Simulation and modeling of natural processes

Week 4: Cellular Automata Modeling

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

1. Definition and basic concepts

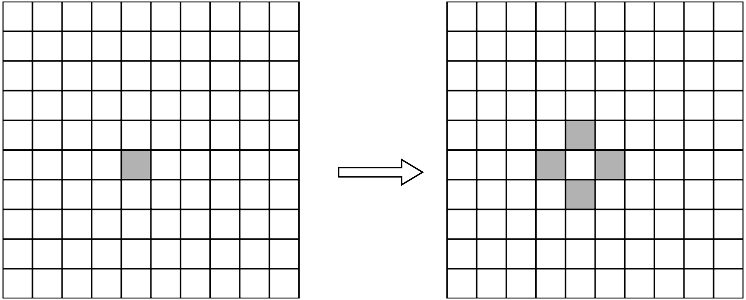
3.1 Définition et concepts de bases

What is a Cellular Automata?

- A mathematical abstraction of the real world, a 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**.

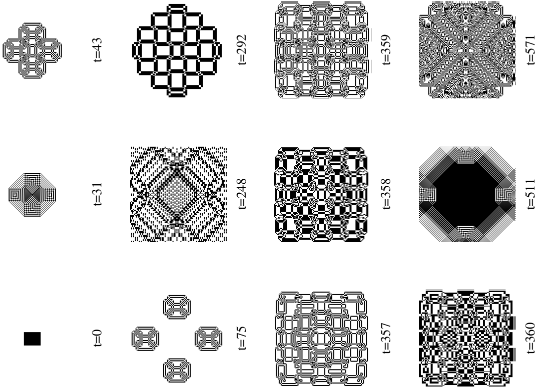
Example: the Parity Rule

- 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

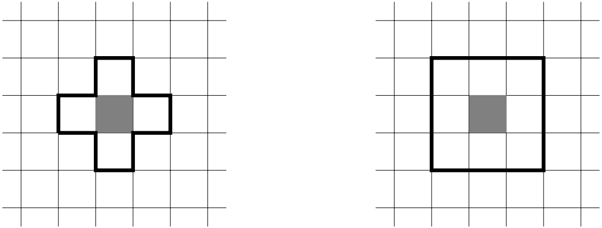


CA Definition

- 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

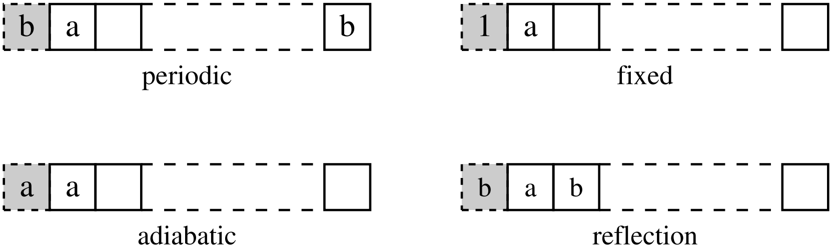
- von Newmann
- Moore
- Margolus
- ...



(a) (b)

Boundary conditions

- periodic
- fixed
- reflexive
- ....



Generalization

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

Implementation of the evolution rule

- On-the-fly calculation

$$s_{ij}(t+1) = s_{i-1,j}(t) \oplus s_{i+1,j}(t) \oplus s_{i,j-1}(t) \oplus s_{i,j+1}(t)$$

- Lookup table

$$\text{index} = s_{i-1,j}(t) + 2s_{i+1,j}(t) + 4s_{i,j-1}(t) + 8s_{i,j+1}(t)$$

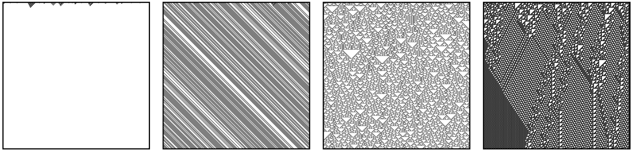
and then

$$s_{ij}(t+1) = \text{Rule}[\text{index}]$$

The possible universes...

- 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.
- Most of them are uninteresting

Wolfram classification of 1D rules with $m = 1$, $k = 3$:



(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

$\boxed{\textit{End of module}}$

Definition and basic concepts

$\boxed{\textit{Coming next}}$

Historical background

2. Historical background

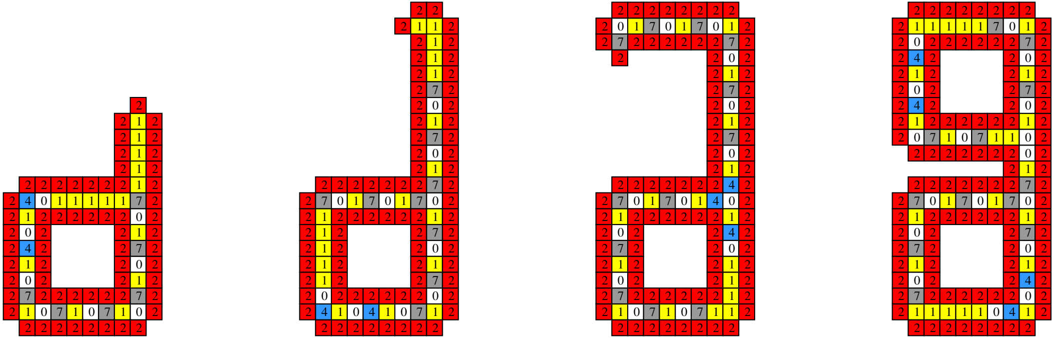
Historical notes

- 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

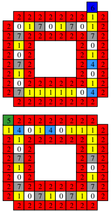
Langton's CA: basic cell replication



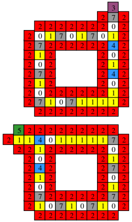
(time 0) (time 35) (time 75) (time 125)

Christopher G. Langton, Physica 10D (1984) 135-144

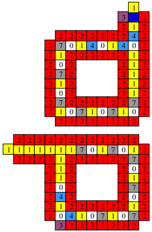
Langton's Automaton : spatial and temporal evolution



iteration=137



iteration=140



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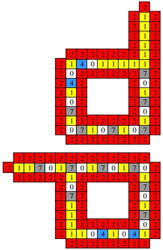
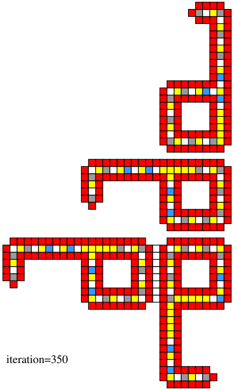
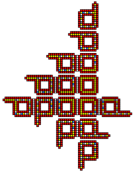


iteration=150



iteration=350

iteration 600



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.

$\boxed{\textit{End of module}}$

Historical background

$\boxed{\textit{Coming next}}$

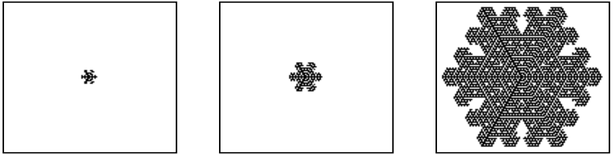
A mathematical abstraction of reality

3. A mathematical abstraction of reality

CA as a mathematical abstraction of reality

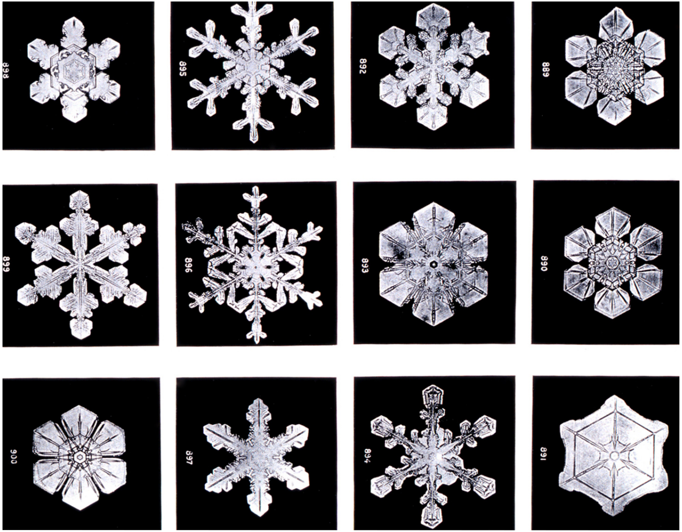
- Several levels of reality: macroscopic, mesoscopic and microscopic.
- The macroscopic behavior depends very little on the details of the microscopic interactions.
- Only "symmetries" or conservation laws survive. The challenge is to find them.
- **Consider a fictitious world, particularly easy to simulate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

A Caricature of reality



What is this ?

The real thing



Wilson Bentley, From Annual Summary of the "Monthly Weather Review", 1902.

Snowflakes model

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

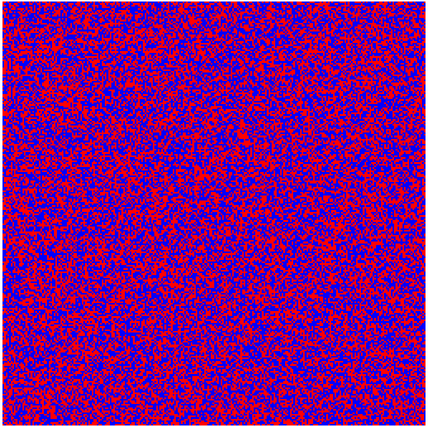
• **A vapor molecule solidifies (→ice) if one and only one already solidified molecule is in its vicinity**
• **Growth is constrained by 60^o angles**

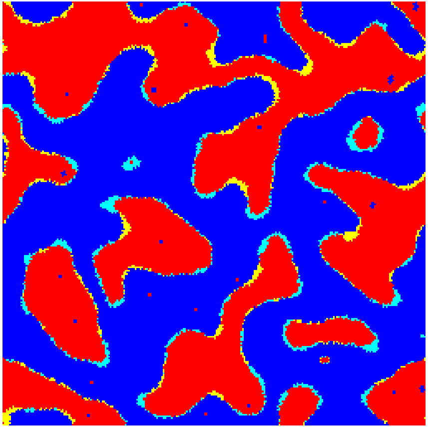
Examples of CA rules

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

Annealing 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





Examples of CA rules

http://cui.unige.ch/~chopard/CA/Animations/img-root.html

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).

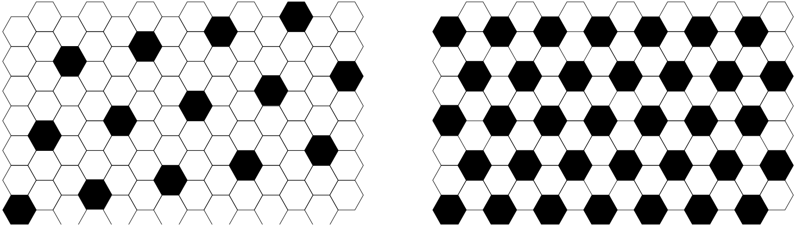
Biological hypotheses:

- 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.

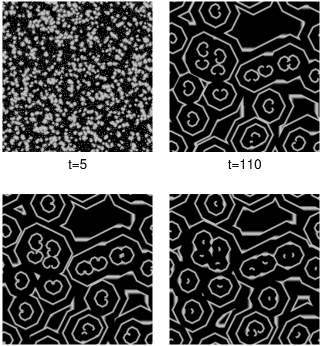
- CA produces situations with about **23%** of active cells, for almost any value of p_{anihil} and p_{growth}.
- Model robust to the lack of details, but need for hexagonal cells

Excitable Media, contagion models

- 3 states: (1) normal (resting), (2) excited (contagious), (3) refractory (immuned)
    1. excited → refractory
    2. refractory→ normal
    3. normal → excited, if there exists excited neighbors (otherwise, normal → 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.

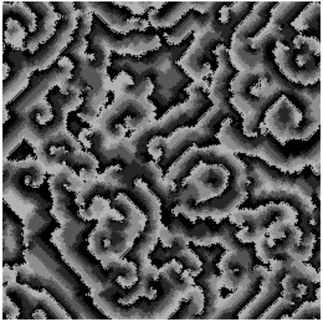


t=5 t=110

t=115 t=120

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;

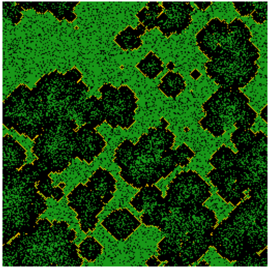
Forest fire

(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).



$\boxed{\textit{End of module}}$

A mathematical abstraction of reality

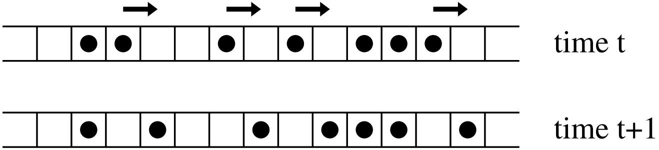
$\boxed{\textit{Coming next}}$

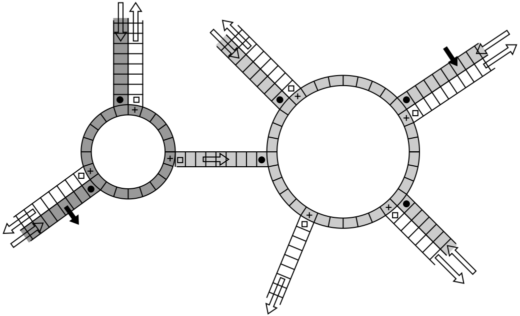
Traffic models

4. Cellular Automata Models for Traffic

Traffic Models

A vehicle can move only when the downstream cell is free (Wolfram rule 184).





Flow diagram

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

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

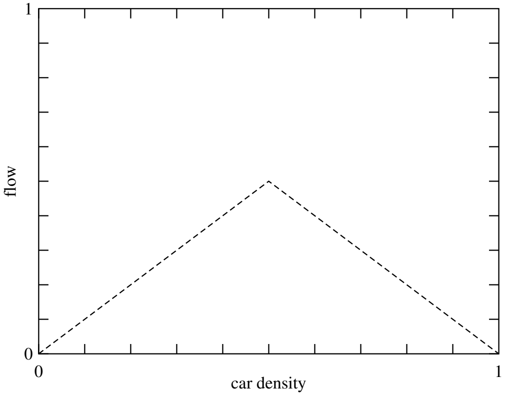
where N is the no of cars along L
The average velocity $< v >$ at time t on this segment is defined as

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

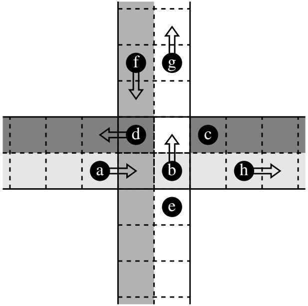
where $M(t)$ is the number of car moving at time t
The traffic flow j is defined as

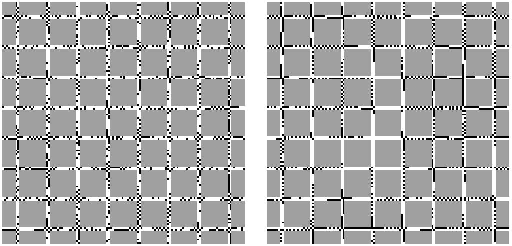
$$j = \rho < v >$$

Flow diagram of rule 184

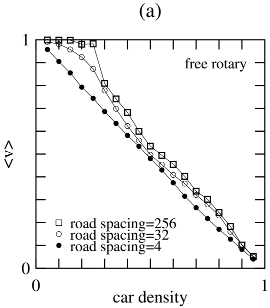


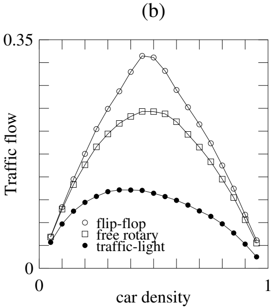
Traffic in a Manhattan-like city





(a) (b)

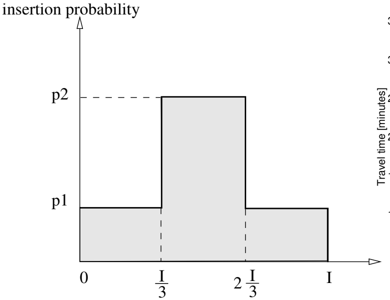


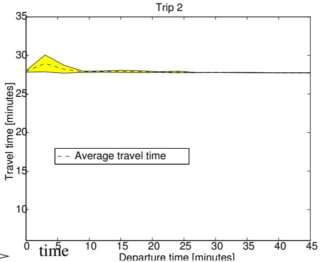


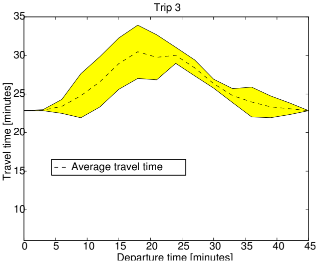
Case of the city of Geneva

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

Travel time during the rush hour







$\boxed{\textit{End of module}}$

Traffic models

$\boxed{\textit{Coming next}}$

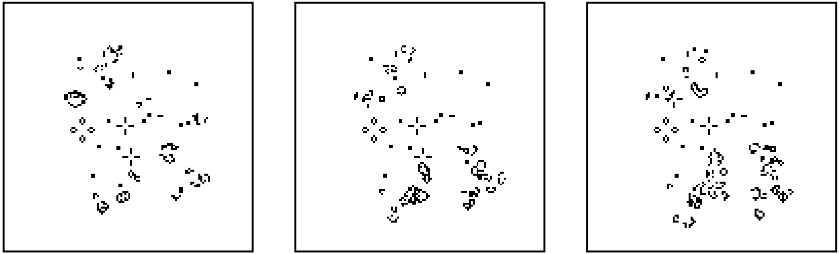
Complex systems

5. Complex systems

Complex systems

Rule of the Conway's Game of Life:

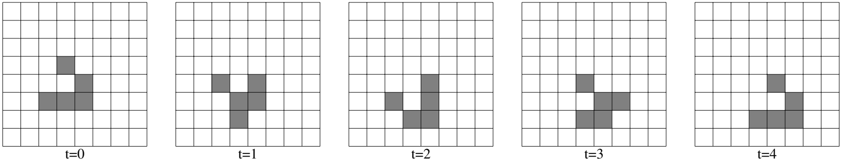
- Square lattice, 8 neighbors
- Cells are dead or alive (0/1)
- Birth if exactly 3 living neighbors
- Death if less than 2 or more than 3 neighbors



t t+10 t+20

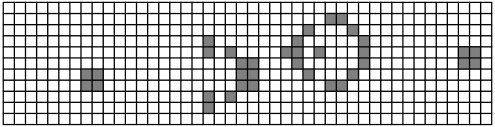
Complex Behavior in the game of life

Collective behaviors develop (beyond the local rule)
“Gliders” (organized structures of cell) can emerge and can **move** collectively.

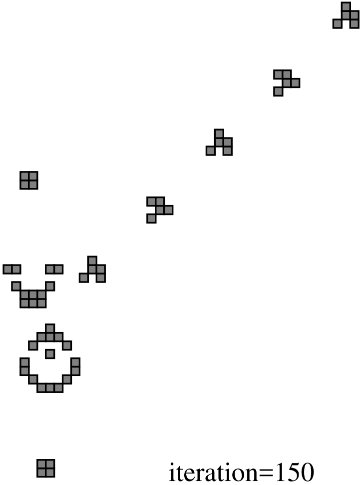


Complex Behavior in the game of life

A glider gun



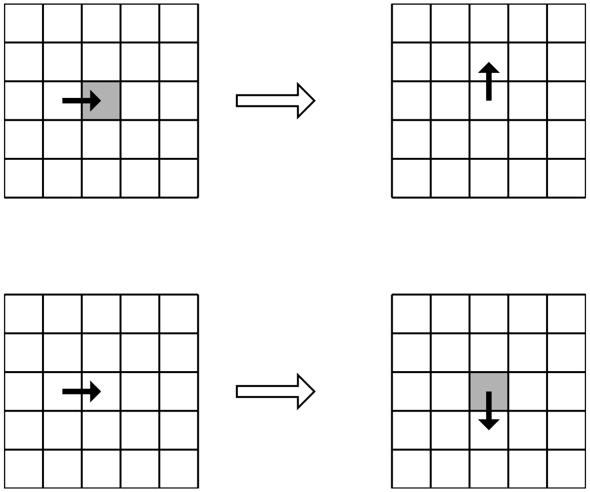
- A *glider gun* is a structure that keeps creating gliders
- There are more complex structures with more complex behavior: a zoology of organisms.
- The game of life is a *Universal computer*



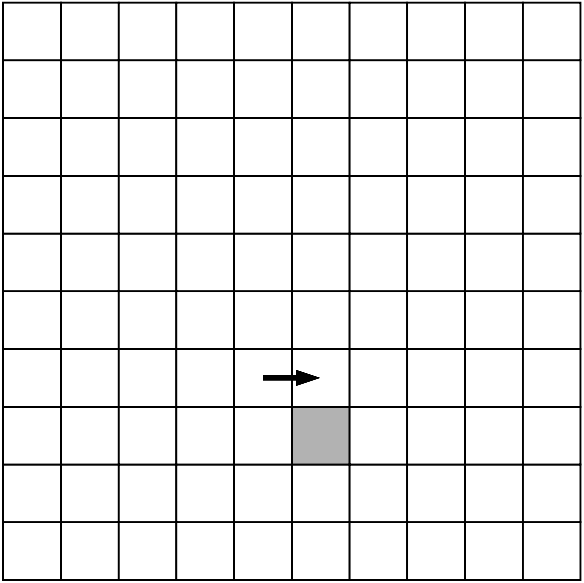
The Langton's Ant

This is a hypothetical animal moving on a 2D lattice, accoring to a simple rule. This rule depends on the “color” of the cell on which the ant is.

The rule of motion



Several steps



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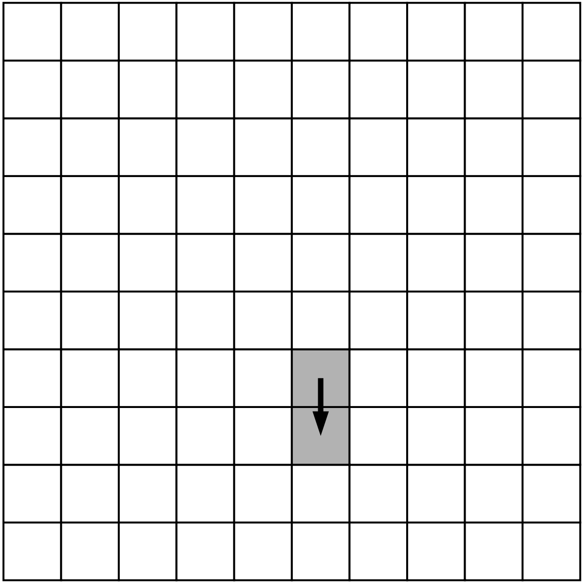
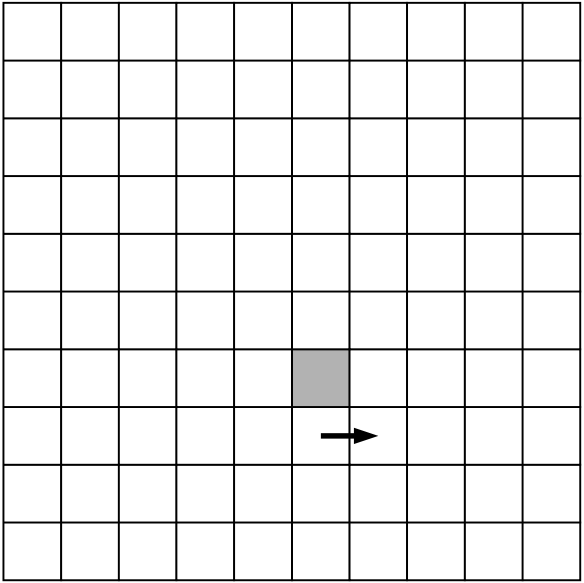


Several steps



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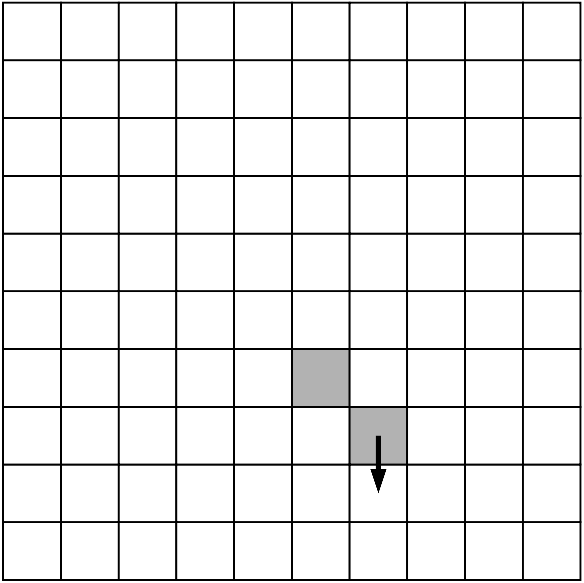

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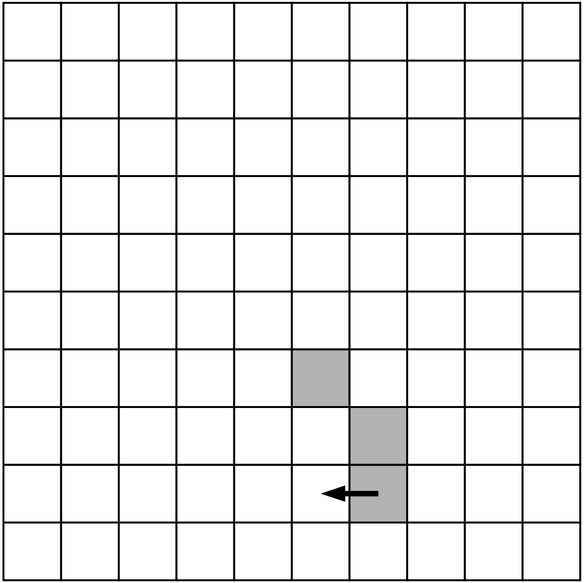

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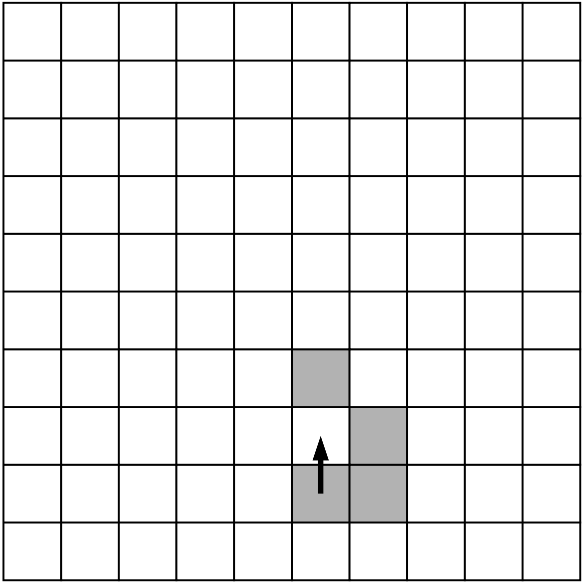

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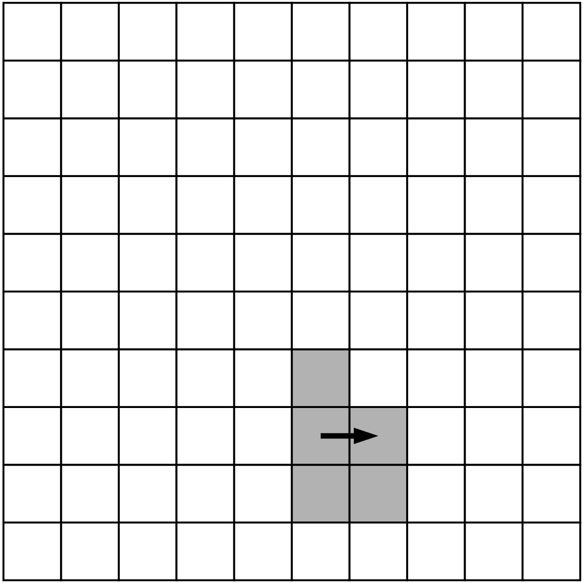

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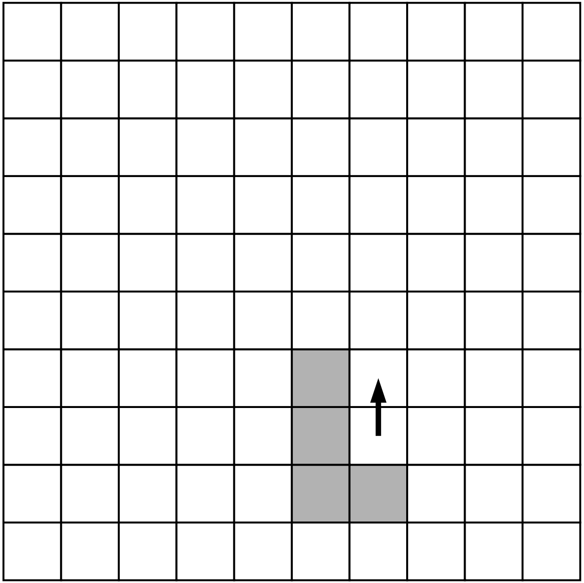
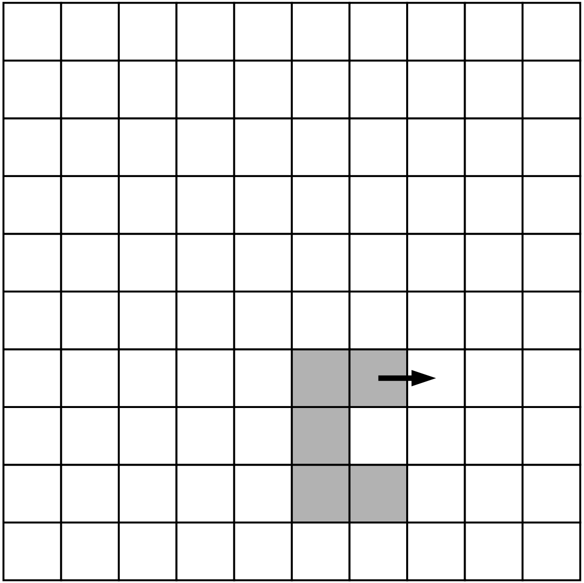


Several steps



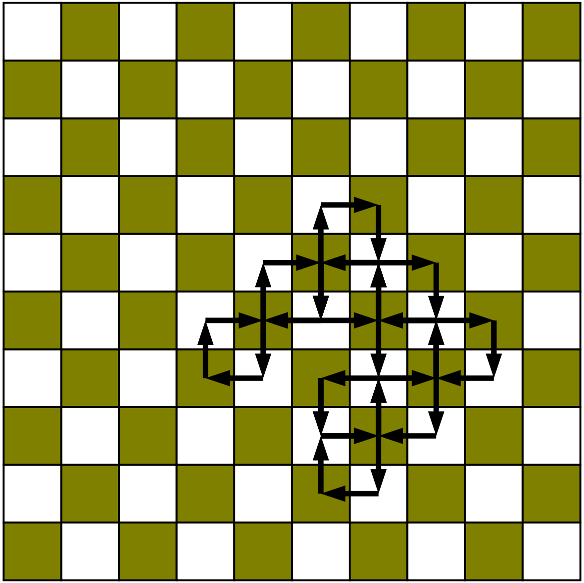
Were does the ant go in the long term?

- Animation...

Were does the ant go in the long term?

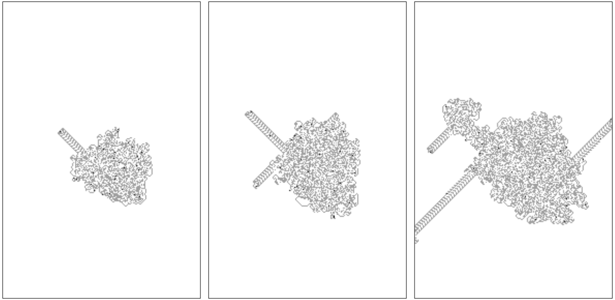
t=6900 t=10431 t=12000

The ants always escape to infinity



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

Impact on the scientific methodolgy

- We know perfectly well the fundamental law governing the system

Impact on the scientific methodolgy

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- ...because we define it ourselves

Impact on the scientific methodolgy

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- However we cannot predict the detailed motion of tha ant (e.g. at what time does the highway appears)

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Impact on the scientific methodolgy

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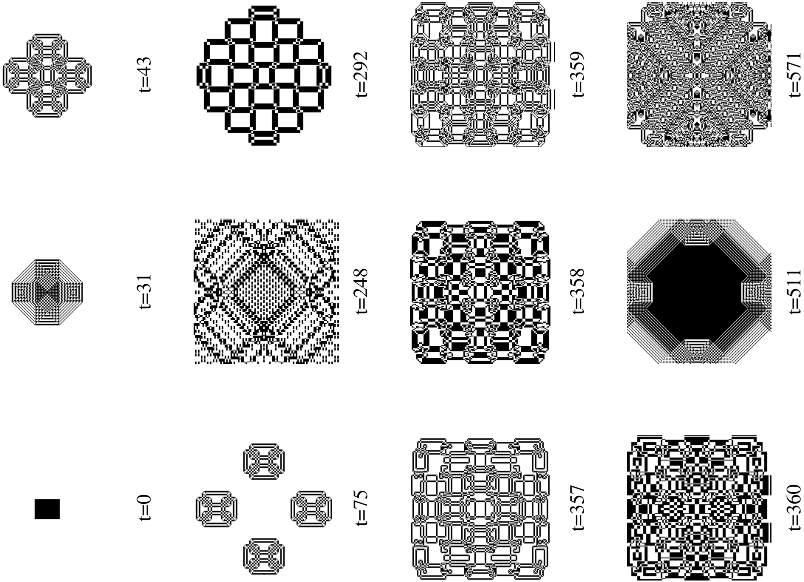
- However we cannot predict the detailed motion of tha ant (e.g. at what time does the highway appears)
- The microscopic description is not always able to predict the macroscopic behavior
- The only solution: **observe** the system
- The only information we get on the trajectory is global and relects the symmetry of the rule.

For other rules, on can be faster than the observation



For other rules, on can be faster than the observation

(a) (b) (c)

- Instead of $n \times n \times T$ computations (direct observation), one can get the results in $n \times n \times \log(T)$ computations

$\boxed{\textit{End of module}}$

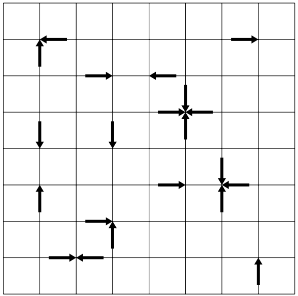
Complex systems

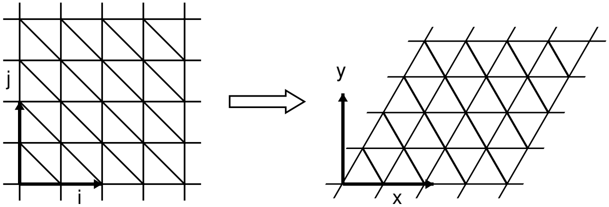
$\boxed{\textit{Coming next}}$

Lattice-gas models

6. Lattice-gas models

Lattice Gas model





Lattice gas Automata (LGA)

- LGA: Lattice Gas automata
- It is a CA that models a gas or a fluid through the dynamics of discrete particles moving on a lattice.
- Fully discrete Molecular Dynamics
- Idealized particles at a **mésoscopic** scale: the microscopic details are simplified
- One can show the equivalence of LGA models with the real phenomena
- Diffusion processes, chemical reactions advection phenomena can also be represented as a LGA

Description

- The particles have a finite number of possible velocities, $\mathbf{v}_i$
- They are such that in a time step Δt of the CA, particles jumps to a neighboring lattice points, thus traveling a distance Δx.
- The choice of the $\mathbf{v}_i$'s is strongly related to the choice of the lattice since $\mathbf{r} + \Delta t \mathbf{v}_i$ must belong to the lattice

Description

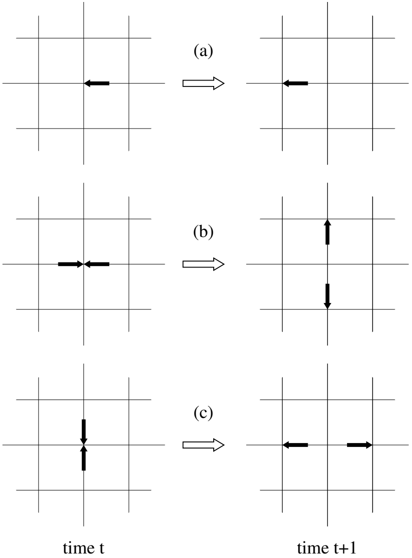
- The state of each cell $\mathbf{r}$ is given by **occupation numbers** $n_i(\mathbf{r}, t)$
- $n_i(\mathbf{r}, t) = 1$ means that a particle enters site $\mathbf{r}$ at time t with velocity $\mathbf{v}_i$.
- $n_i = 0$ means the absence of such a particle

Exclusion principle

- $n_i \in \{0, 1\}$ is Boolean number: there is at most 1 particle per site and per direction at a given time.
- A finite number of bits is sufficient to fully describe the state of the system.

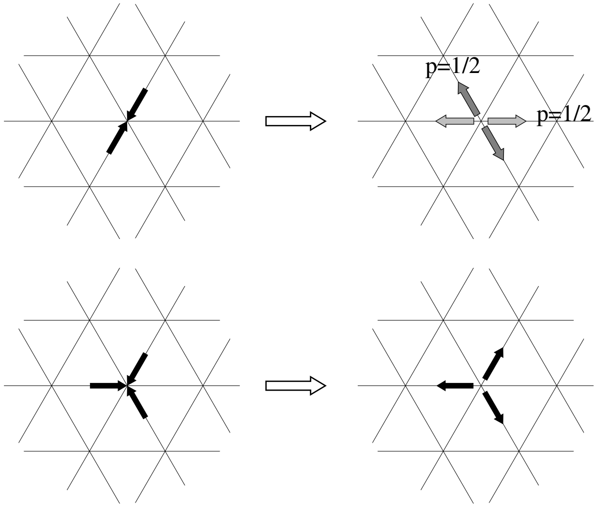
Example: HPP model collision rules

- 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.)



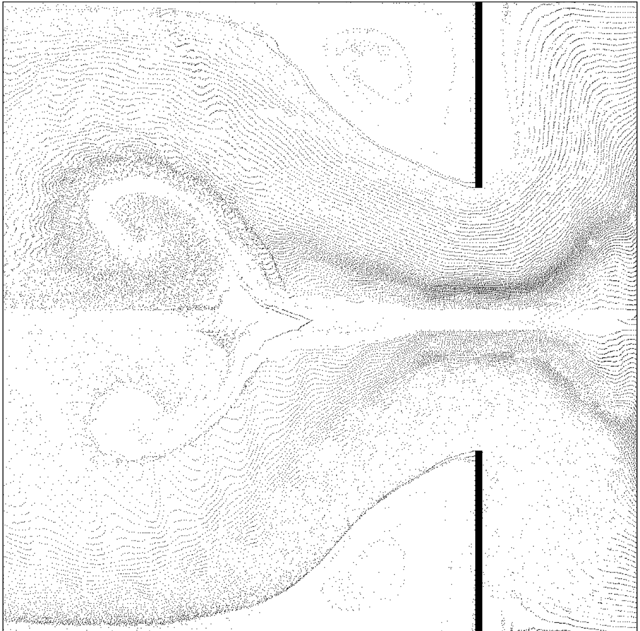
Exact mass and momentum conservation: that is what really matters for a

FHP model



Stochastic rule with Conservation of mass and momentum.

Flow past an obstacle (FHP)



$\boxed{\textit{End of module}}$

Lattice-gas models

$\boxed{\textit{Coming next}}$

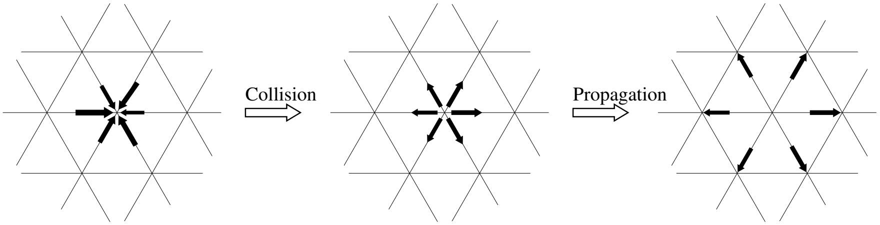
Microdynamics of LGA

7. Microdynamics of LGA

Microdynamics of LGA

It consists of two steps. We define $n_i^{in} = n_i$ and n_i^{out} to better specify them

- **Collision step:** The quantities n_i^{in} "collide" locally. Particles are deviated and new values n_i^{out} are computed at each lattice site, according to a pre-defined collision operator $\Omega_i(n)$
- **Propagation step:** The quantitiy $n_i^{out}(\mathbf{r})$ is sent to the neighboring site along lattice direction $\mathbf{v}_i$.



Microdynamics of LGA

In formula, we get

- collision: $n_i^{out}(\mathbf{r}, t) = n_i^{in}(\mathbf{r}, t) + \Omega_i(n^{in}(\mathbf{r}, t)$
- propagation: $n_i^{in}(\mathbf{r} + \mathbf{v}_i \Delta t, t + \Delta t) = n_i^{out}(\mathbf{r}, t)$

where Δt carry the time units and $\mathbf{v}_i$ has the unit of a velocity. Particle with velocity n_i travels in direction $\mathbf{v}_i$ and will thus reach lattice site $\mathbf{r} + \mathbf{v}_i$, still with velocity $\mathbf{v}_i$.

Microdynamics of LGA

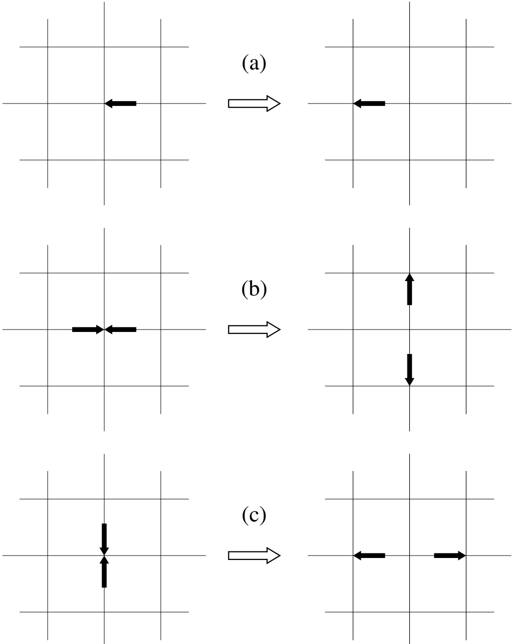
The above formula reflects how the LGA microdynamics is implemented in a computer. But mathematically, one ca combine the collision and propagation steps into:

$$n_i(\mathbf{r} + \mathbf{v}_i \Delta t, t + \Delta t) = n_i(\mathbf{r}, t) + \Omega_i(n(\mathbf{r}, t)$$

where $n_i \equiv n_i^{in}$

Note: if $\Omega_i = 0$, we obtain a free particle motion or streaming

HPP model



HPP model: Computer Implementation

Admitted velocities

$$\mathbf{v}_1 = (1,0), \quad \mathbf{v}_2 = (0,1), \quad \mathbf{v}_3 = (-1,0) \quad \mathbf{v}_4 = (0,-1)$$

Microdynamics:

$$n_i^{out} = n_i - n_i n_{i+2}(1-n_{i+1})(1-n_{i+3}) + n_{i+1}n_{i+3}(1-n_i)(1-n_{i+2})$$

and

$$n_i(\mathbf{r}) = n_i^{out}(\mathbf{r} - \mathbf{v}_i)$$

Mass conservation

The incoming mass is

$$\rho^{in}(\mathbf{r},t) = \sum_i n_i^{in}(\mathbf{r},t)$$

the outgoing mass is

$$\rho^{out}(\mathbf{r},t) = \sum_i n_i^{out}(\mathbf{r},t)$$

It is easy to check that the HPP collision rule is such that

$$\rho^{in}(\mathbf{r},t) = \rho^{out}(\mathbf{r},t)$$

Momentum conservation

Similarly, **momentum** is the defined as

$$j(\mathbf{r},t) \equiv \rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \sum_i \mathbf{v}_i n_i(\mathbf{r},t)$$

and it is easy to show that HPP conserves it during collision

Demos and discussion

- Pressure/density wave: anisotropy
- Reversibility: exact calculation
- Spurious invariants: momentum along each line and column, checkerboard invariant

More demos and discussion

- Sound wave propagation for FHP
- Snow transport by wind
- Diffusion, DLA, hour-glass,...

$\boxed{\textit{End of module}}$

Microdynamics of LGA

$\boxed{\textit{End of Week 4}}$

Thank you for your attention!