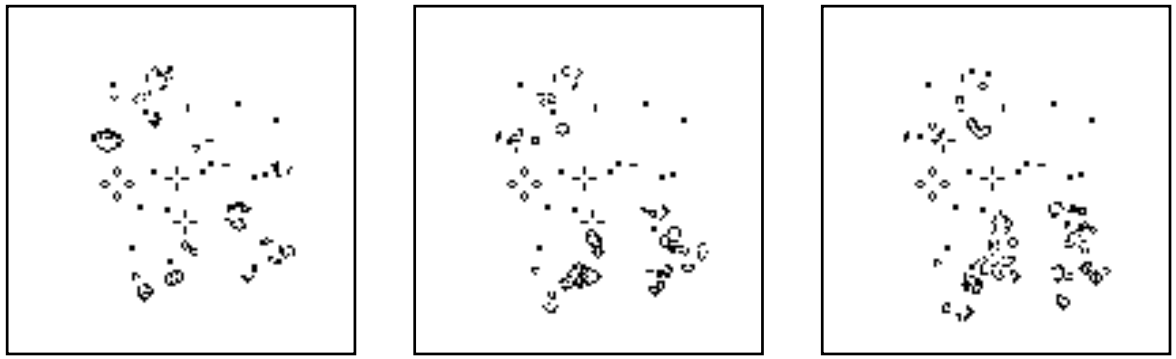
(4) A tree without a burning nearest neighbor becomes a burning tree during one time step with probability f (lightning).



Complex systems

Rule of the Game of Life :

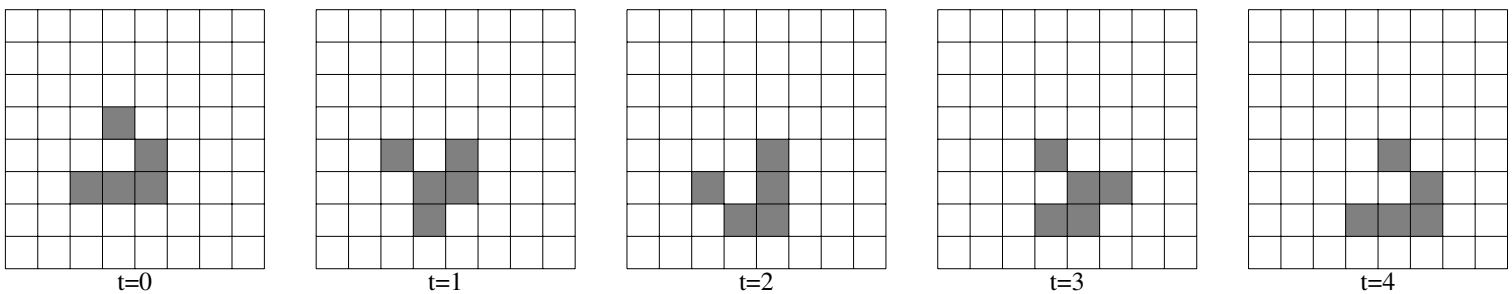
- Square lattice, 8 neighbors
- Cells are dead or alive (0/1)
- Birth if exactly 3 living neighbors
- Death if less than 2 or more than 3 neighbors



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.



Complex Behavior in the game of life

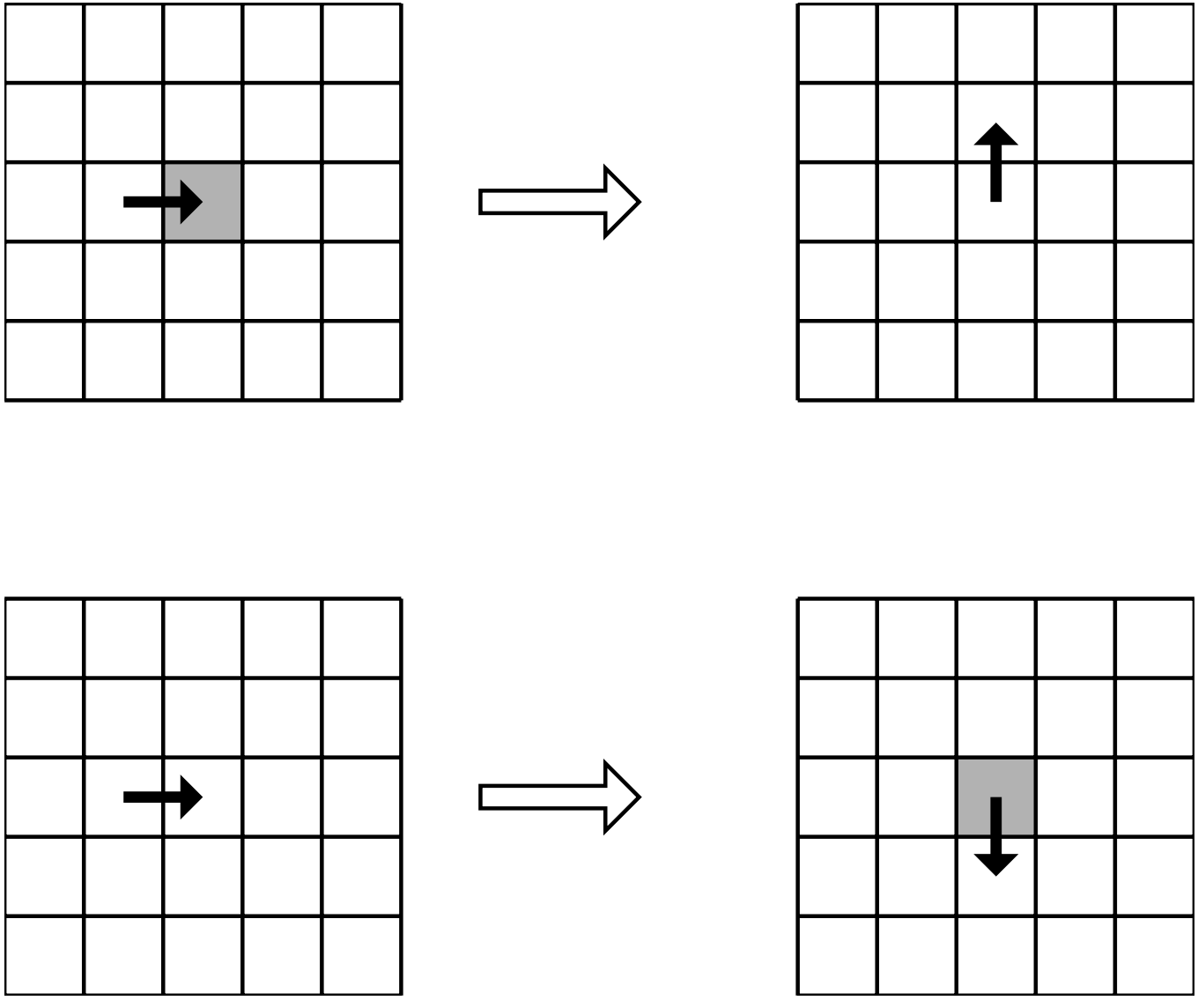
A glider gun (image : Internet)

- There are more complex structures with more complex behavior : a zoology of organisms.
- The game of life is a *Universal computer*

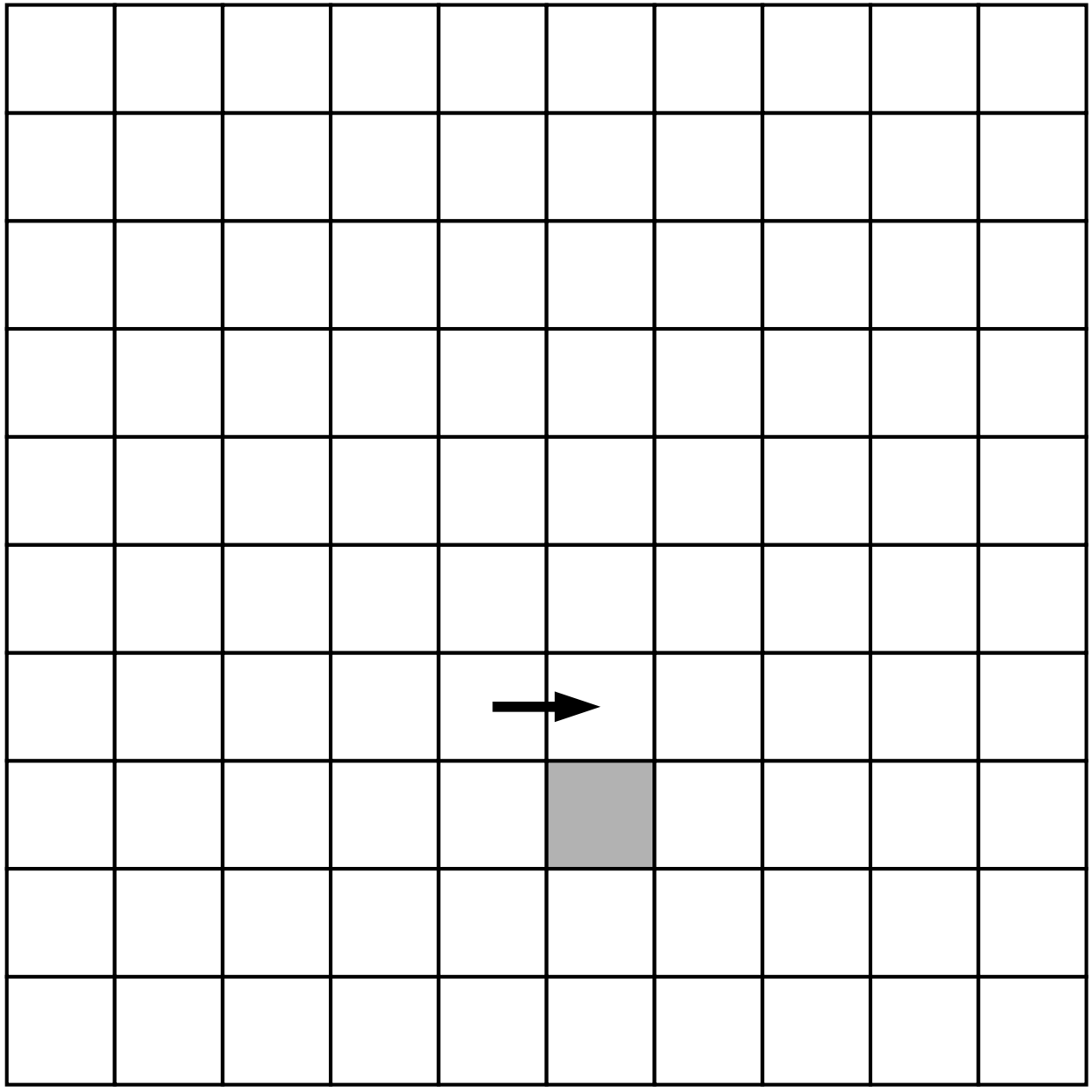
Langton's ant

This is an hypothetical animal moving on a 2D lattice, acoring to simple rules, which depend on the color of the cell on which the ant sits.

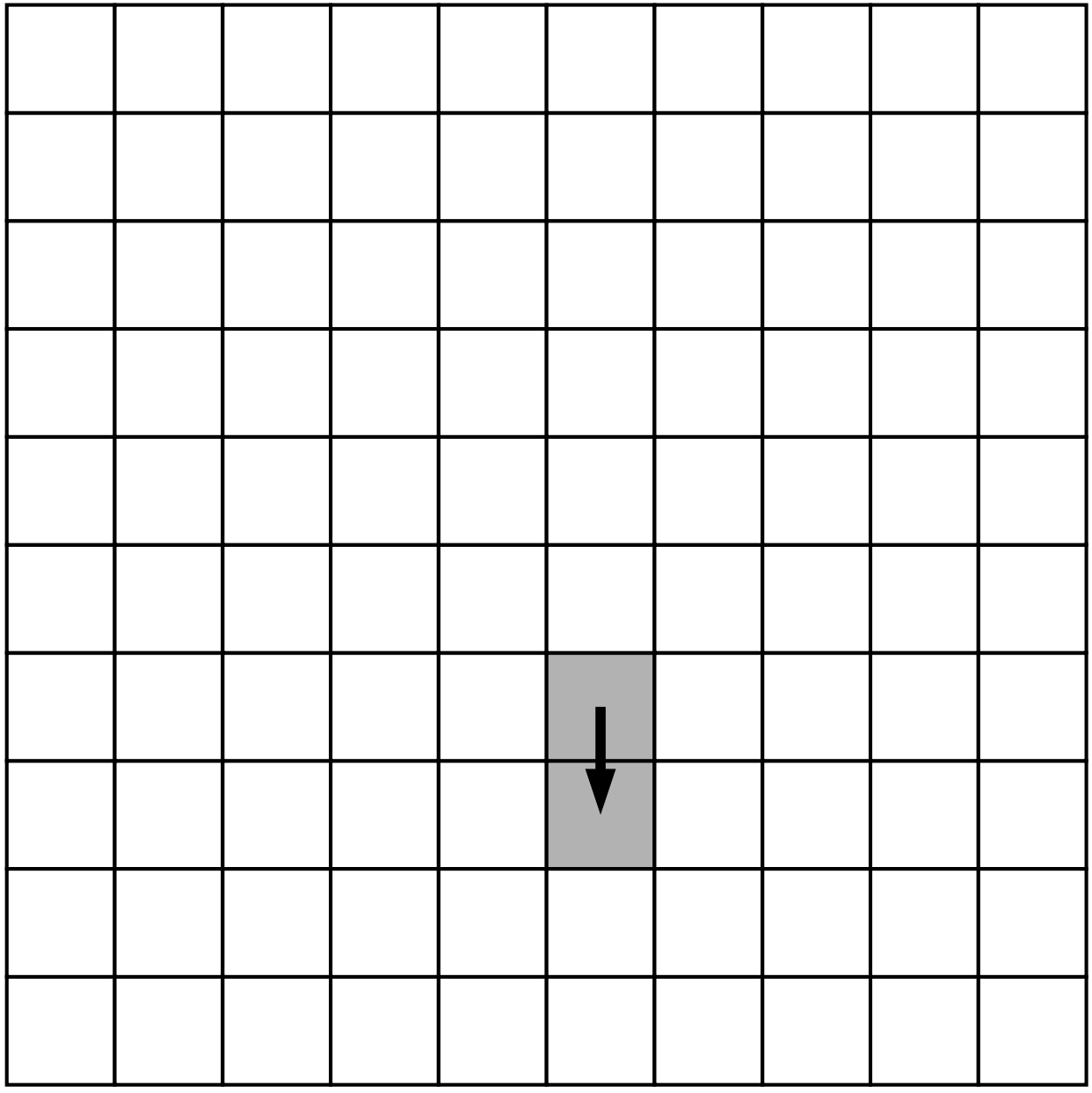
The rules



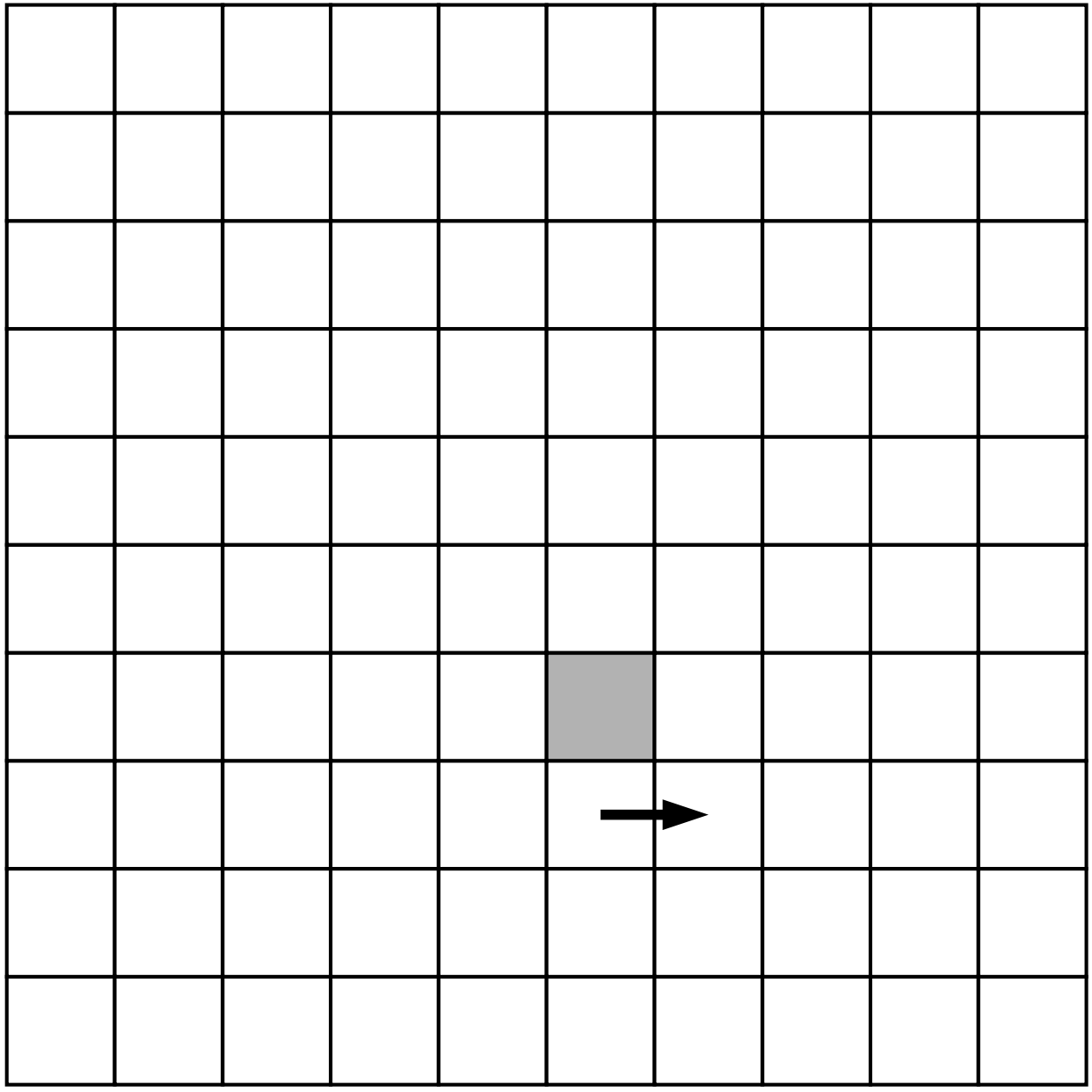
Some evolution steps



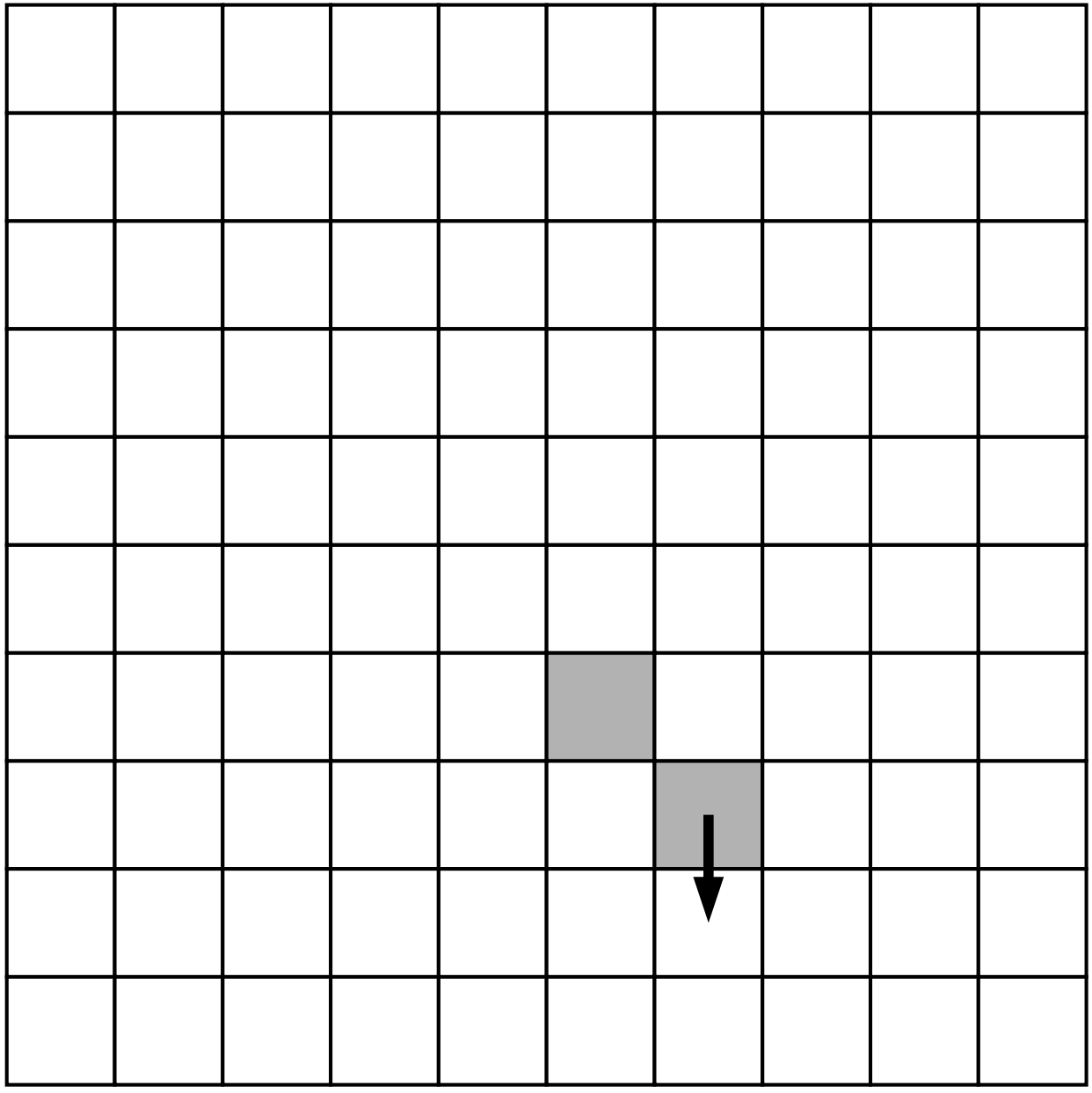
Some evolution steps



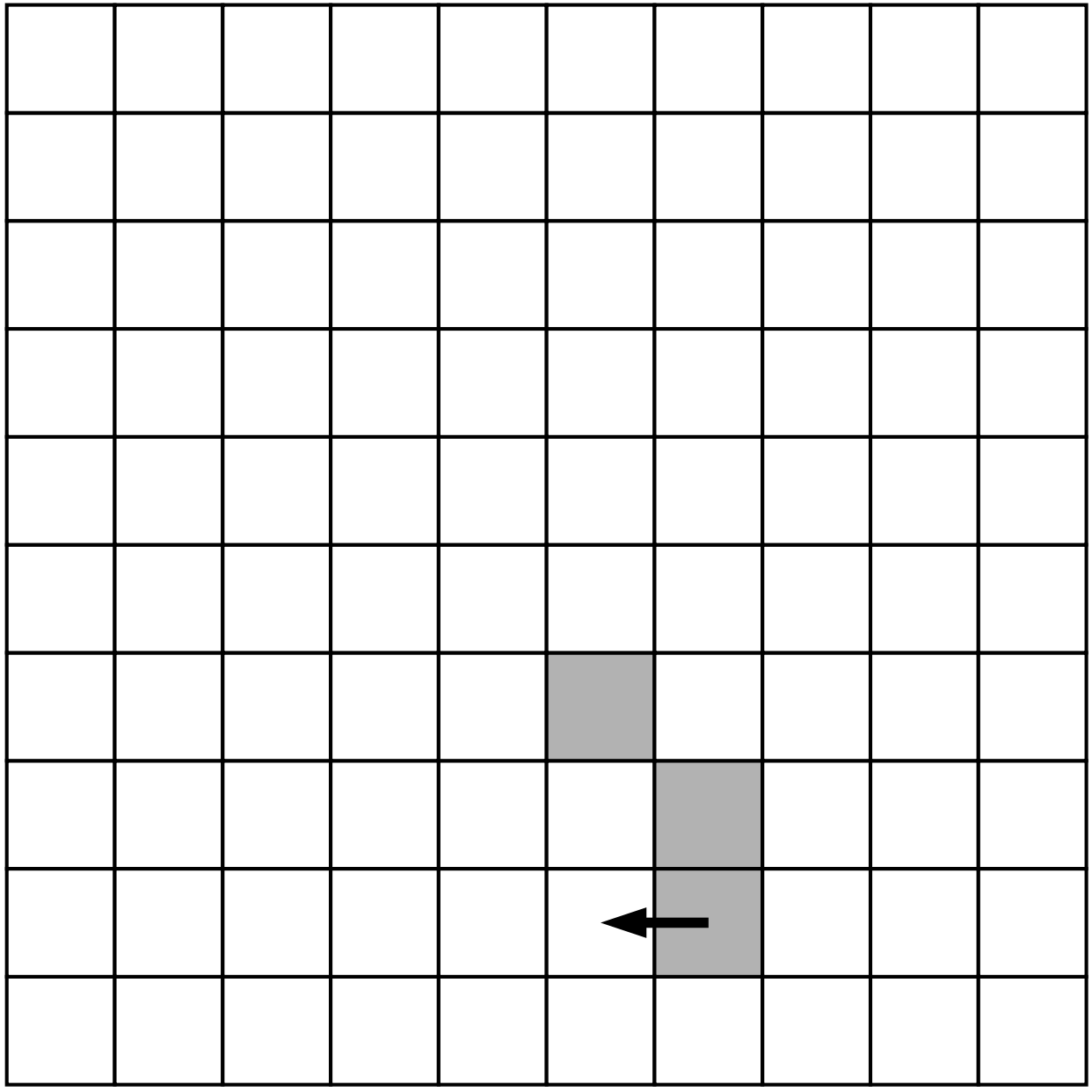
Some evolution steps



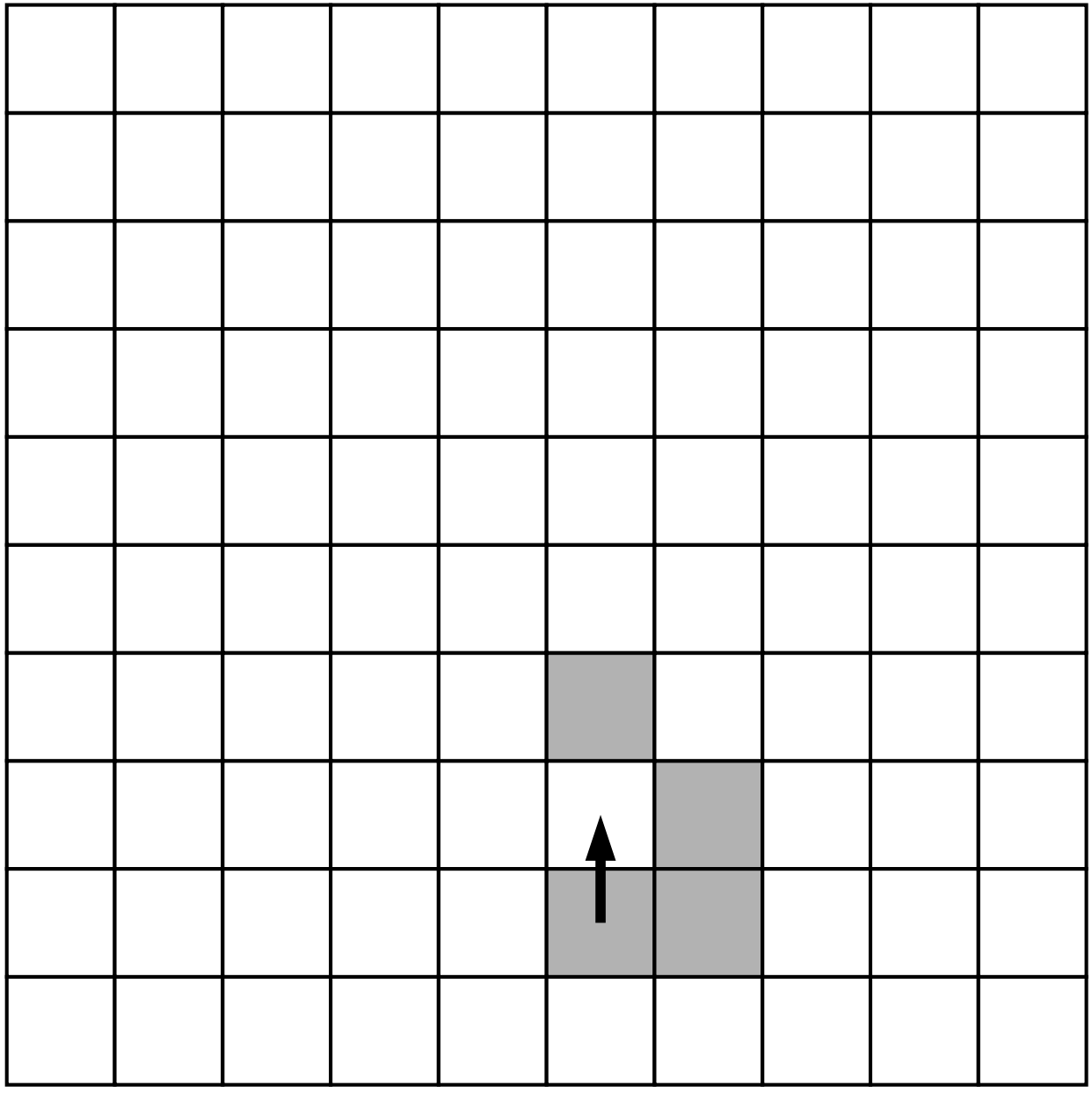
Some evolution steps



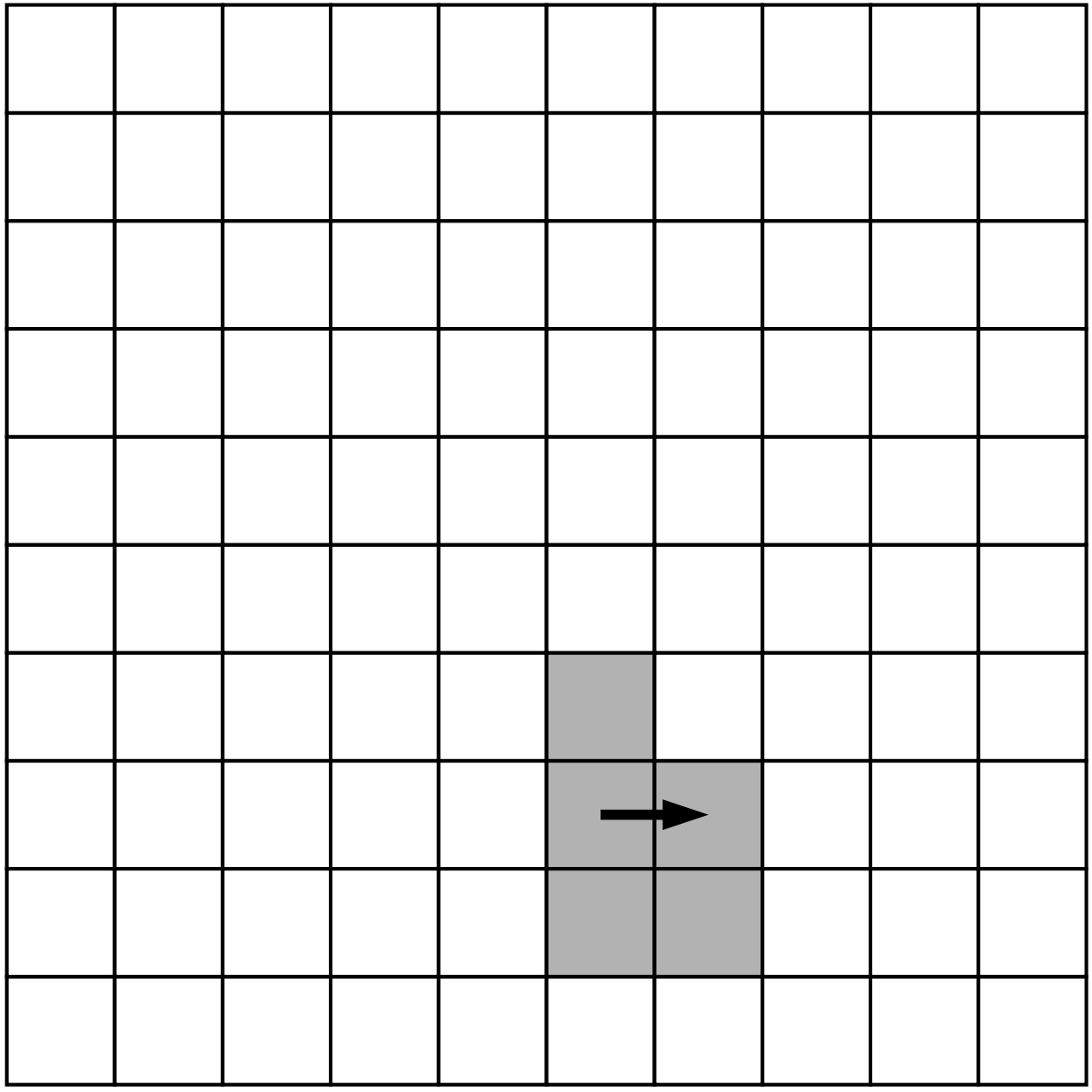
Some evolution steps



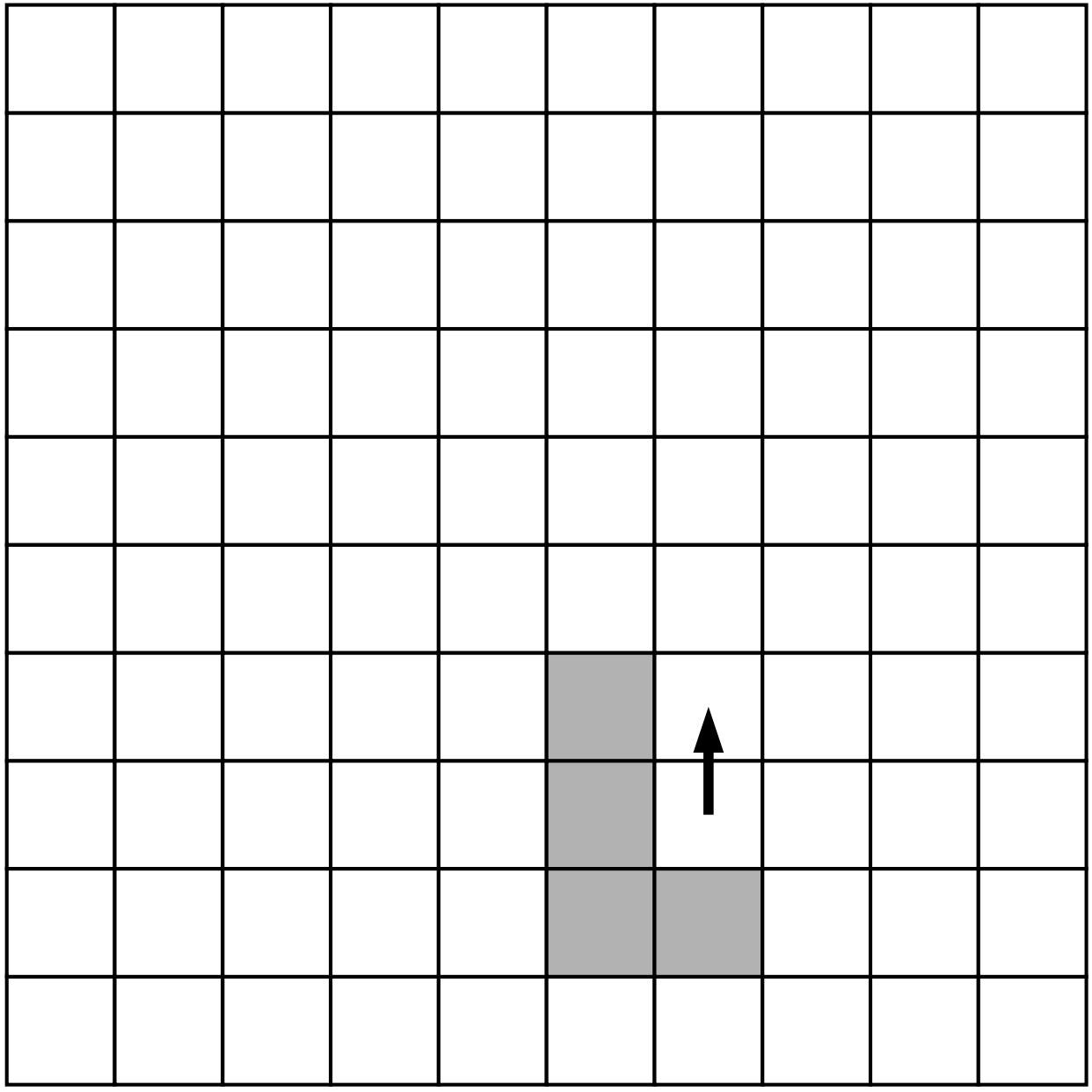
Some evolution steps



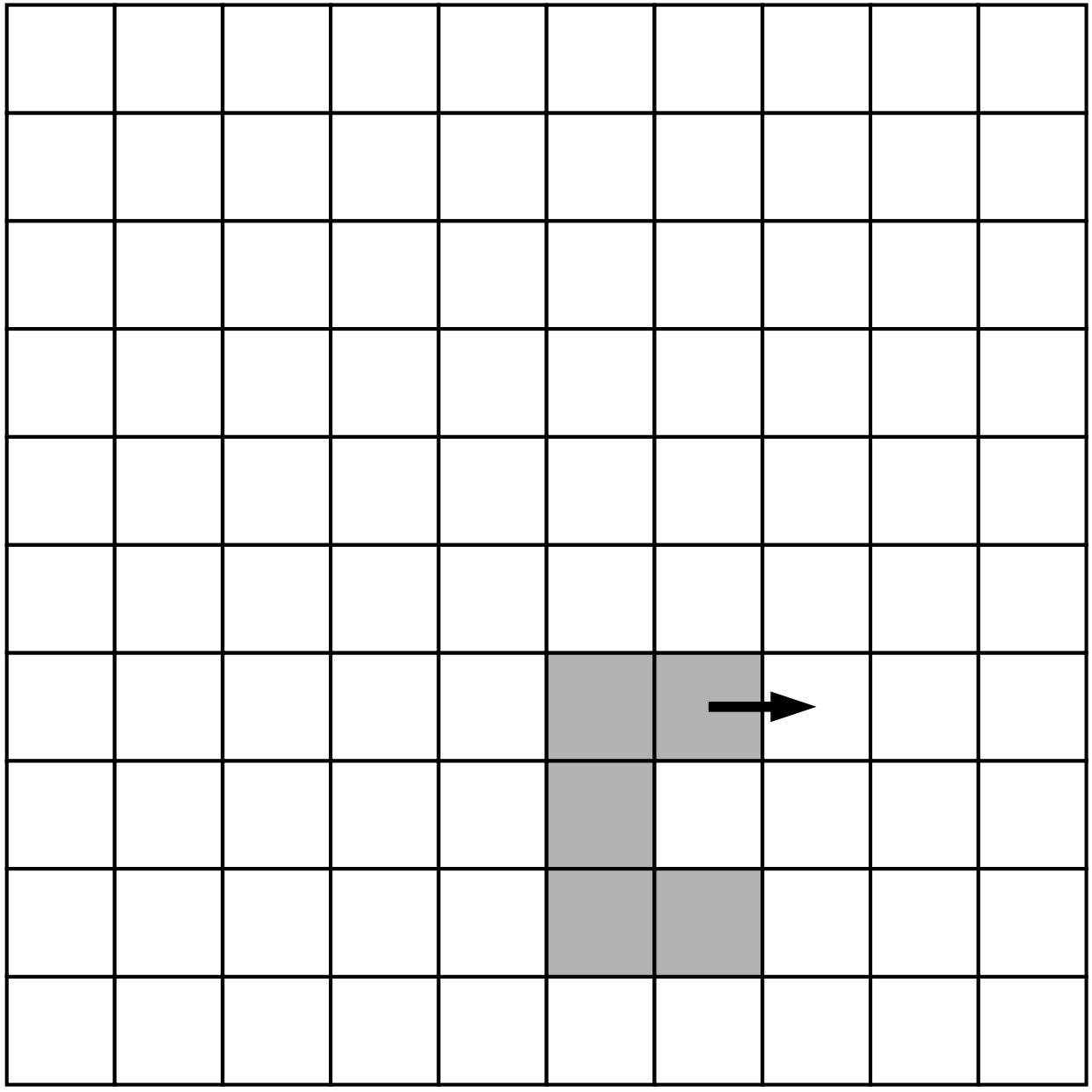
Some evolution steps



Some evolution steps



Some evolution steps

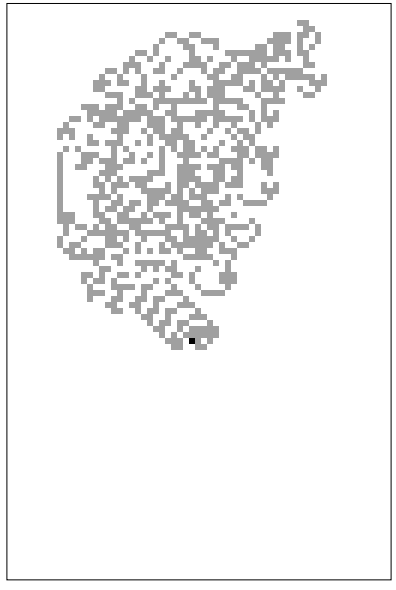


Where does the ant go in the long run

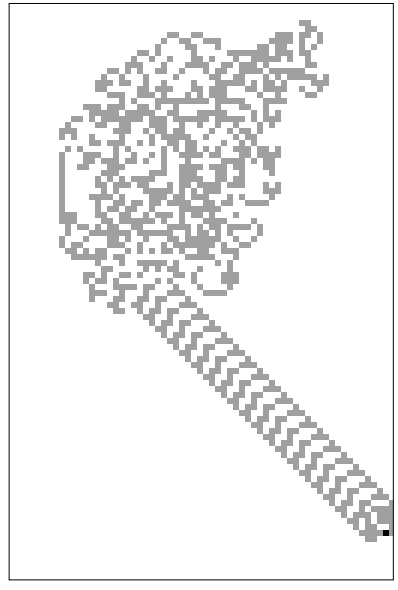
- Animation...

Where does the ant go in the long run

t=6900

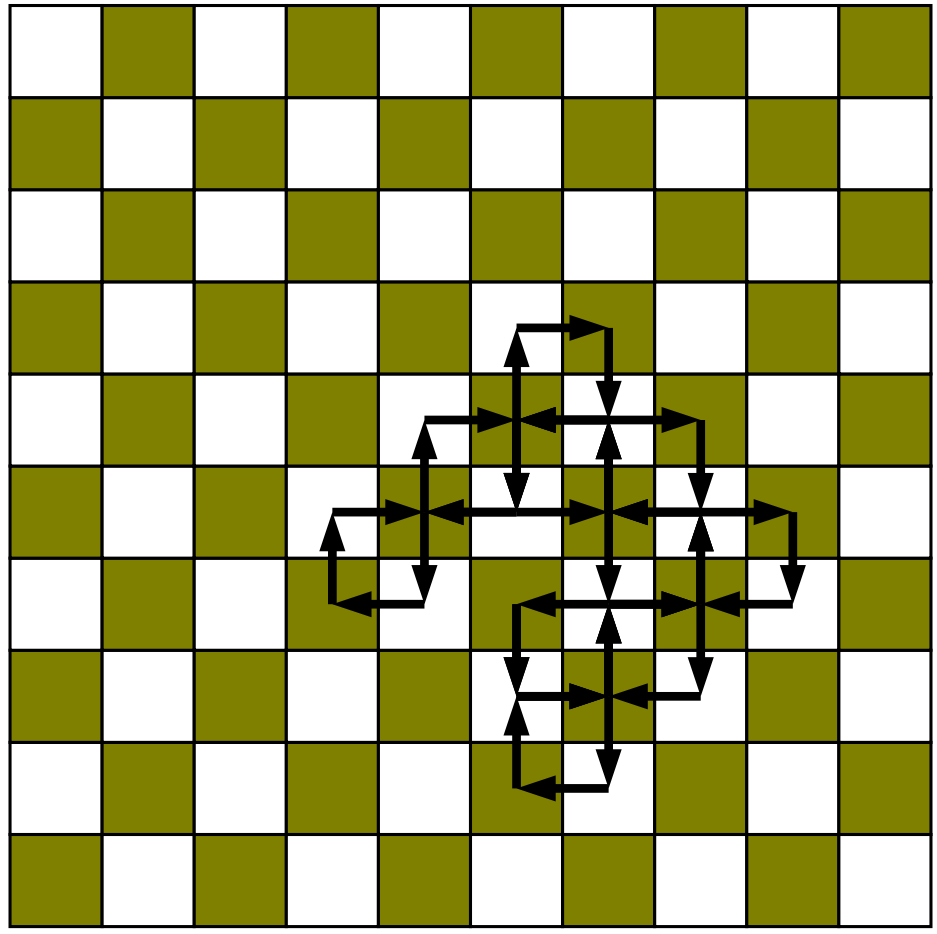


t=10431



t=12000

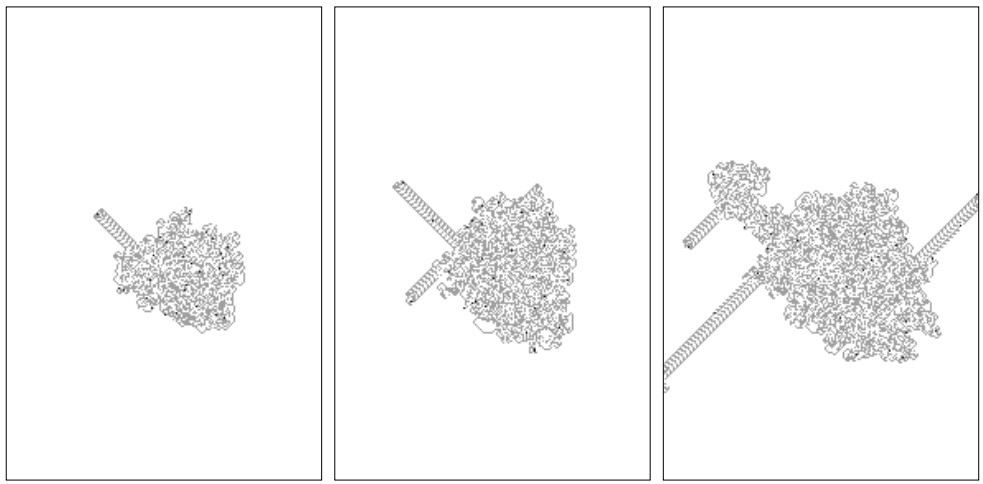
The ants always escape to infinity



for any initial coloration of the cells

What about many ants ?

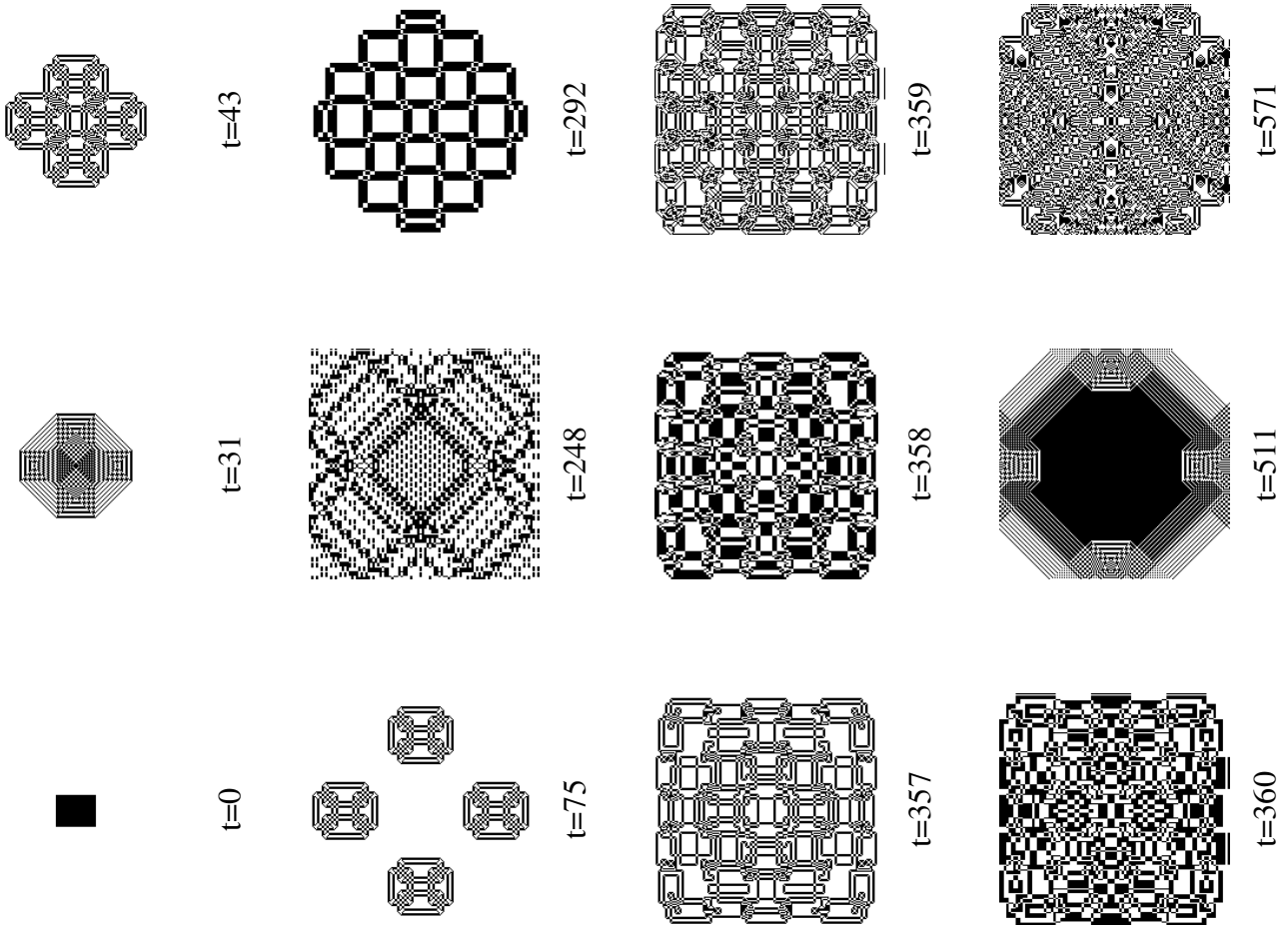
- Adapt the “change of color” rule
- Cooperative and destructive effects
- The trajectory can be bounded or not
- Past/futur symmetry explains periodic motion



Impact on the scientific methodolgy

- The laws are perfectly known
- But we cannot predict the details of the movements (when does a highway appears)
- Microscopic knolwdge is not enough to predict the macroscopic behavior
- Then, the only solution is the **observe** the behavior
- The only information we have on the trajectory are the reflect of the symmetries of the rule

Prediction means to compute faster than reality

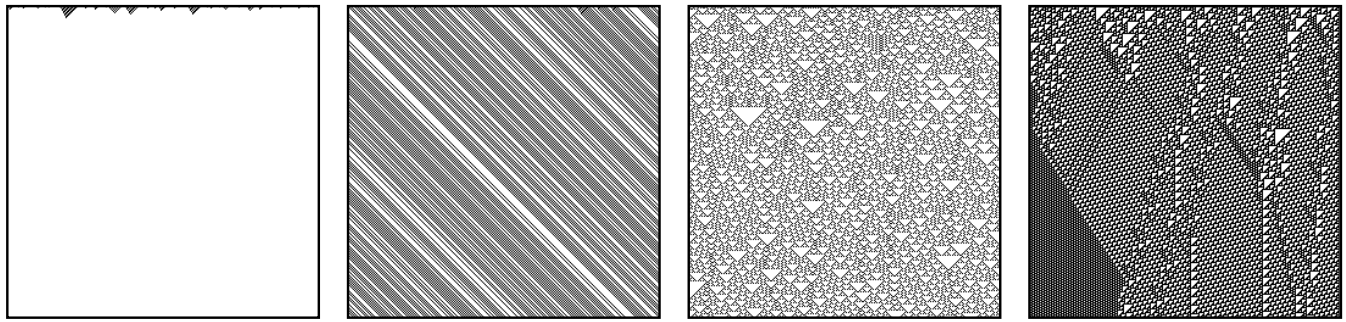


Prediction means to compute faster than reality

(a) (b) (c)

Wolfram's rules

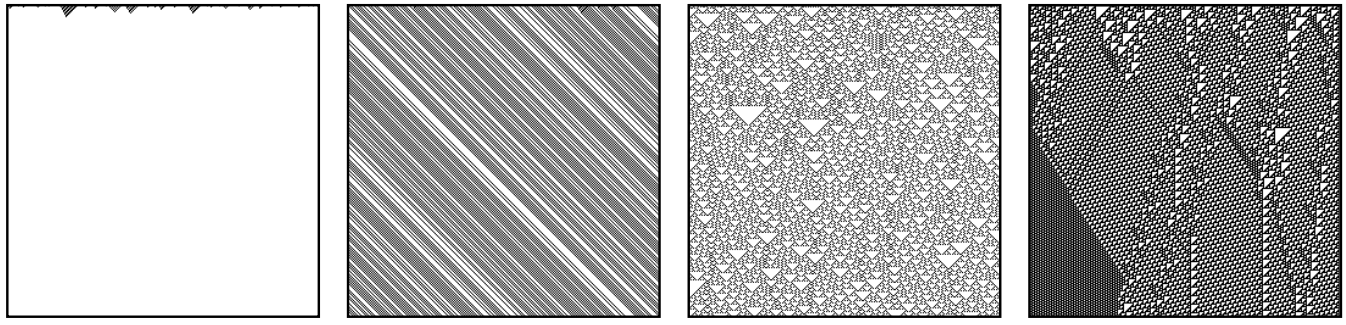
256 one-dimensional, 3 neighbors Cellular Automata :



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

Coombs, Stephen 2009, The Geometry and Pigmentation of Seashells

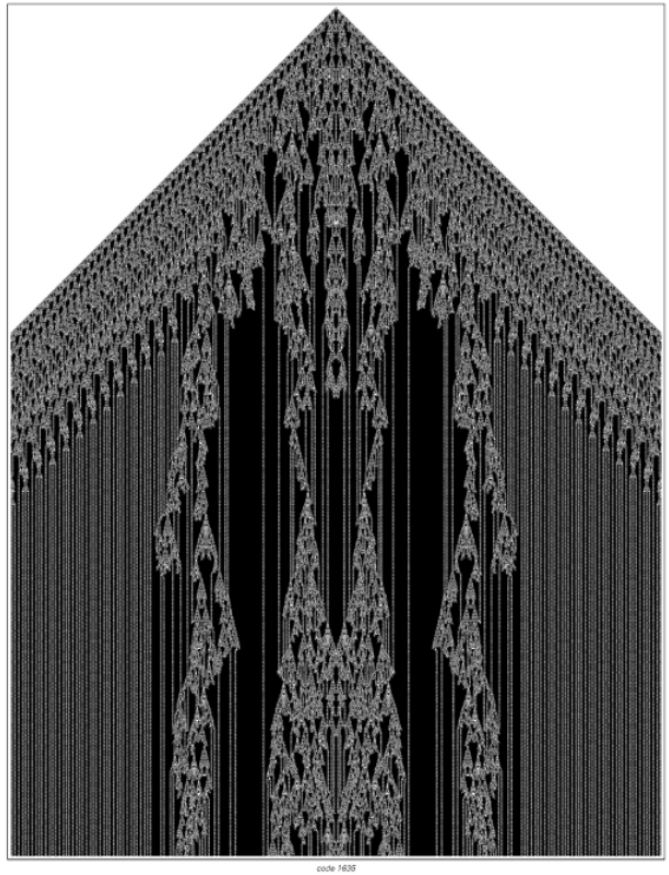
Wolfram's rules : complexity classes



- **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.

Wolfram's rules : 1D, 5 neighbors



Other simple rules

- time-tunnel

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

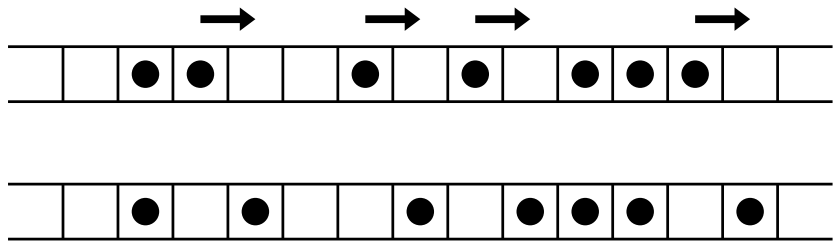
- random

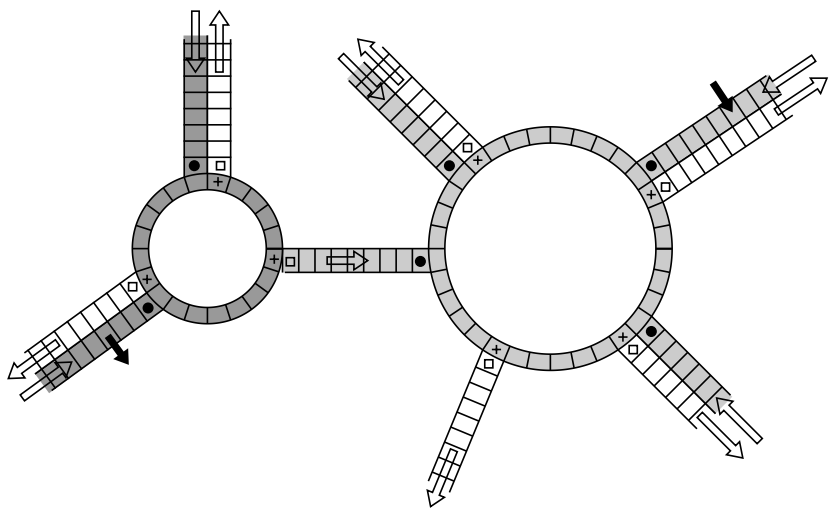
$$C(t+1) = (S(t).and.E(t)).xor.W(t).xor.N(t).xor.C(t)$$

- string : a one-dimensional spring-bead system

Traffic Models

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





Flow diagram

The car density at time t on a road segment of length L is defined as

$$\rho(t) = \frac{N(t)}{L}$$

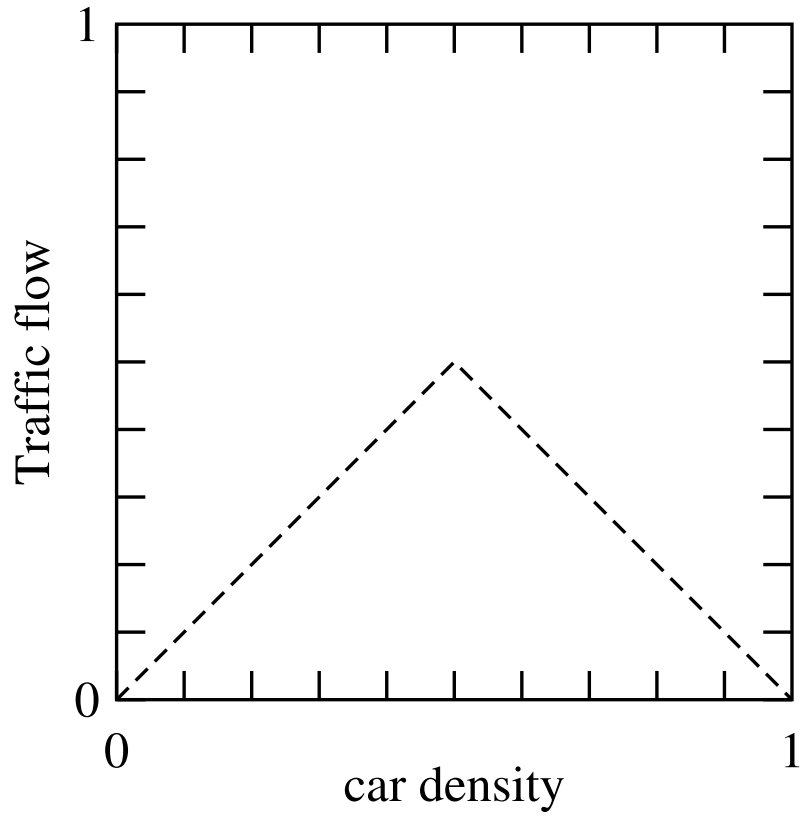
where N is the no of cars along L
The average velocity $< v >$ at time t on this segment is defined as

$$< v >= \frac{M(t)}{N(t)}$$

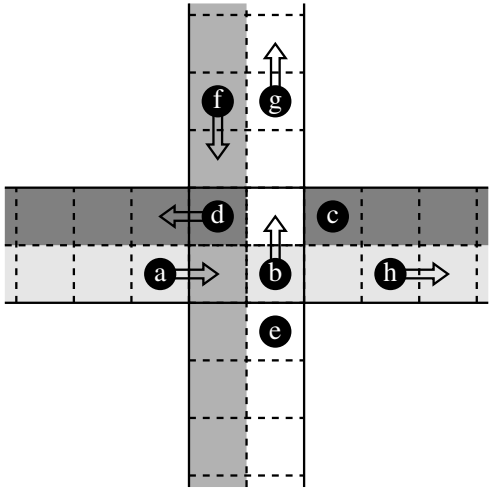
where $M(t)$ is the number of car moving at time t
The traffic flow j is defined as

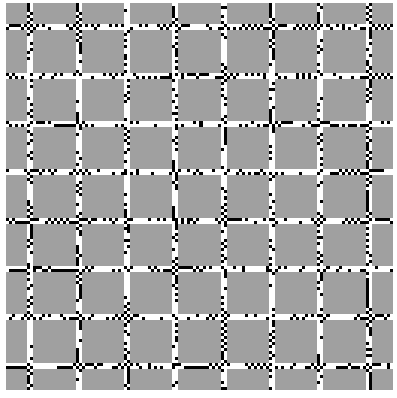
$$j = \rho < v >$$

Flow diagram of rule 184

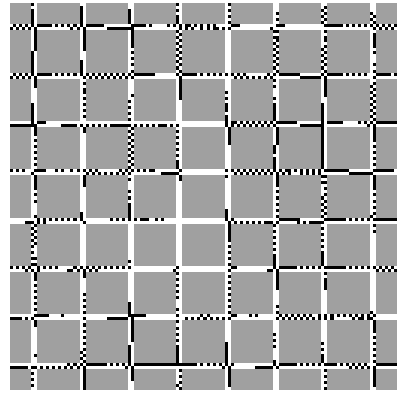


Traffic in a Manhattan-like city



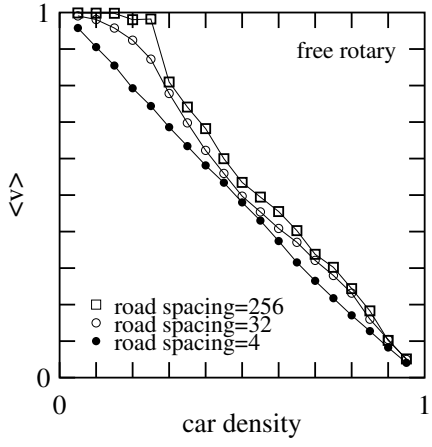


(a)

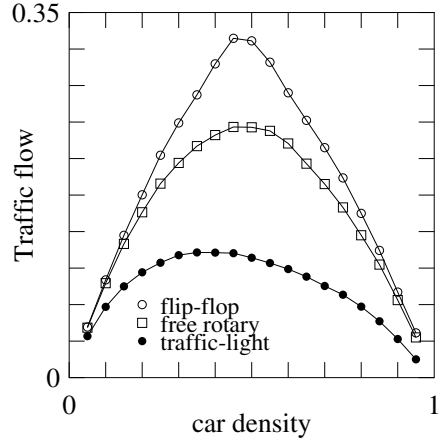


(b)

(a)

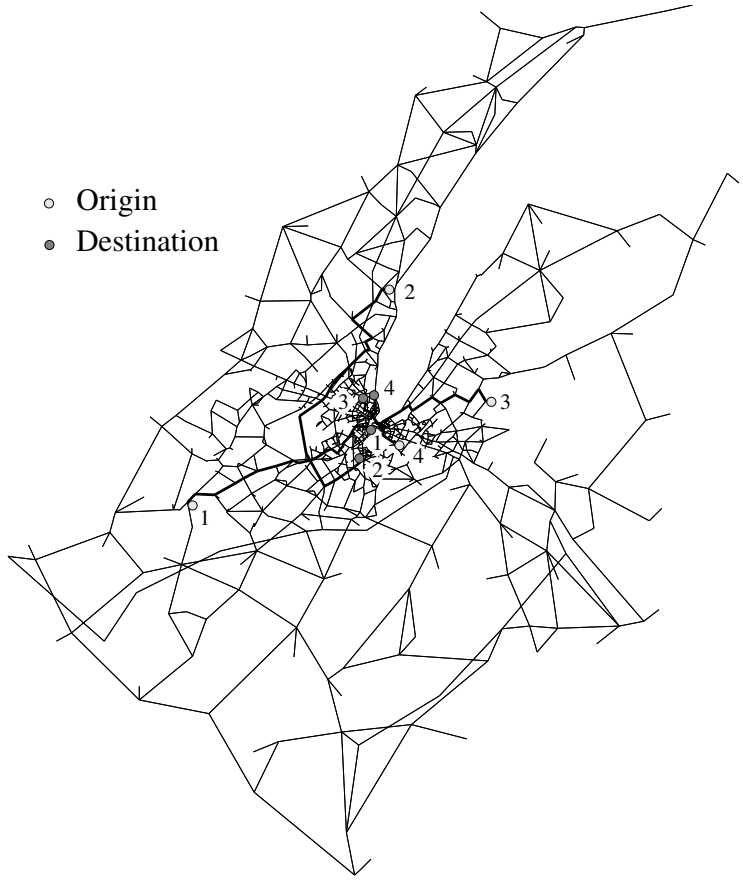


(b)

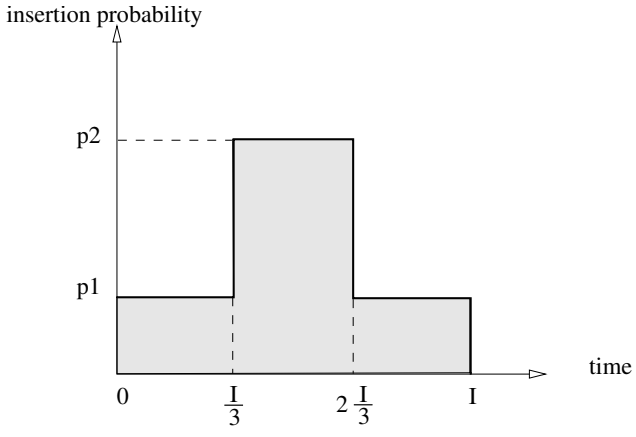


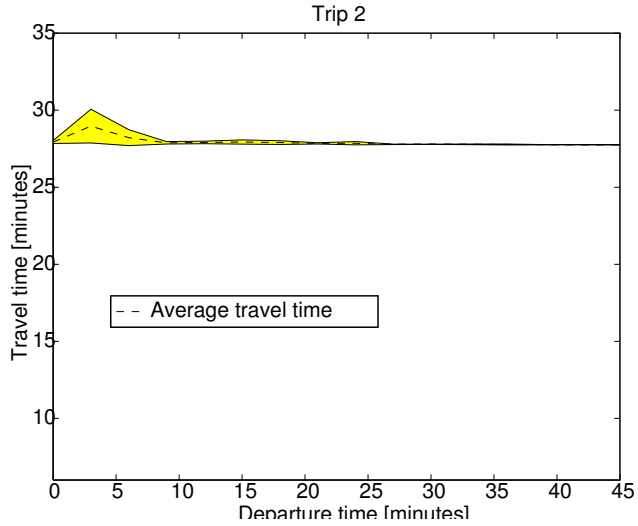
Case of the city of Geneva

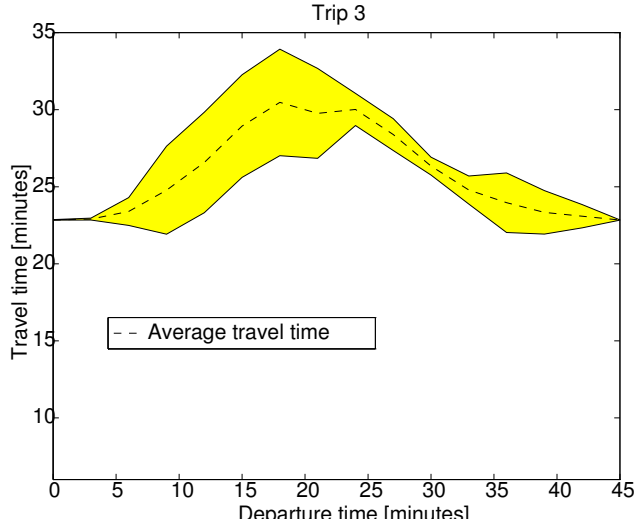
- 1066 junctions
- 3145 road segments
- 560886 road cells
- 85055 cars



Travel time during the rush hour

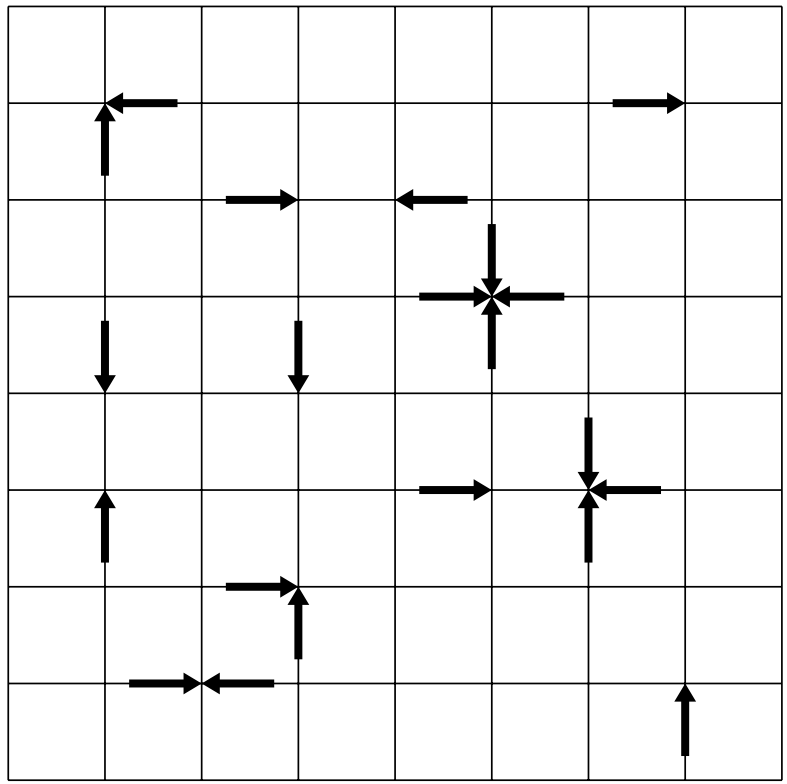






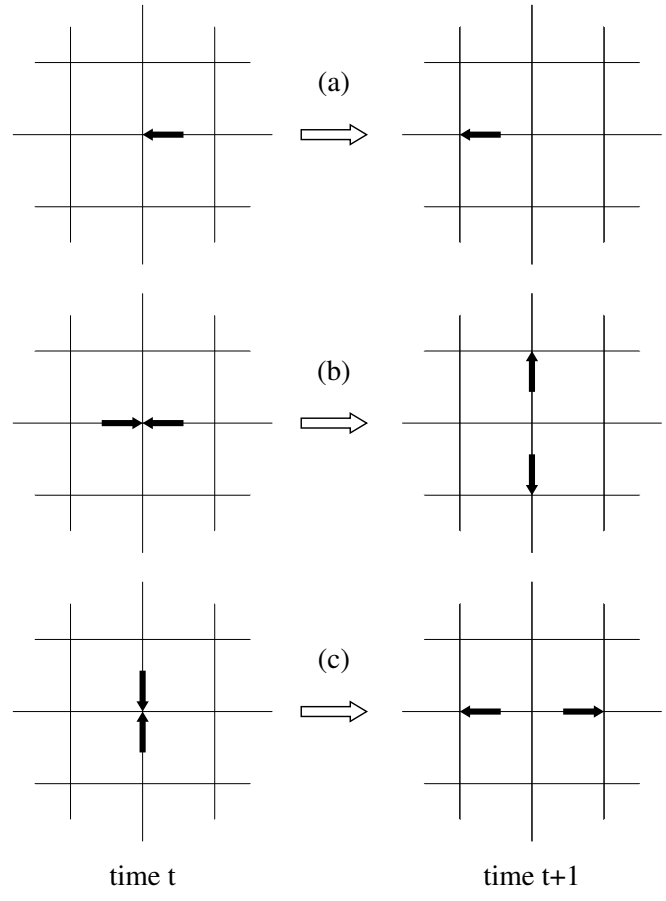
Lattice gases

Fully discrete molecular dynamics



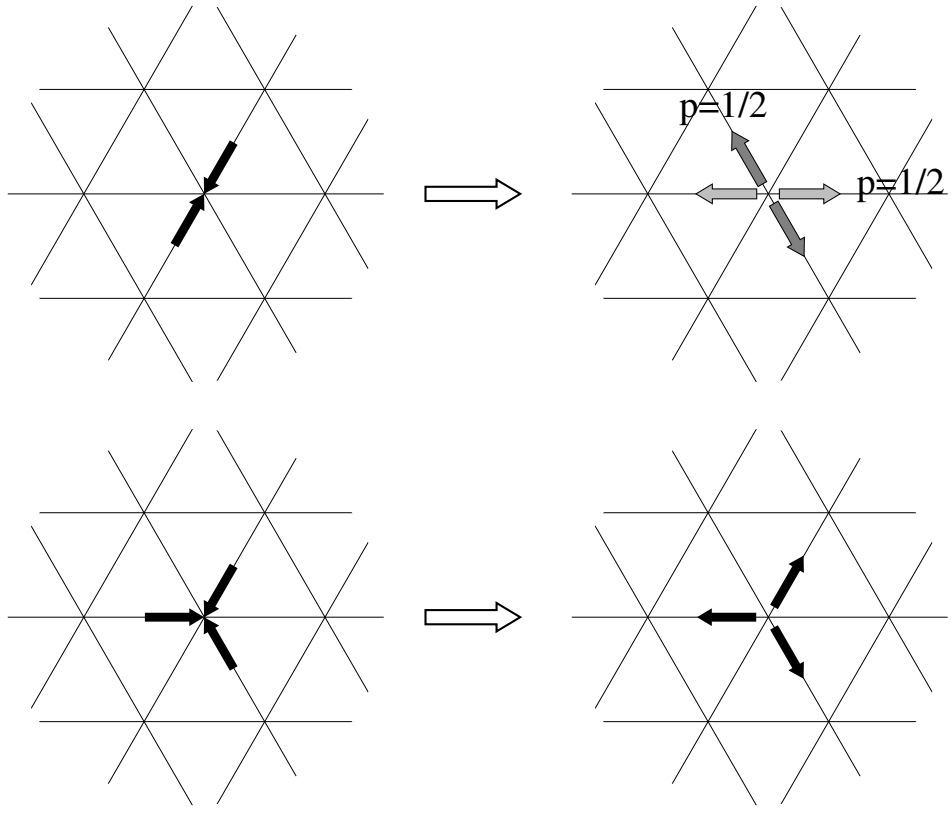
Example : HPP model collision rules

- HPP : Hardy, Pomeau, de Pazzis, 1971 : kinetic theory of point particles on the D2Q4 lattice
- FHP : Frisch, Hasslacher and Pomeau, 1986 : first LGA reproducing a (almost) correct hydrodynamic behavior (Navier-Stokes eq.)



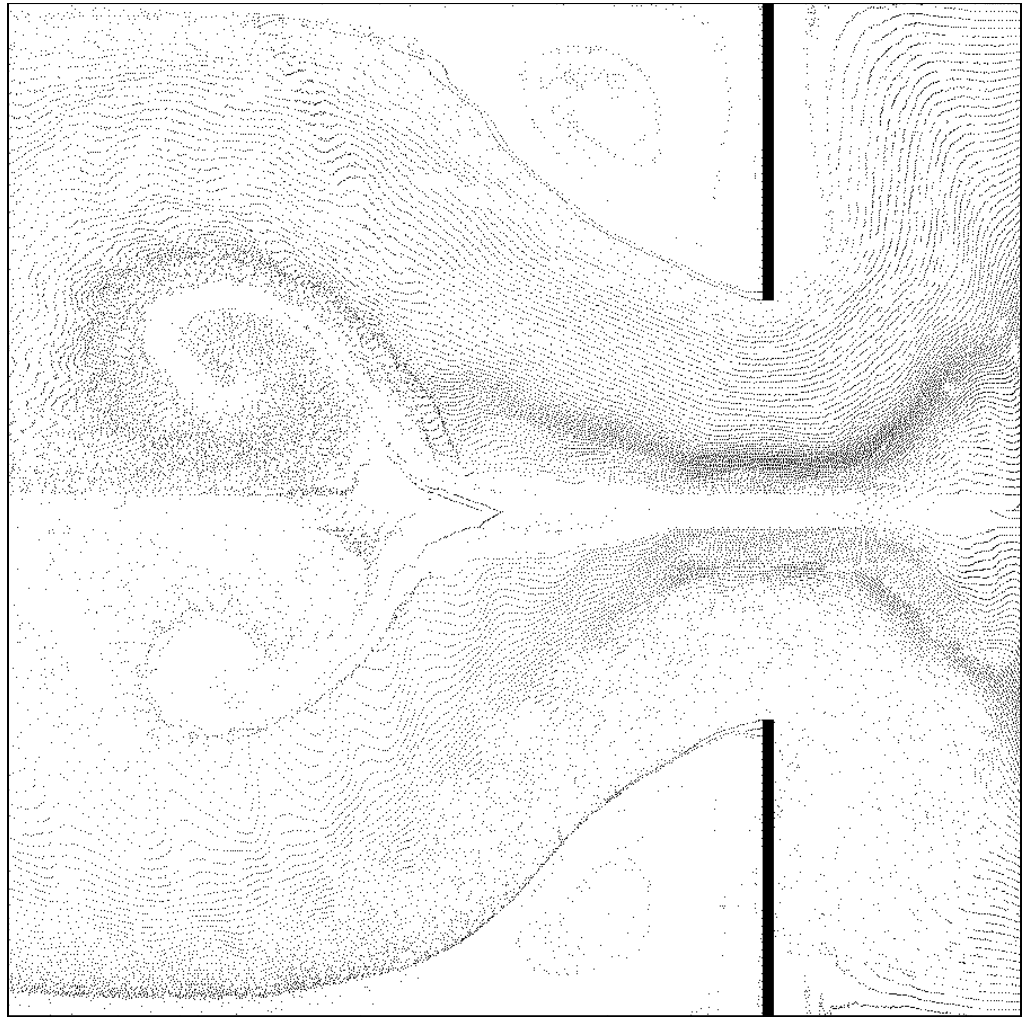
Exact mass and momentum conservation : that is what really matters for a fluid ! ! !

FHP model



Stochastic rule with Conservation of mass and momentum.

Flow past an obstacle (FHP)



Why can such a simple model work ?

- At a macroscopic scale, the detail of the interaction does not matter so much
- Only conservation laws and symmetries are important
- We can invent our own fluid, especially one adapted to computer simulation

Demos

- Pressure/density wave : aniotropy
- Reversibility
- Spurious invariants : momentum along each line and column, checkerboard invariant
- Diffusion, DLA, reaction-diffusion models
- Snow transport by wind

Lattice Boltzmann (LB) models

- Lattice Gases implement an exact dynamics
- But they require large simulations, statistical averages and have little freedom to adjust problem parameters
- In the early 1990s, the discrete Boltzmann equation describing the average dynamics of a lattice Gas was re-interpreted (with improvements) as a flow solver
- $\rightarrow$ Lattice Boltzmann models

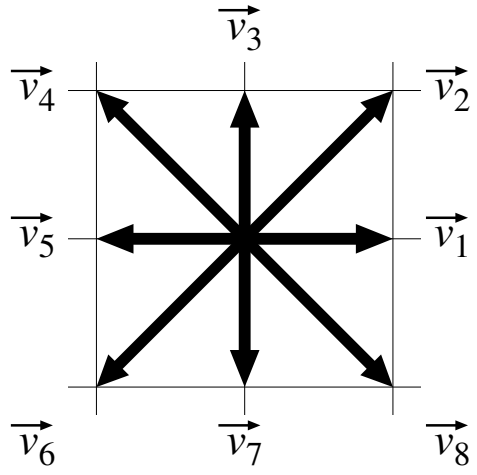
The lattice Boltzmann (LB) method : the historical way

- Historically, LB was born from **Lattice Gases**, discrete kinetic models of colliding particles
- Now the LB method is often derived by a discretization procedure (in velocity, space and time variables) of the standard Boltzmann equation

$$\partial_t f(v, r, t) + v \cdot \partial_r f(v, r, t) = \Omega(f)$$

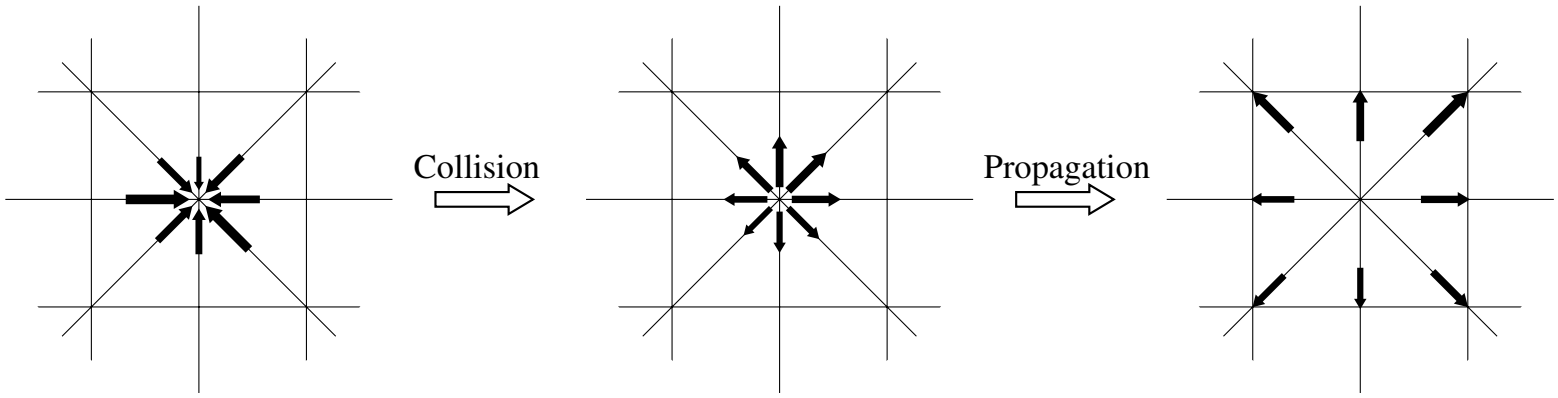
- where $f(v, r, t)$ is the density distribution of particles at location r, time t, with velocity v.

The Lattice Boltzmann scheme : definitions



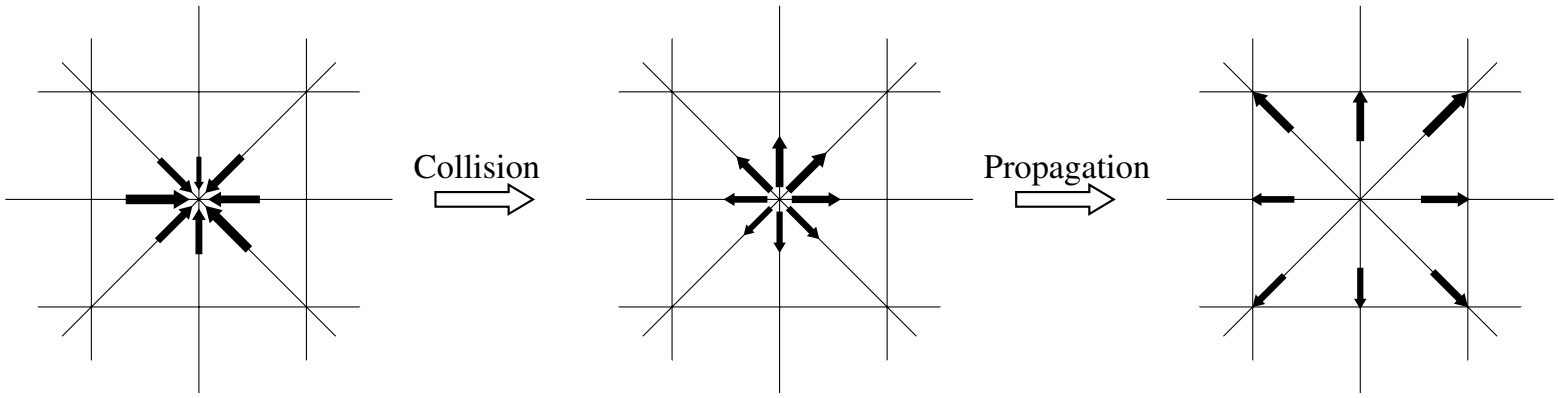
- Possible particle velocities : $\mathbf{v}_i$, $i = 0, 1, ..., q-1$
- Lattice spacing : Δx, time step : Δt, $|v_i| = \Delta x / \Delta t$.

The Lattice Boltzmann scheme : definitions



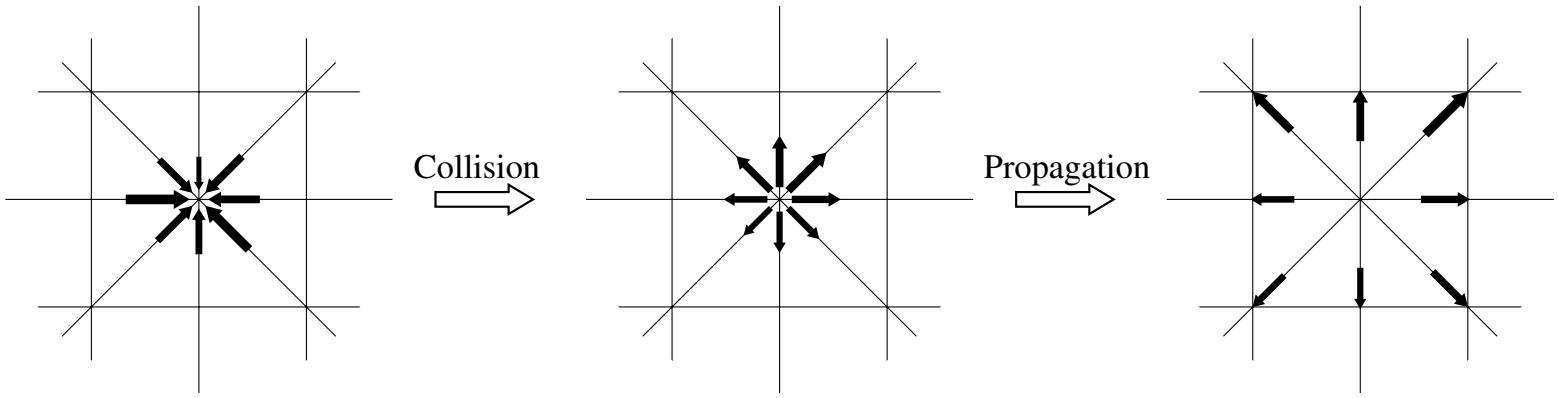
- Possible particle velocities : $\mathbf{v}_i$, $i = 0, 1, ..., q-1$
- Lattice spacing : Δx, time step : Δt, $|v_i| = \Delta x / \Delta t$.
- $f_i^{in}(\mathbf{r}, t)$ is the density of particle entering site $\mathbf{r}$ with velocity $\mathbf{v}_i$, at time t.

The Lattice Boltzmann scheme : definitions



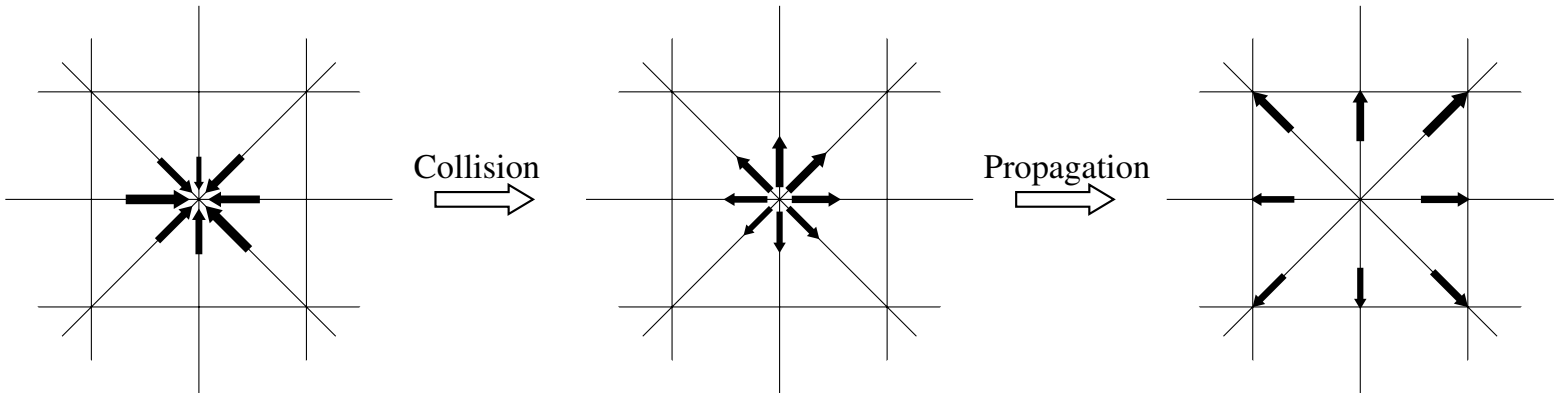
- Possible particle velocities : $\mathbf{v}_i$, $i = 0, 1, ..., q-1$
- Lattice spacing : Δx, time step : Δt, $|v_i| = \Delta x/\Delta t$.
- $f_i^{in}(\mathbf{r}, t)$ is the density of particle entering site $\mathbf{r}$ with velocity $\mathbf{v}_i$, at time t.
- Density : $\rho(\mathbf{r}, t) = \sum_i f_i^{in}$;

The Lattice Boltzmann scheme : definitions



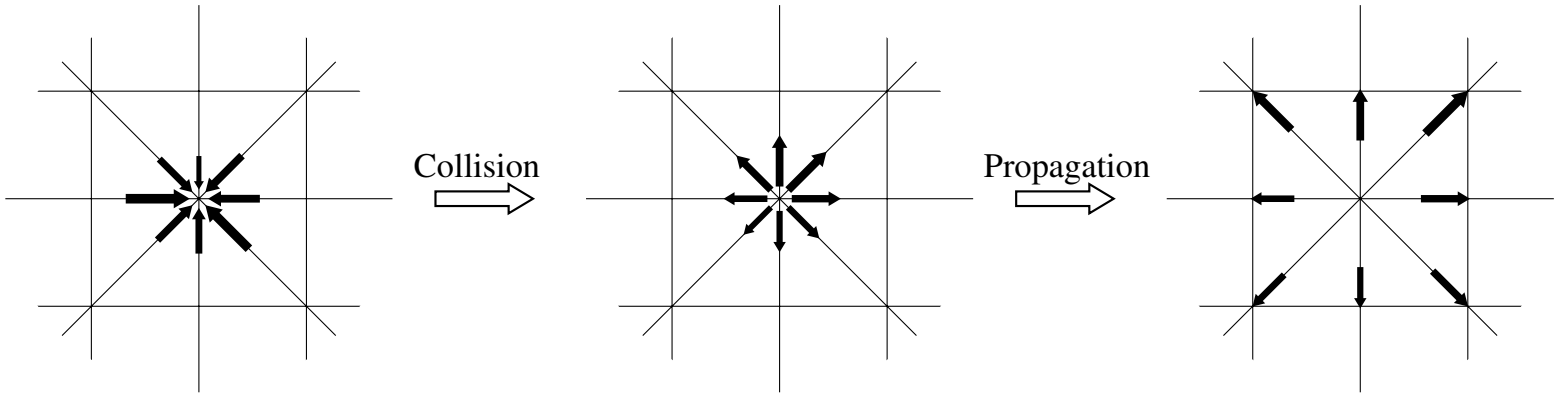
- Possible particle velocities : $\mathbf{v}_i$, $i = 0, 1, ..., q-1$
- Lattice spacing : Δx, time step : Δt, $|v_i| = \Delta x/\Delta t$.
- $f_i^{in}(\mathbf{r}, t)$ is the density of particle entering site $\mathbf{r}$ with velocity $\mathbf{v}_i$, at time t.
- Density : $\rho(\mathbf{r}, t) = \sum_i f_i^{in}$;
- Velocity : $\rho\mathbf{u} = \sum_i f_i^{in}\mathbf{v}_i$

The Lattice Boltzmann scheme : definitions



- Possible particle velocities : $\mathbf{v}_i$, $i = 0, 1, ..., q-1$
- Lattice spacing : Δx, time step : Δt, $|v_i| = \Delta x/\Delta t$.
- $f_i^{in}(\mathbf{r}, t)$ is the density of particle entering site $\mathbf{r}$ with velocity $\mathbf{v}_i$, at time t.
- Density : $\rho(\mathbf{r}, t) = \sum_i f_i^{in}$;
- Velocity : $\rho\mathbf{u} = \sum_i f_i^{in}\mathbf{v}_i$
- Momentum tensor $\Pi_{\alpha\beta} = \sum_i f_i^{in}(\mathbf{r}, t) v_{i\alpha} v_{i\beta}$

The Lattice Boltzmann scheme : dynamics



- Collision : $f_i^{out} = f_i^{in} + \Omega_i(f)$
- Propagation : $f_i^{in}(\mathbf{r} + \Delta t \mathbf{v}_i, t + \Delta t) = f_i^{out}(\mathbf{r}, t)$

Collision and Propagation :

$$f_i(\mathbf{r} + \Delta t \mathbf{v}_i, t + \tau) = f_i(\mathbf{r}, t) + \Omega_i(f) \qquad (1)$$

where $f = f^{in}$

The single relaxation time LB scheme (BGK)

The collision term Ω_i is a relaxation towards a prescribed **local equilibrium** distribution

$$\Omega_i(f) = \frac{1}{\tau}(f_i^{eq}(\rho, \mathbf{u}) - f_i) \tag{2}$$

where

$$f_i^{eq} = \rho w_i(1 + \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2} + \frac{1}{c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta) \tag{3}$$

contains the desired physics (here hydrodynamics) and $Q_{i\alpha\beta}$ is

$$Q_{i\alpha\beta} = v_{i\alpha} v_{i\beta} - c_s^2 \delta_{\alpha\beta}$$

τ is a constant called the **relaxation time**

Choice of the $\mathbf{v}_i$ and lattice weight w_i

The "microscopic" velocities $\mathbf{v}_i$ must be such that there exists constants w_i and c_s^2 so that :

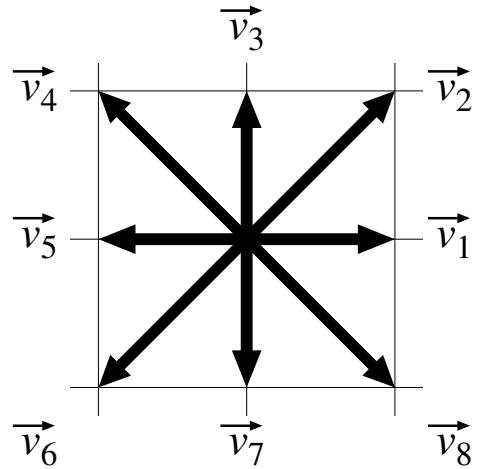
$$
\begin{aligned}
\sum_i w_i &= 1 \\
\sum_i w_i \mathbf{v}_i &= 0 \\
\sum_i w_i v_{i\alpha} v_{i\beta} &= c_s^2 \delta_{\alpha\beta} \\
\sum_i w_i v_{i\alpha} v_{i\beta} v_{i\gamma} &= 0 \\
\sum_i w_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} &= c_s^4 \left(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}\right) \\
\sum_i w_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} v_{i\epsilon} &= 0 \qquad (4)
\end{aligned}
$$

Lattice Geometries DdQq

d is the space dimension and q the number of microscopic velocities

- D2Q9 : 2D, square lattice with diagonals and rest particles.
- D3Q19 : 3D, with rest particles

have enough symmetries.



$$w_0 = 4/9 \qquad w_1 = w_3 = w_5 = w_7 = 1/9$$

$$w_2 = w_4 = w_6 = w_8 = 1/36$$

Continuous limit

Up to order $\mathcal{O}(\Delta x^2)$ and $\mathcal{O}(\Delta t^2)$, and provied that $Ma << 1$, the LB eq.

$$f_i(\mathbf{r} + \Delta t \mathbf{v}_i, t + \tau) = f_i(\mathbf{r}, t) + \frac{1}{\tau}(f_i^{eq} - f_i) \tag{5}$$

is equivalent to Navier-Stokes equations

$$\begin{cases} \partial_t \rho + \partial_\alpha \rho u_\alpha = 0 \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} \end{cases} \tag{6}$$

for $\rho = \sum_i f_i$ and $\rho \mathbf{u} = \sum_i f_i \mathbf{u}$.

Properties :

Viscosity :

$$\nu = c_s^2 \Delta t(\tau - 1/2)$$

Pressure :

$$p = \rho c_s^2$$

Thus, LB-fluids are compressible

Relations between the f_i's and the hydrodynamic quantites

Hydrodynamic quantities from the f_i	f_i from the hydrodynamic quantities
▶ $\rho = \sum_i f_i$ ▶ $\rho \mathbf{u} = \sum_i f_i \mathbf{v}_i$ ▶ $\Pi_{\alpha\beta} = \sum_i v_{i\alpha} v_{i\beta} f_i$	▶ $f = f^{eq} + f^{neq}$ ▶ $f_i^{eq} = \rho w_i (1 + \frac{\mathbf{v}_i \cdot \mathbf{u}}{c_s^2} + \frac{1}{2c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta)$ ▶ $f_i^{neq} = -\Delta t \tau \frac{w_i}{c_s^2} Q_{i\alpha\beta} \rho S_{\alpha\beta}$

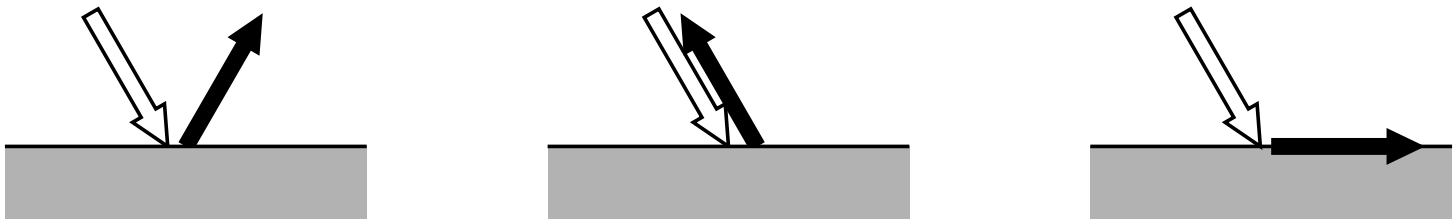
where

$$S_{\alpha\beta} = (1/2)(\partial_\alpha u_\beta + \partial_\beta u_\alpha)$$

and

$$Q_{i\alpha\beta} = v_{i\alpha} v_{i\beta} - c_s^2 \delta_{\alpha\beta}$$

Boundary conditions

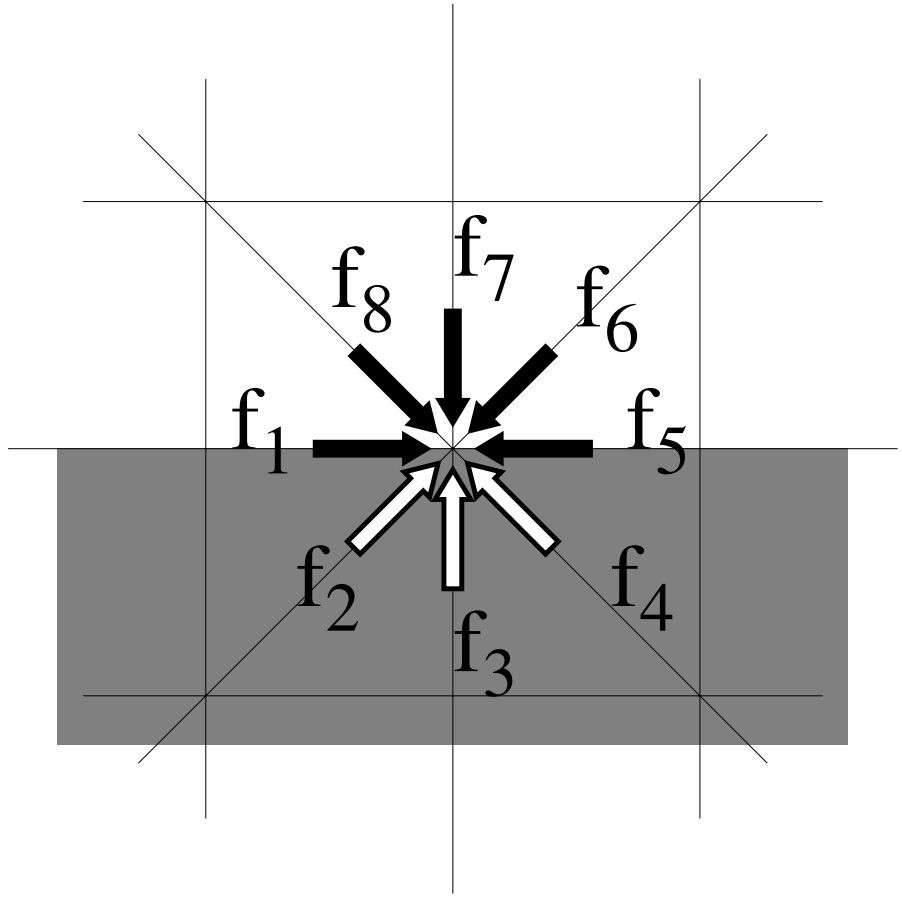


(a) Specular reflection, (b) bounce back condition and (c) trapping wall condition

The **Bounce Back rule** implements a no-slip condition. It is the most common choice :

$$f_i^{out} = f_{-i}^{in}$$

Boundary conditions : beyond bounce-back



Compute the missing population so as to have the desired physical properties

Pros and cons on the LB method

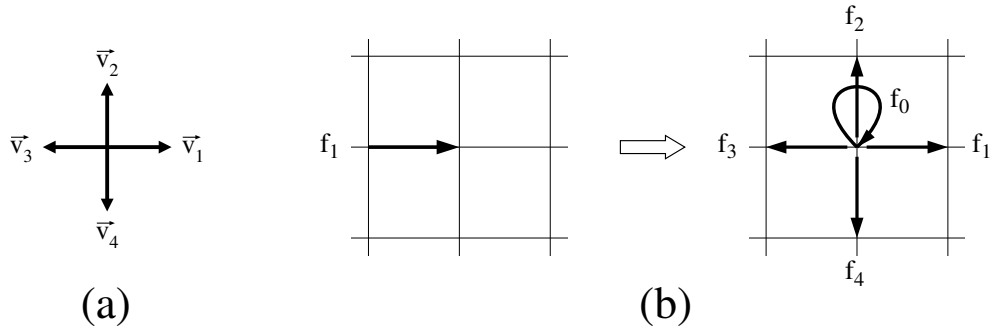
+ Closer to physics than to mathematics
+ Quite flexible to new developments, intuitive, multiphysics
+ Complicated geometries, cartesian grids
+ no need to solve a Poisson equation
+ Parallelization

- Recent methods
- No efficient unstructured grids
- Intrinsically a time dependent solver
- Not always so easy
- Still some work to have a fully consistent thermo-hydrodynamical model.

More advantages...

- Streaming is exact
- Non-linearity is local
- Numerical viscosity is negative
- Extended range of validity for larger Knudsen numbers
- Palabos open source LB software (http ://www.palabos.org)

Wave equation



$$f_i(\mathbf{r} + \tau\mathbf{v}_i, t + \tau) = f_i(\mathbf{r}, t) + 2(f_i^{eq} - f_i) \tag{7}$$

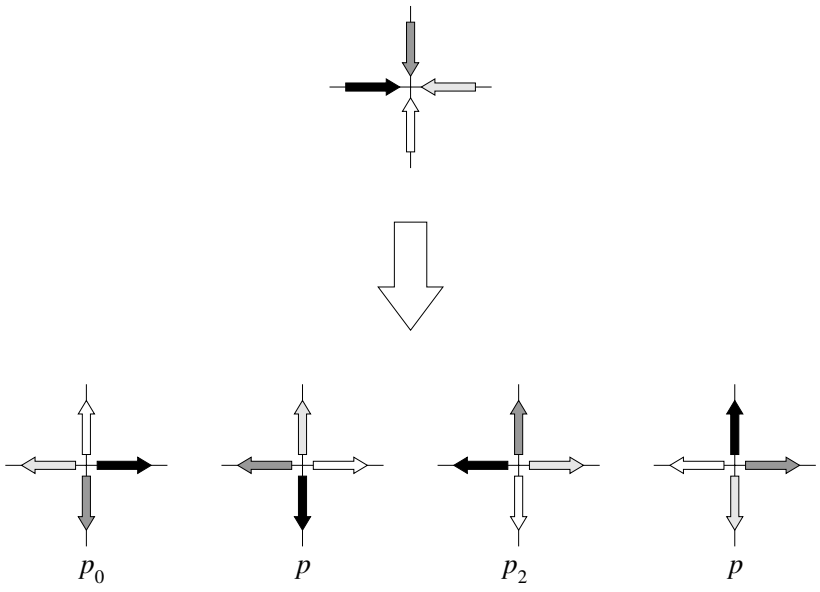
$$f_i^{eq} = a\rho + b\mathbf{u} \cdot \mathbf{v}_i$$

Conservation of ρ, its current $\mathbf{u}$ and time reversibility. Note that $\sum f_i^2$ is also conserved.

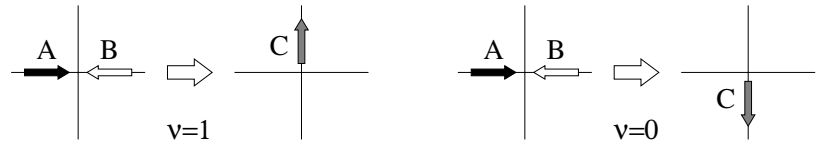
This is equivalent to

$$\partial_t^2 \rho + c^2 \nabla^2 \rho = 0$$

CA for Reaction-Diffusion processes



Diffusion



Reaction

LB Reaction-Diffusion

$$f_i(\mathbf{r} + \Delta t \mathbf{v}_i, t + \tau) = f_i(\mathbf{r}, t) + \omega(f_i^{eq} - f_i) + \frac{\Delta t}{2d} R \qquad (8)$$

with R the reaction term (for instance $R = -k\rho^2$). and

$$f^{eq} = \frac{1}{2d}\rho$$

This is equivalent to

$$\partial_t \rho = D\nabla^2 \rho + R$$

Demos

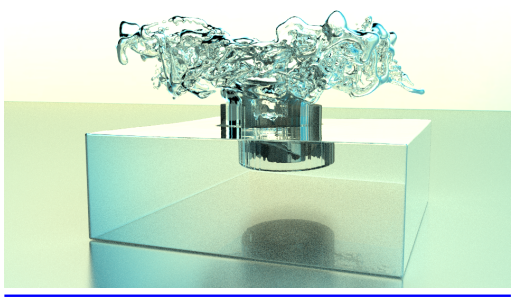
http ://cui.unige.ch/∼chopard/CA/Animation/root.html

Palabos : an Open-Source solver (UNIGE)

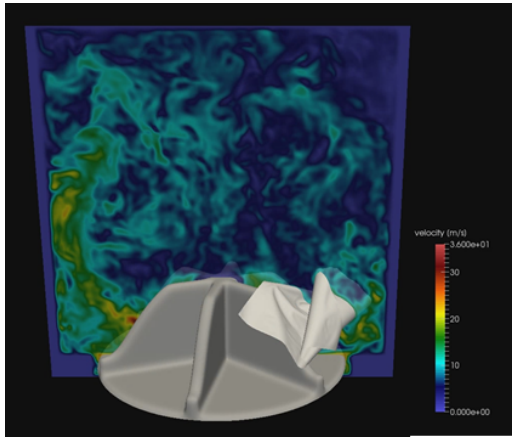
Multiphysics, same code from laptop to massively parallel computer : (www.palabos.org)

Droplet

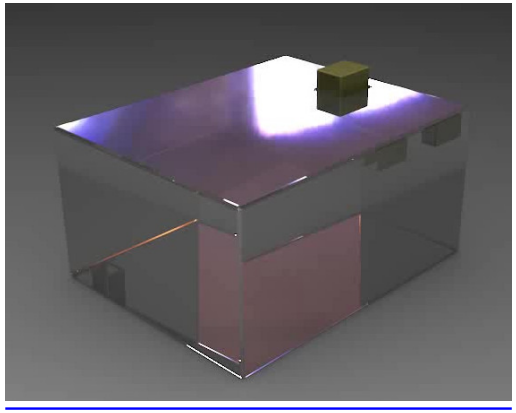
Pumps



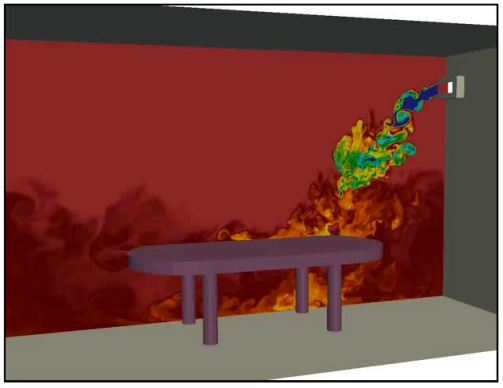
Washing machines



Energy converter

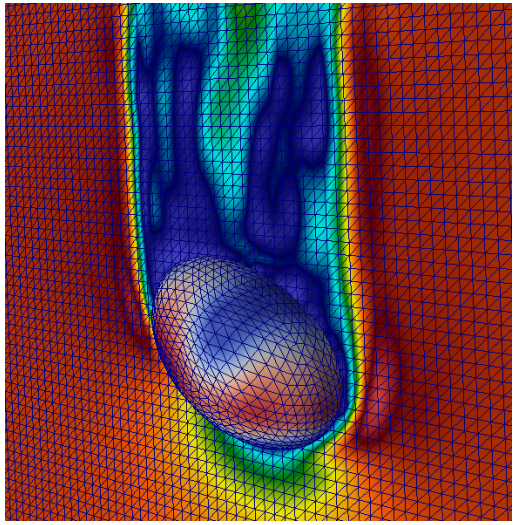


Air conditioning

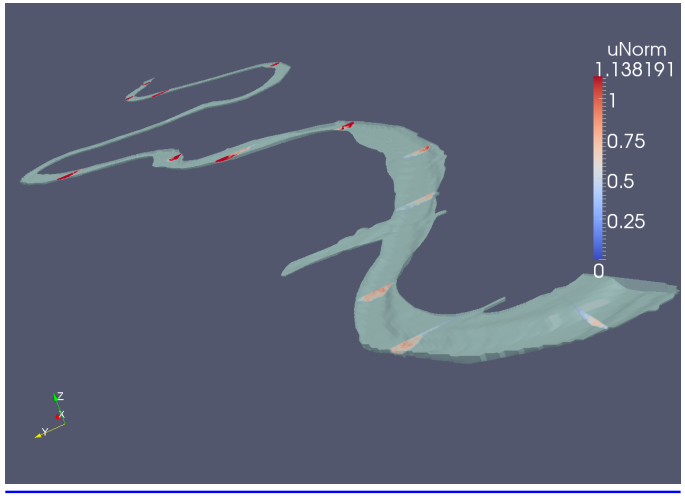


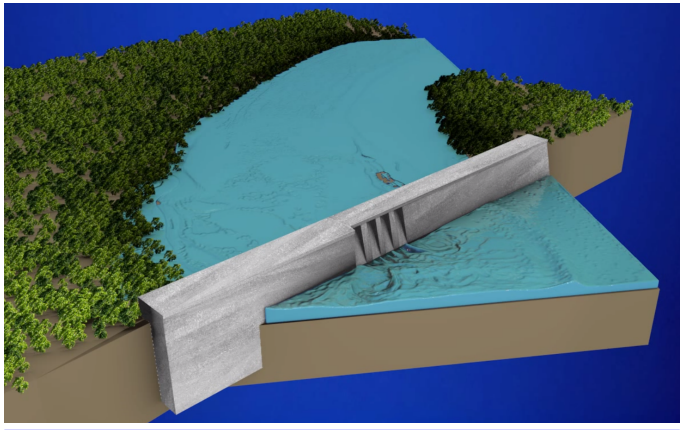
Fixed air-conditioner

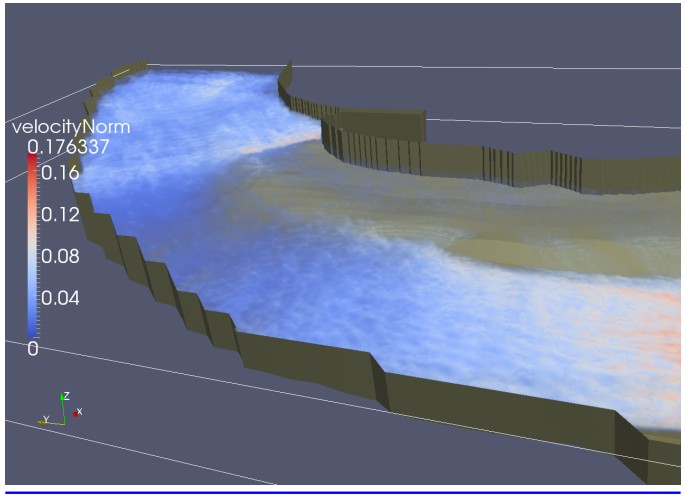
sedimentation



Simulation of river Rhone in Geneva

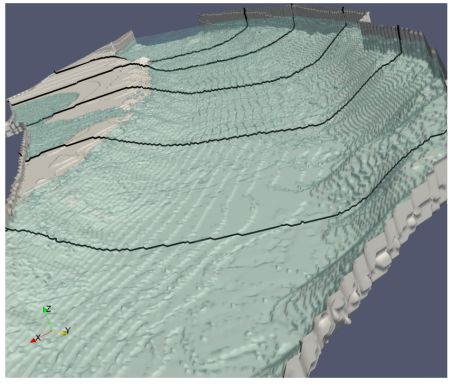






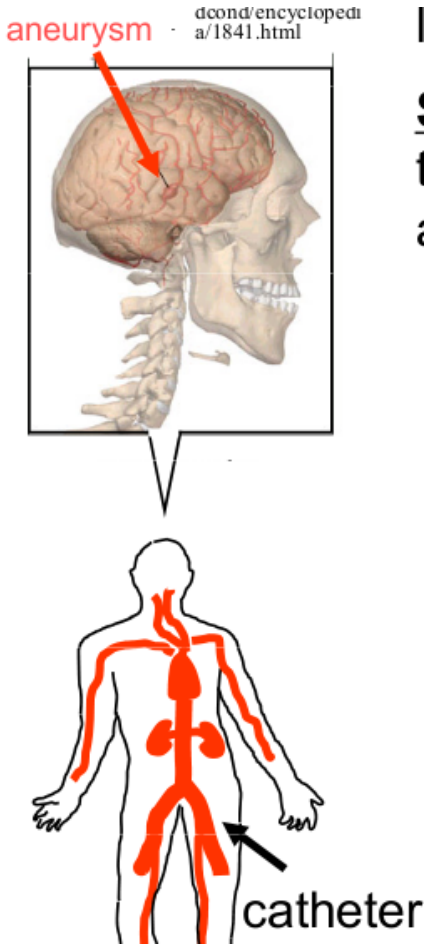
Draining of the river Rhône, with riverbed erosion.

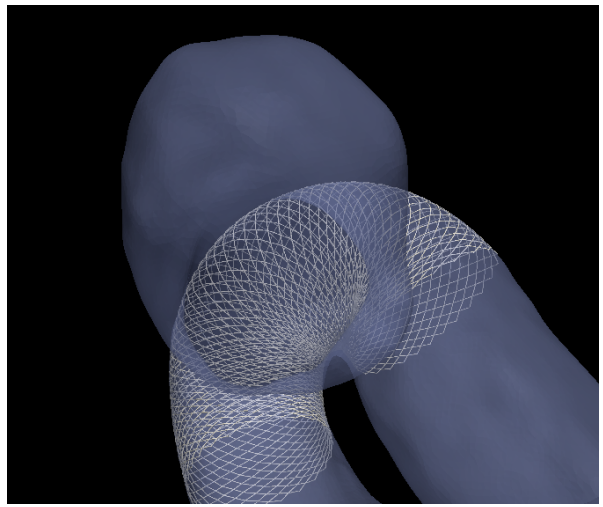
Water level is shown in semi-transparent light-blue color.

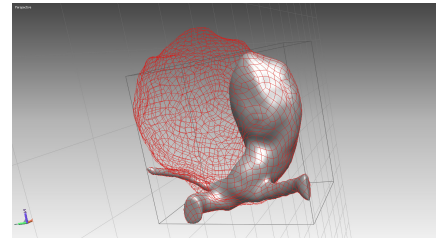


palabos.org

How to treat cerebral aneurysms : flow diverters







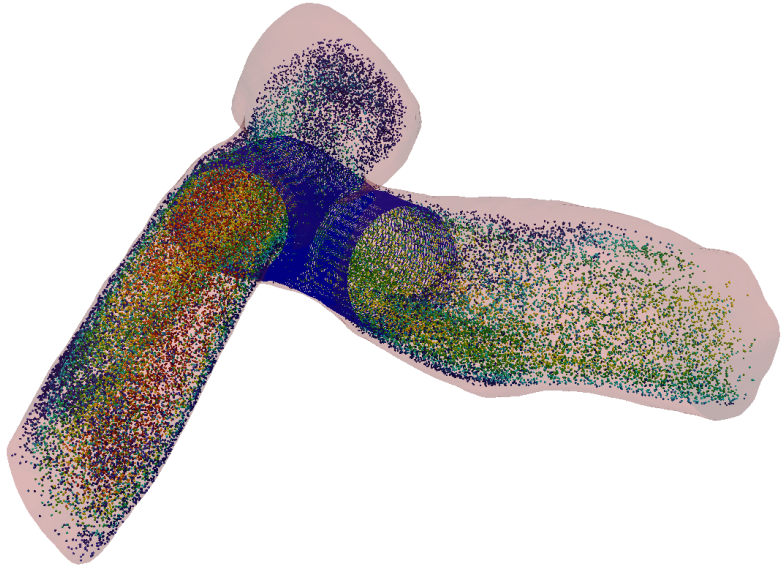
- The stent **reduces bloodflow** in the aneurysm
- Clotting is induced in the aneurysm

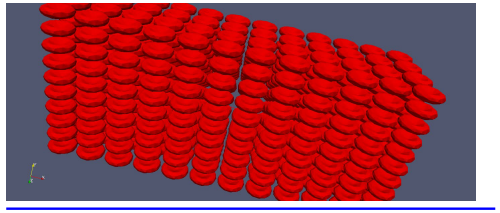
Our goal is to elucidate the mechanisms leading to thrombus formation from biological knowledge and numerical modeling

Fully resolved simulation with a flow diverter

Pipeline flow diverter from EV3-COVIDIEN

Δx	Δt	diameter	# fluid nodes	Re
25 μm	1 μs	3.7 mm	40 millions	≈ 300

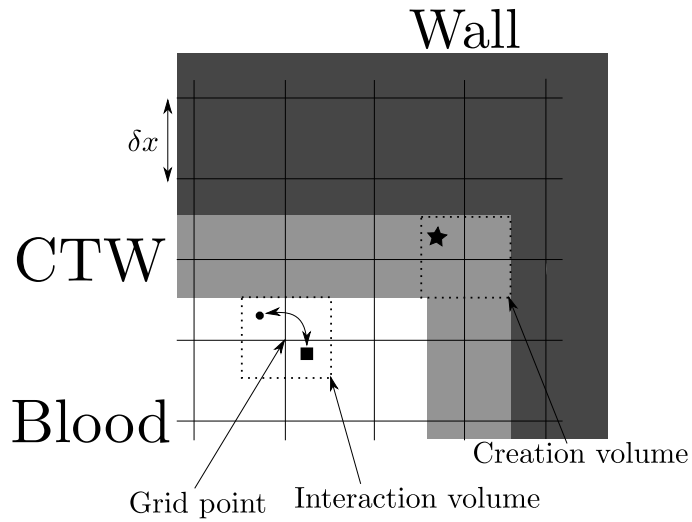




CPU time : 10 days (on 120 Westmere Intel cores)

Spatio-temporal Thrombosis Model

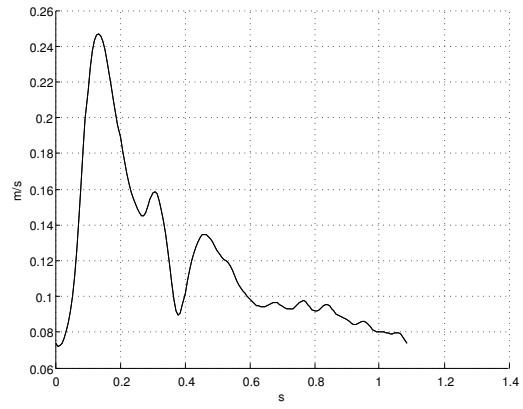
- Low shear : creation of TF, then thrombin from endothelial cells
- Fibrinogen and anti-thrombin are in suspension, brought by fresh blood
- thrombin+fibrinogen $\rightarrow$ fibrin (=clot)
- thrombin+anti-thrombin $\rightarrow$ 0
- Platelets attach to the fibrin, compact the clot and allow re-endothelialization
- Clot stops to grow when all thrombin molecules have been consumed



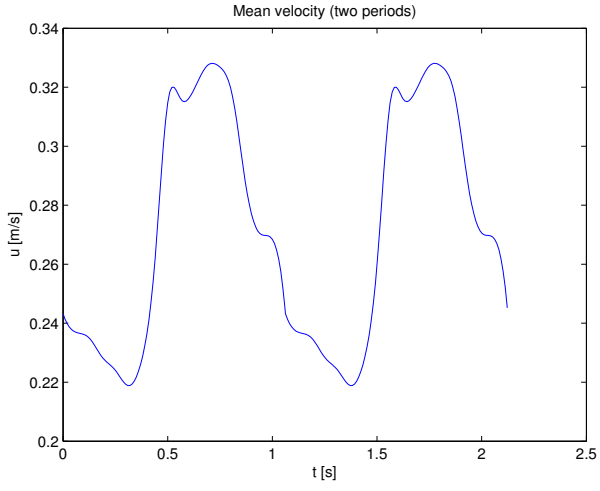
Need clever multiscale solutions for the numerical implementation

Thrombosis Model

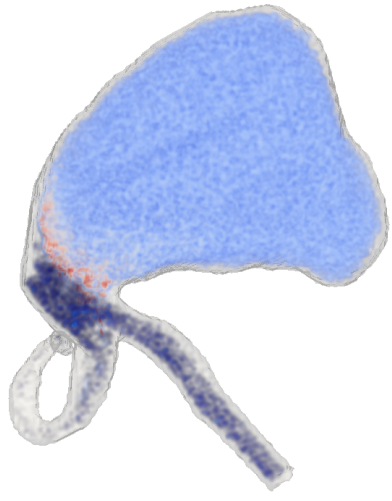
Pulsatile versus steady flow



Simulation of the thrombus in giant aneurysm



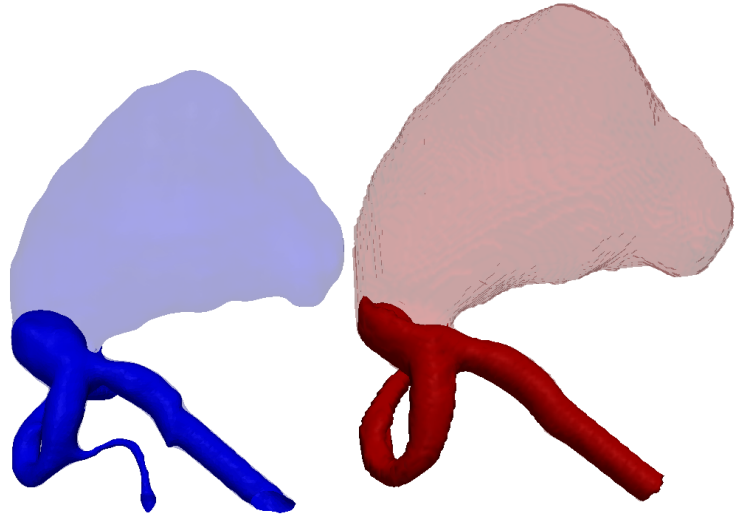
- movie
- accelerated for 2200 heart cycles

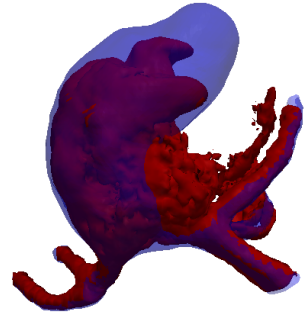


ν	ρ	inlet diam.	aneurysm size	inlet flow
3.7e-6 m^2/s	1080 kg/m^3	0.8 mm	8 cm	4×10^{-6} m^3/s

Validation with a patient

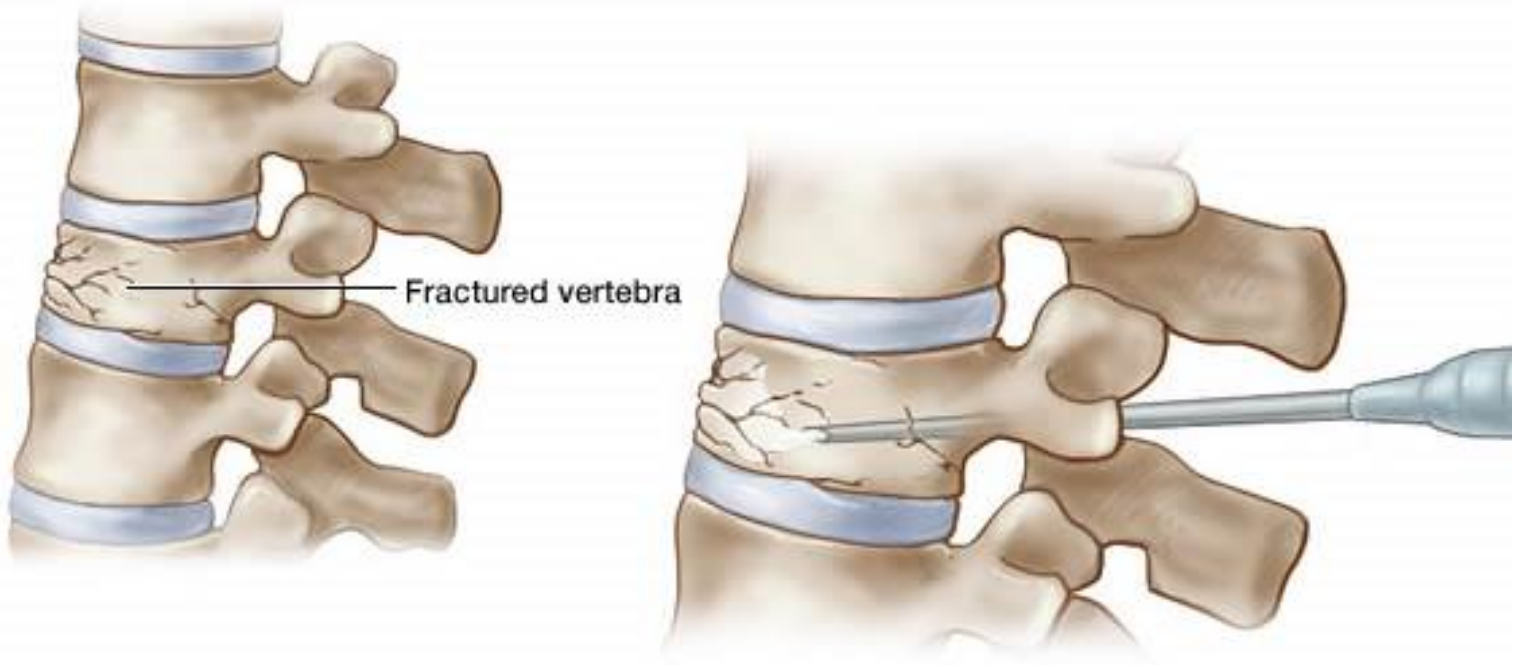
Blue : patient Red : simulation





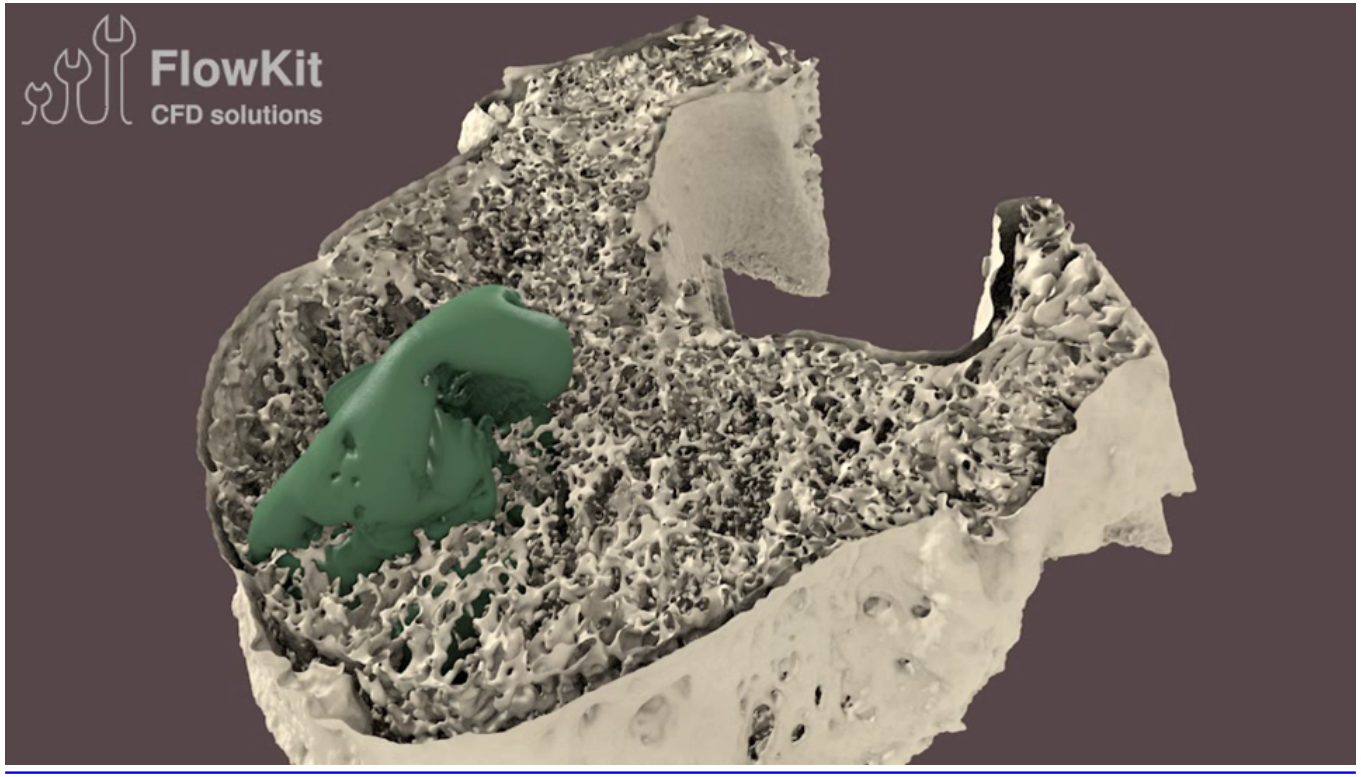
Another case

Vertebroplasty



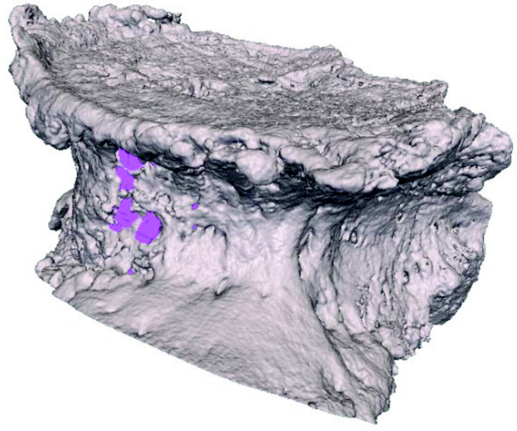
Quick setting bone cement injected into fractured vertebra

Palabos Simulation

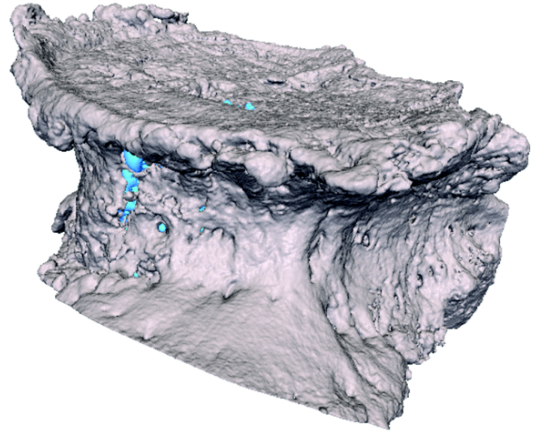


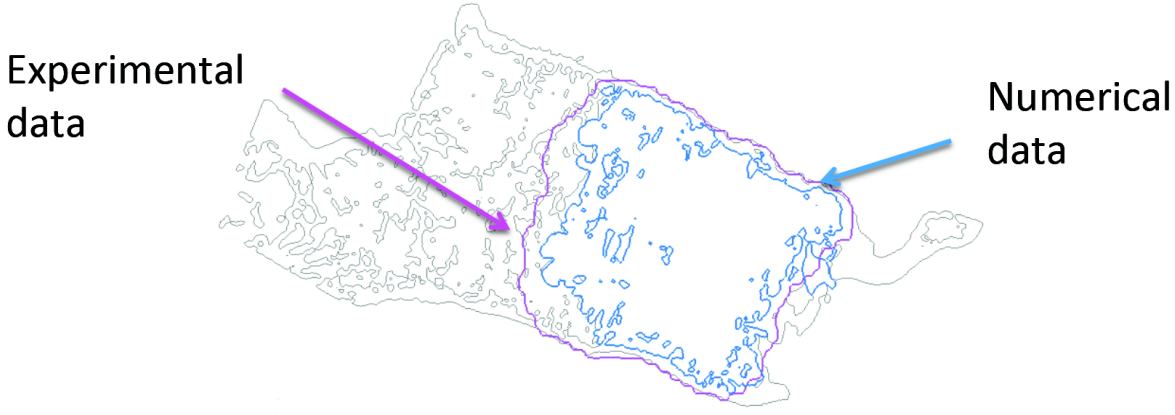
Experiment versus simulation

After 6 ml



After 7 ml

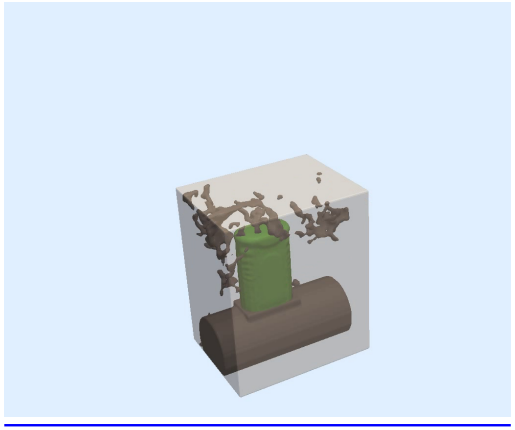


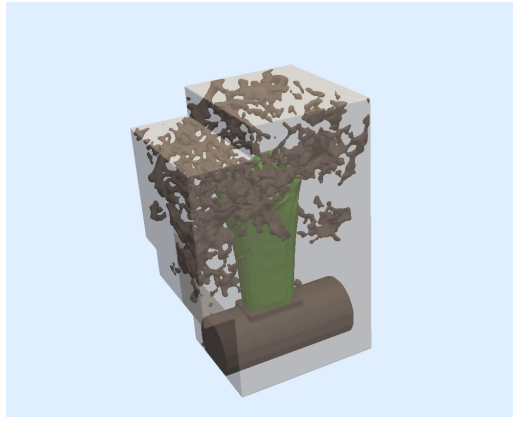


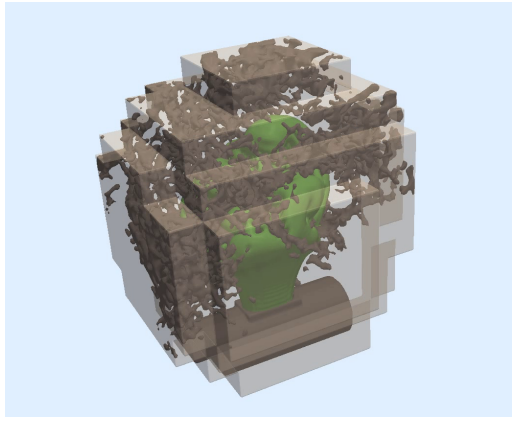
Good agreement within experimental errors

Dynamical load balancing on Palabos

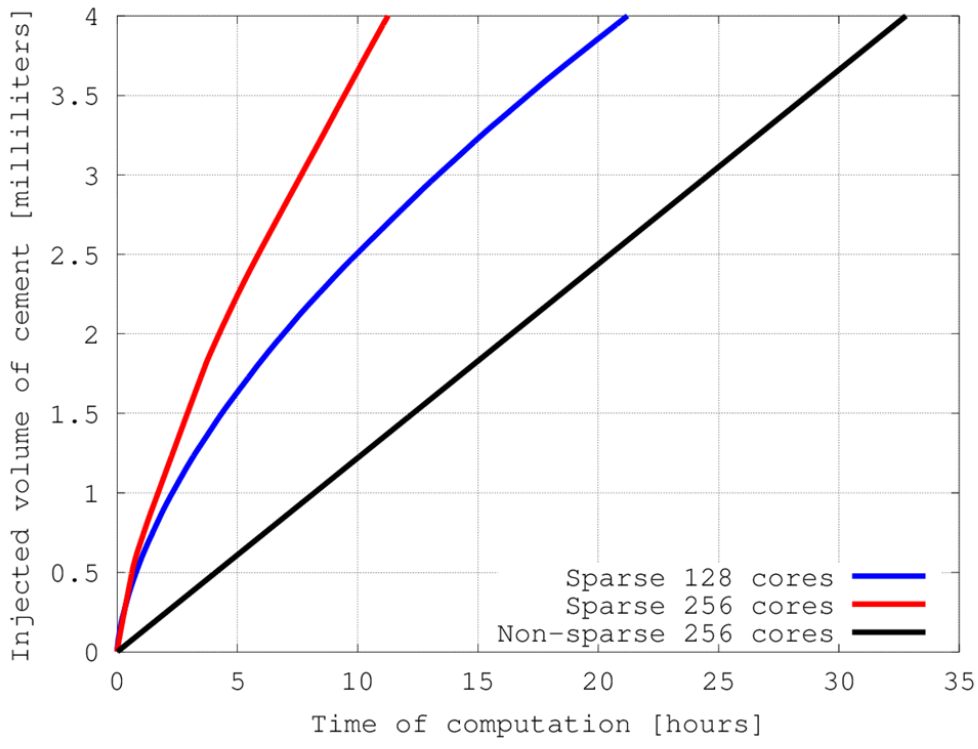
Domains reallocation at regular time intervals







Performance with and without data migration



Exercices

- Play with a python code producing a 2D flow around a sphere **(d2q9.py)**. For instance, change the Reynolds number RE
- Play with a python code modeling the movement of bacteria in a field of nutrients **(bacteria.py)**. Try to add a source and diffusion of nutrients, and the change in concentration when eaten by the bacteria

http://cui.unige.ch/~chopard/FTP/USI/

Acknowledgments

- Jonas Latt
- Yann Thorimbert
- Orestis Malaspinas