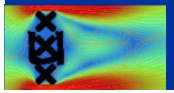
Modeling Complex Systems with Cellular Automata

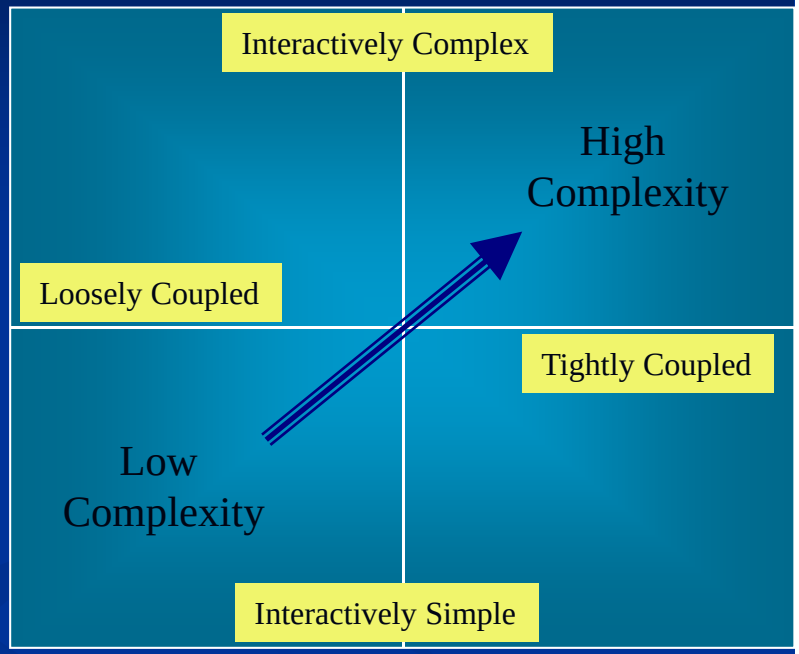
What is a complex System?

- Consists of a large number of interacting components (agents, cells…)
- Exhibit Emergence; A *self-organizing* collective behavior difficult to anticipate form the knowledge of the individual components' behavior
- Emergence is not a result of the existence of a central controller



Complex Systems

- Large number of interacting parts
- Difficult to understand behavior
- Hard to comprehend the structure that binds the components
- Nontrivial and complicated interaction between components
- Unpredictable emergent behavior



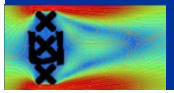
Perrow's Framework of Complexity

ACM Communications; May 2005 -- *Adaptive Complex Enterprises*

Complexity exists at the "edge of chaos" somewhere between too much and too little order. :-)

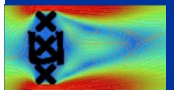
Examples

- Ant colony
- Coral reefs
- (Social) (Biological) Networks
- Earth quakes
- Traffic flow
- …



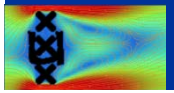
Some Characteristics

- Multi-scale-temporal
- Fractal dimensionality
- Scale invariance
- Non-equilibrium (exception Ising Spin)
- 1/f noise
- Self-organized criticality
- Phase transistions



Not (necessary) chaotic

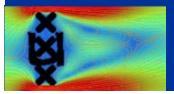
- A chaotic system:
  - Sensitive to initial conditions
  - Topological Transitive
  - Has periodic points that are dense in a set



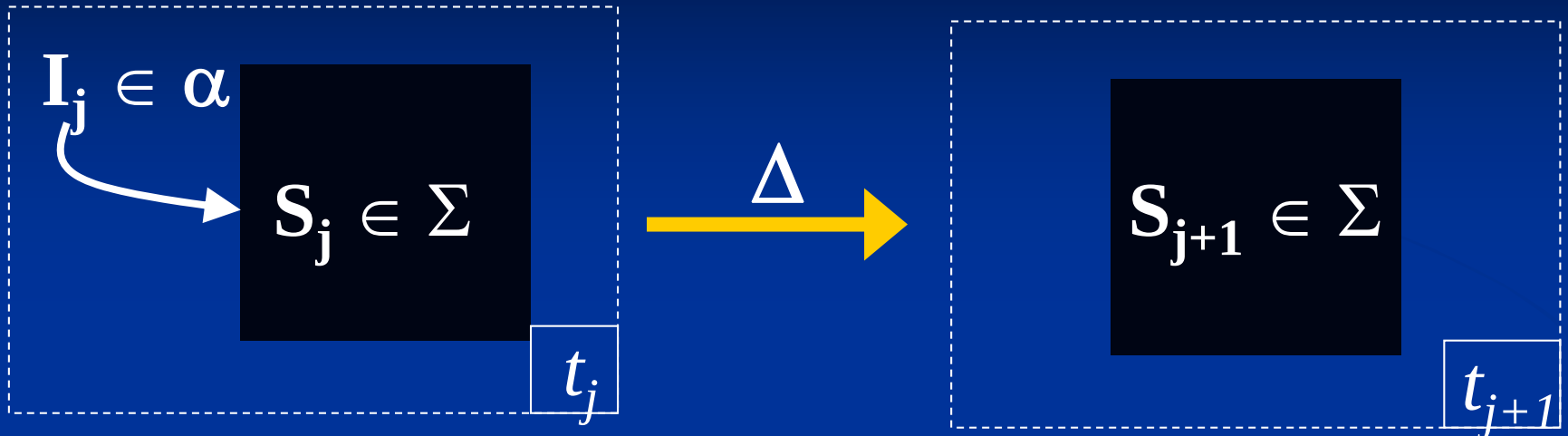
Modeling the world

Model/Variable	State	Space	Time
PDE's	C	C	C
Integro-difference Equations	C	C	D
Coupled ODEs	C	D	C
Interacting Particle Systems	D	D	C
Coupled map lattices, systems of difference equations, LBE models	C	D	D
Cellular Automata and Lattice Gas Automata	D	D	D

Table I: Mathematical and numerical modeling approaches to spatio-temporal processes. PDE: Partial Differential Equation; ODE: Ordinary Differential Equation; LBE: Lattice Boltzmann Equation. For more details see **Sloot & Hoekstra CRC Handbook**



Finite State Machine (FSM)



Define sets α, Σ:

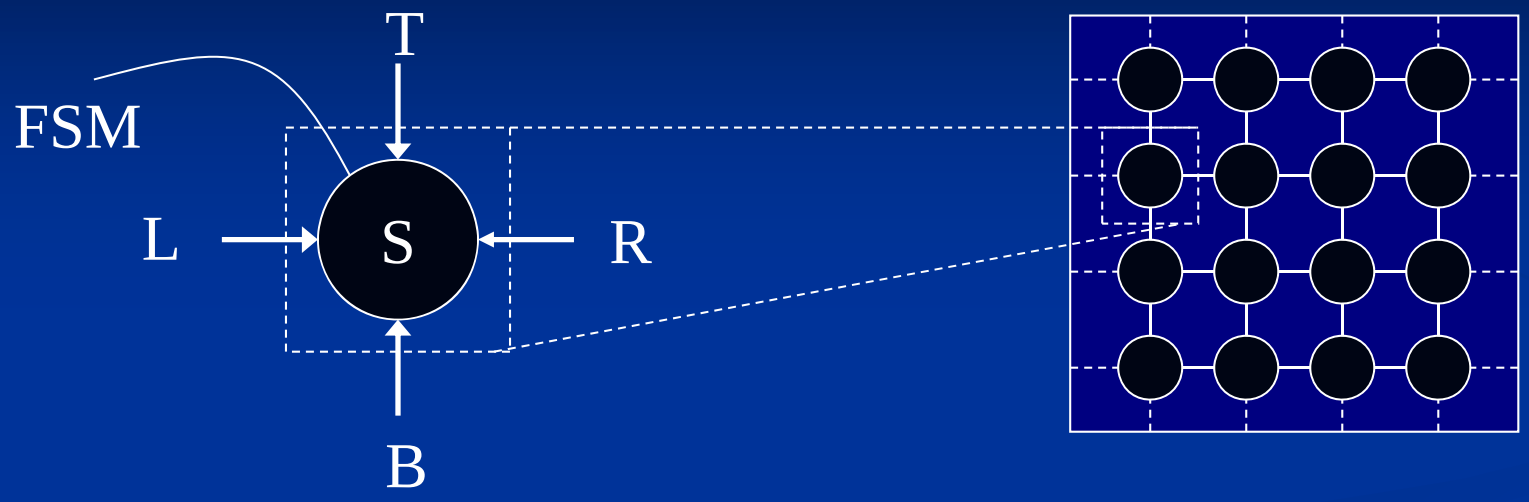
$\alpha = \{a_1, \ldots, a_n\}$ = finite input alphabet

$\Sigma = \{\sigma_1, \ldots, \sigma_m\}$ = finite set of states

And a function:

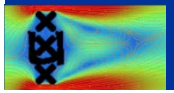
$\Delta: (\alpha, \Sigma) \rightarrow \Sigma$ = transition function

Cellular Automata

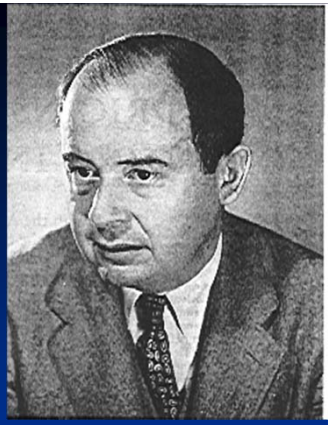


- D-dimensional lattice of FSMs.
- Each cell has N neighbors ($\alpha = \Sigma^N$).
- Transition function identical at every cell:

$$\Delta : \underbrace{\Sigma \times \Sigma \times \ldots \times \Sigma}_{N} \rightarrow \Sigma$$



Cellular Automata

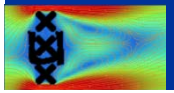


- 1966 Introduced by John von Neumann
- 1985 Stephen Wolfram suggested CA are capable of Universal Computation
- 1990 Lindgren et al., proved UC in 1D CA

  (Complex Systems, vol. 4, 299-318, 1990. 32)

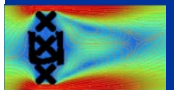
Lindgren & Nordahl (1990)

- Discovered computation-universal 1D cellular automata for:
  - $r = 1$, $k = 7$
  - $r = 2$, $k = 4$
- Proved:
  - A Turing Machine with m tape symbols and n internal states can be simulated by a CA with $r = 1$ and $k = m + n + 2$.



Turing Machine Example

- http://www.win.tue.nl/~aeb/ca/turing/turing.html
- Universal



Wolfram 2,3 Turing Machine Research Prize: The Solution - Mozilla Firefox

File Edit View History Bookmarks Tools Help

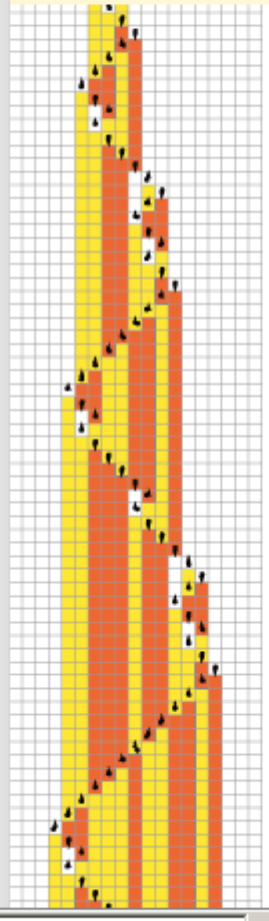
http://www.wolframscience.com/prizes/tm23/solved.html

"Wandering Camera"... Why STELLA? Het Nederlands Insti... Hotel MOSCOW, St.P... 1998 ACM Computin... 7th International Su... Abbaye in France

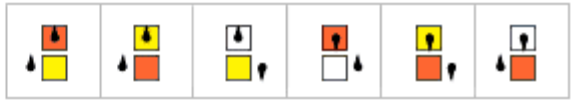
Wolfram 2,3 Turing Machine Res...

THE WOLFRAM 2,3 TURING MACHINE RESEARCH PRIZE

HOME



Wolfram's 2,3 Turing machine is universal!



The lower limit on Turing machine universality is proved—

providing new evidence for Wolfram's Principle of Computational Equivalence.

The Wolfram 2,3 Turing Machine Research Prize has been won by 20-year-old Alex Smith of Birmingham, UK.

Smith's Proof (to be published in Complex Systems):
Prize Submission » *Mathematica* Programs »

News Release » Technical Commentary »

Stephen Wolfram's Blog Post »

Media Enquiries »

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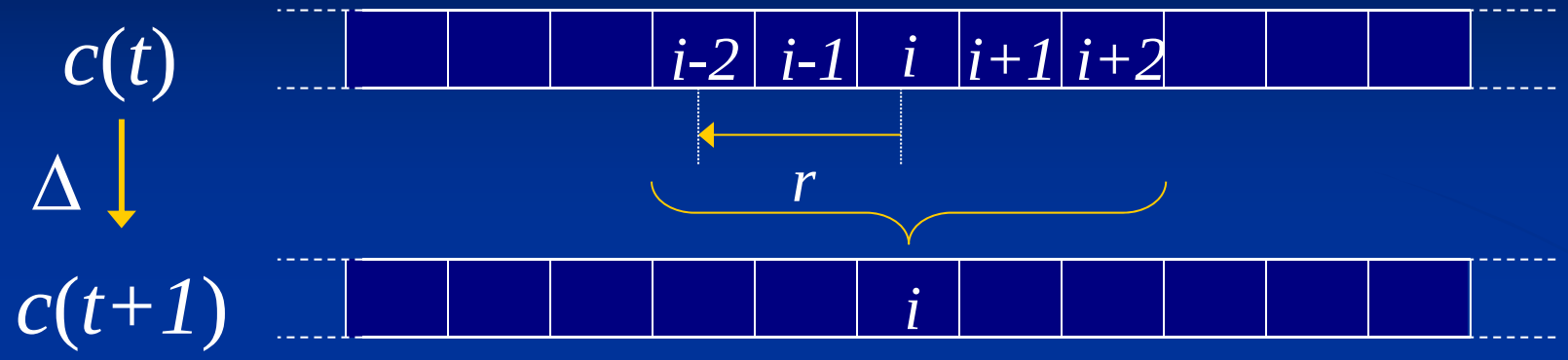
One-dimensional CA

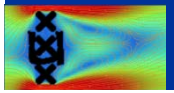


- $c_i(t) \in \Sigma$: value of i^{th} cell at time t.
- r : range (on left and right)
- Δ : transition (update) function.
- CA states evolve as:
  - $c_i(t) = \Delta(c_{i-r}(t - 1), c_{i-r+1}(t\text{-}1), \ldots , c_{i+r-1}(t\text{-}1), c_{i+r}(t\text{-}1))$

Rule-space for 1D CA

$c_{i-r}(t-1)$	$c_{i-r+1}(t-1)$	…	$c_i(t-1)$	…	$c_{i+r}(t-1)$	$c_i(t)$
0	0		0		0	$\Delta(0,0,\ldots,0)$
0	0		0		1	$\Delta(0,0,\ldots,1)$
:	:		:		:	:
k	k	…	k	…	k	$\Delta(k,k,\ldots,k)$

- Each cell takes on $k = |\Sigma|$ possible states.
- Δ assigns any of k values to each of the k^{2r+1} possible tuples.
- Total of $|\Delta| = k^{(k^{(2r+1)})}$ possible rules.
  - For nearest neighbors (r=1) and k = 2, $|\Delta| = 2^8 = 256$



Rule Codes for $r = 1$, $k = 2$

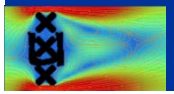
$\Sigma = \{0, 1\}$

$\alpha = \{111, 110, 101, 100, 011, 010, 001, 000\}$

111	110	101	100	011	010	001	000
↓	↓	↓	↓	↓	↓	↓	↓
$\Delta_{1,1,1}$	$\Delta_{1,1,0}$	$\Delta_{1,0,1}$	$\Delta_{1,0,0}$	$\Delta_{0,1,1}$	$\Delta_{0,1,0}$	$\Delta_{0,0,1}$	$\Delta_{0,0,0}$

- Define the rule code **R**[Δ] as:

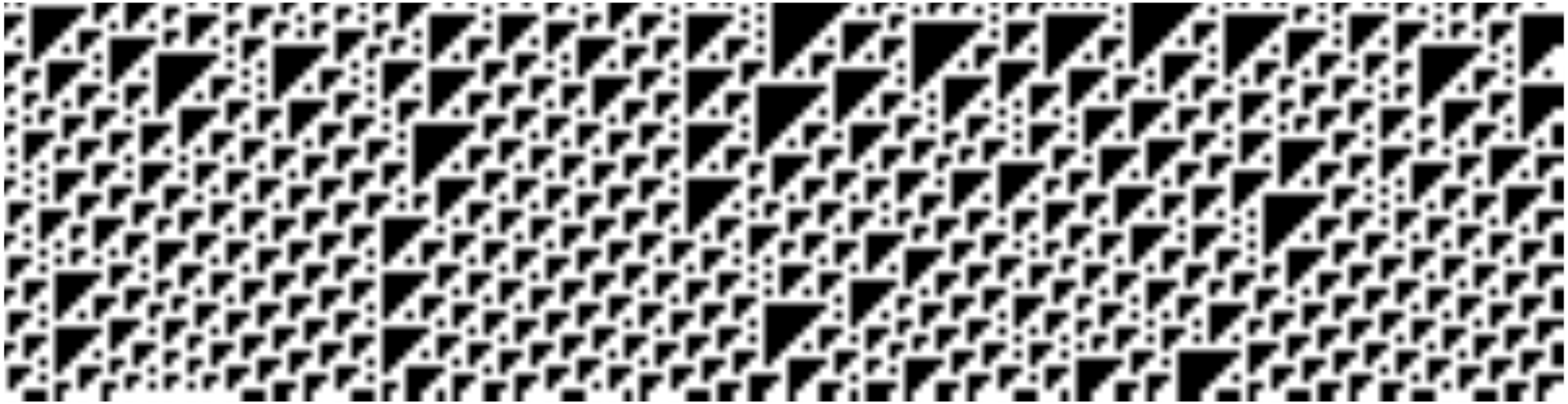
$$\mathbf{R}[\Delta] = 2^7 \cdot \Delta_{1,1,1} + 2^6 \cdot \Delta_{1,1,0} + 2^5 \cdot \Delta_{1,0,1} + 2^4 \cdot \Delta_{1,0,0} + 2^3 \cdot \Delta_{0,1,1} + 2^2 \cdot \Delta_{0,1,0} + 2^1 \cdot \Delta_{0,0,1} + 2^0 \cdot \Delta_{0,0,0}$$



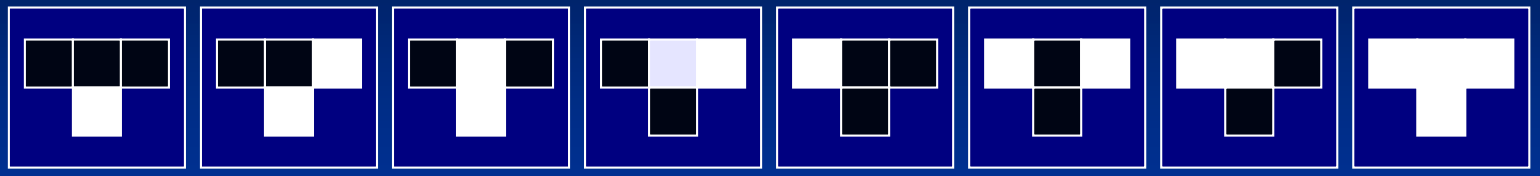
Productie Regel 110

111	110	101	100	011	010	001	000
0	1	1	0	1	1	1	0

Time Evolution of 1D Cellular Automata 110



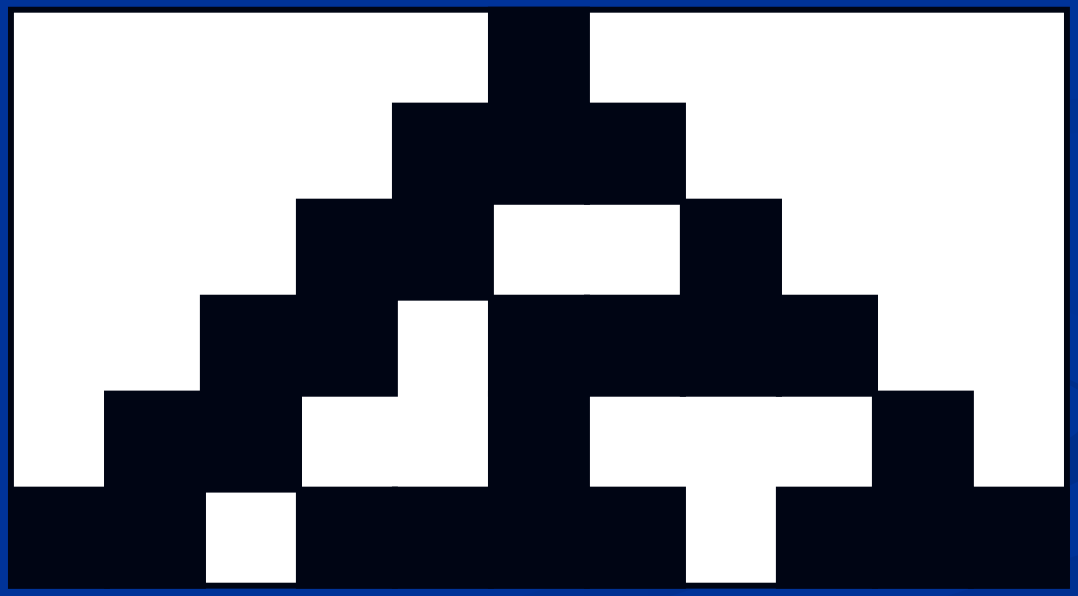
Example: R30



0 0 0 1 1 1 1 0

$(00011110)_2 = 30$

time = 0
time = 1
time = 2
time = 3
time = 4
time = 5



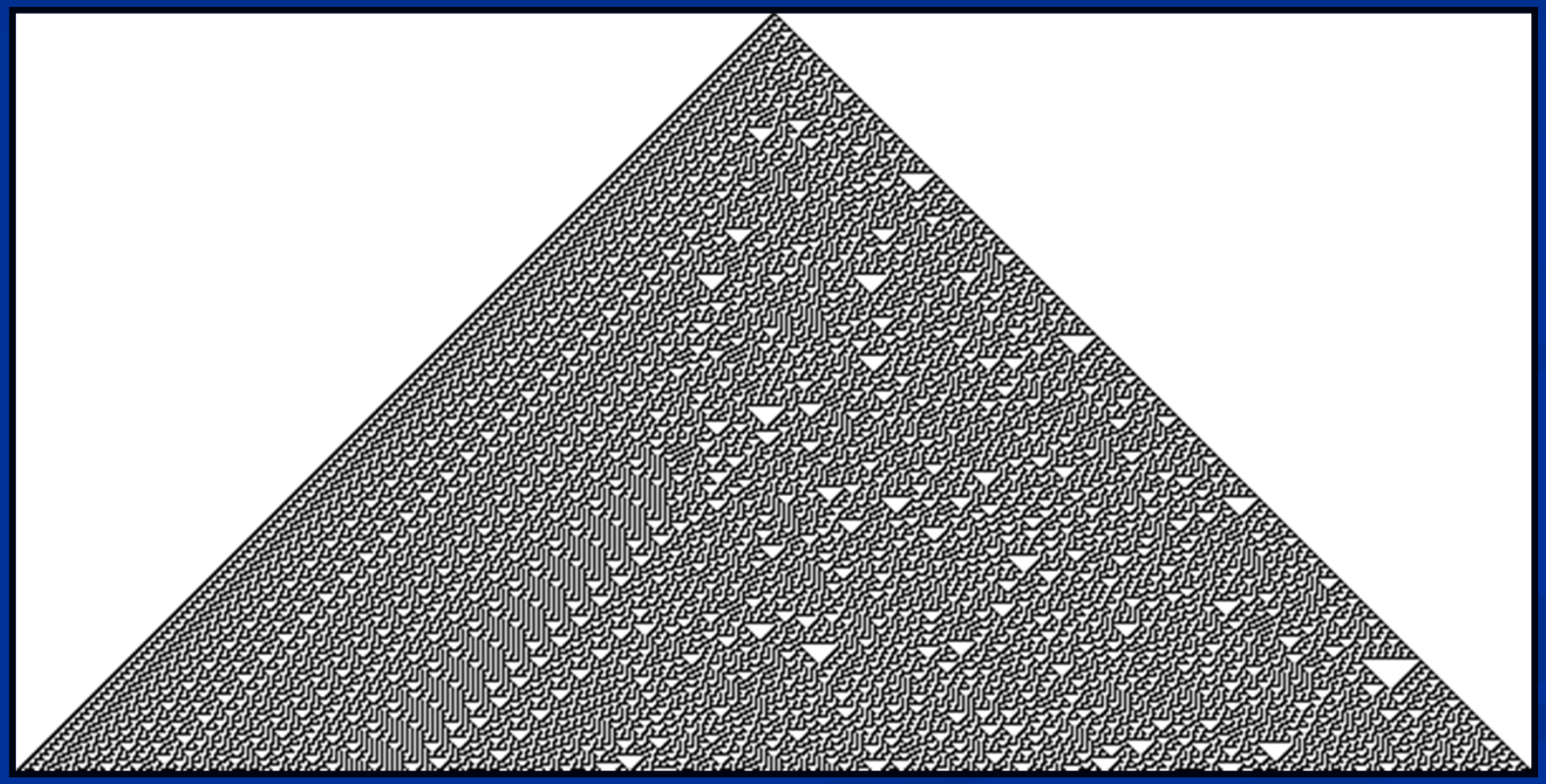
■: c = 1
□: c = 0

5 generations

Space-time pattern for R30

space →

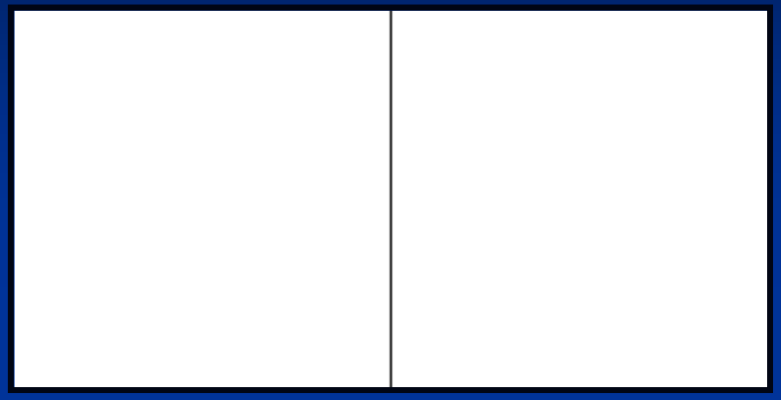
time ↓



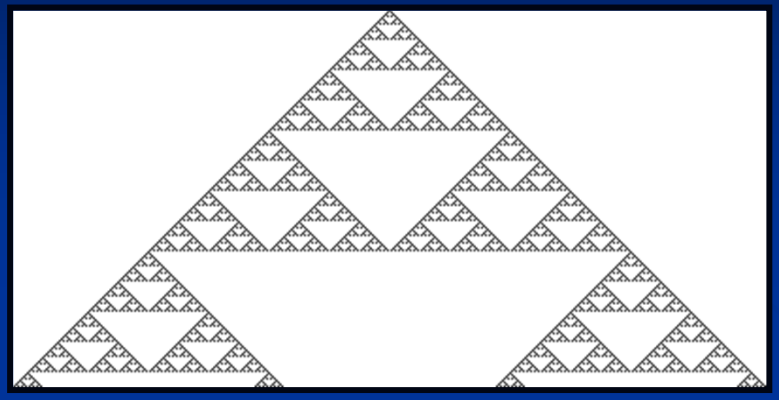
300 generations

Peter Sloot: Computational Science, University of Amsterdam, The Netherlands.

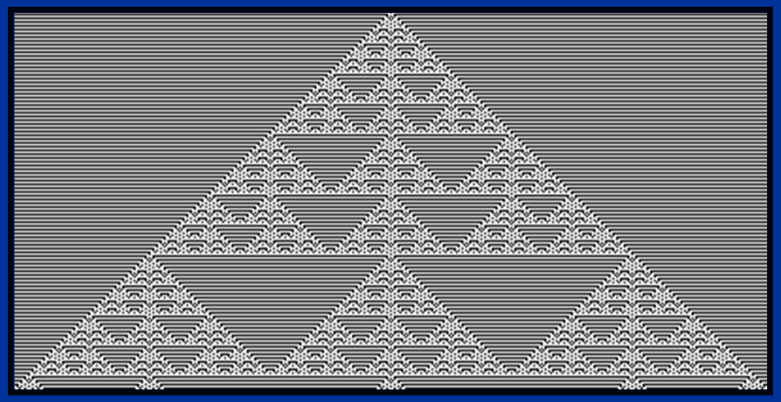
Patterns from a single seed



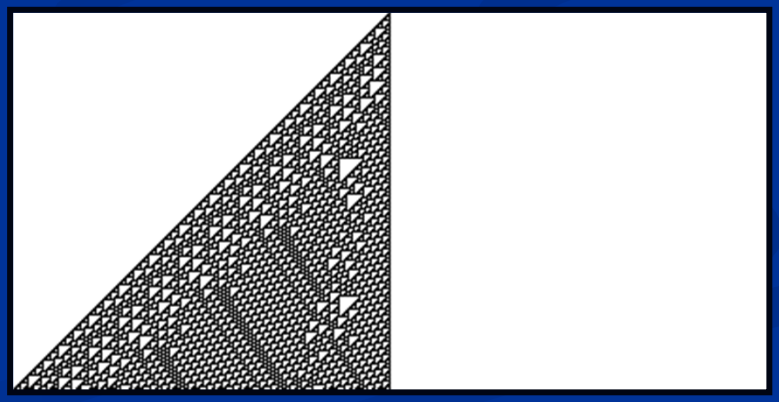
R4



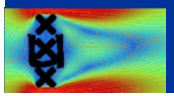
R18



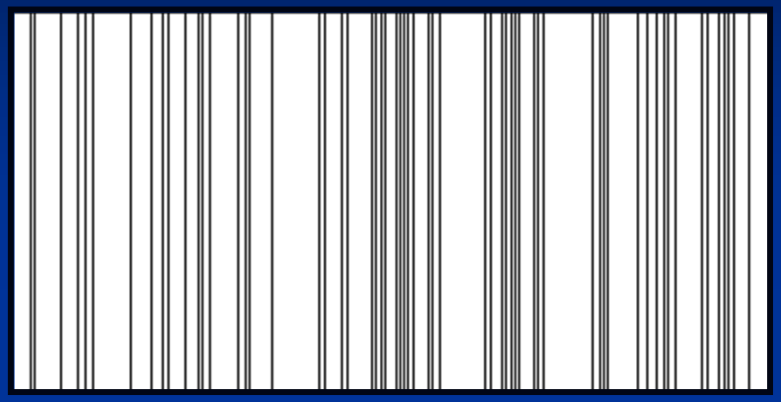
R105



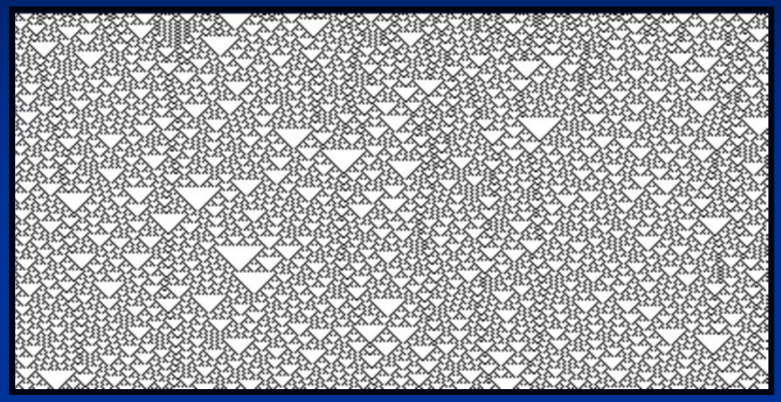
R110



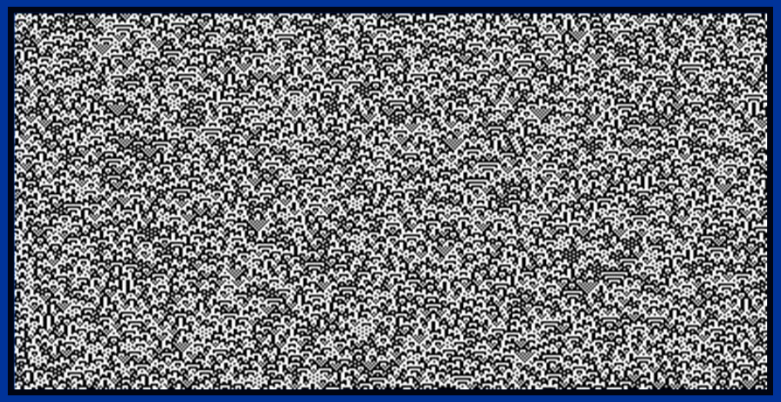
Patterns from a random seed



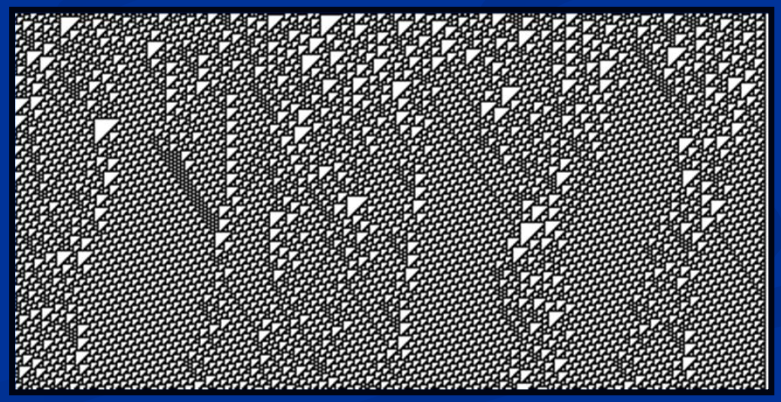
R4



R18



R105

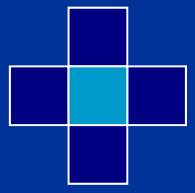


R110

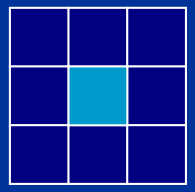
Peter Sloot: Computational Science, University of Amsterdam, The Netherlands.

Two-dimensional CA

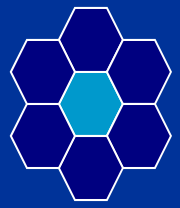
- Lattice is a 2D grid.
- Commonly-used neighborhoods:



von Neumann

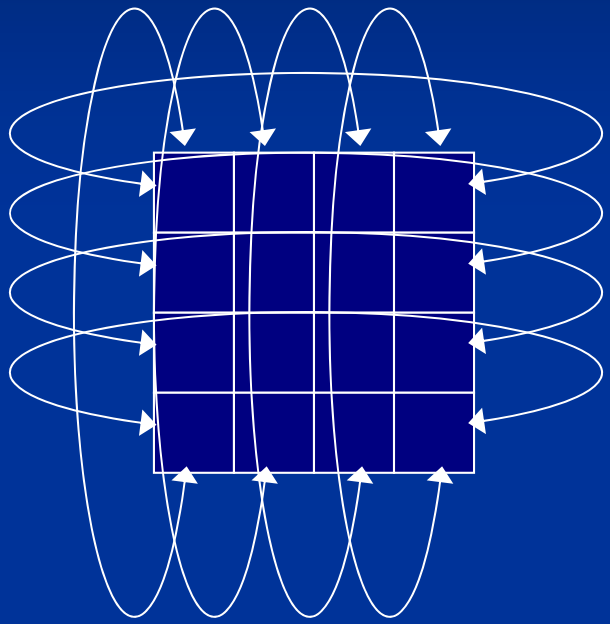


Moore

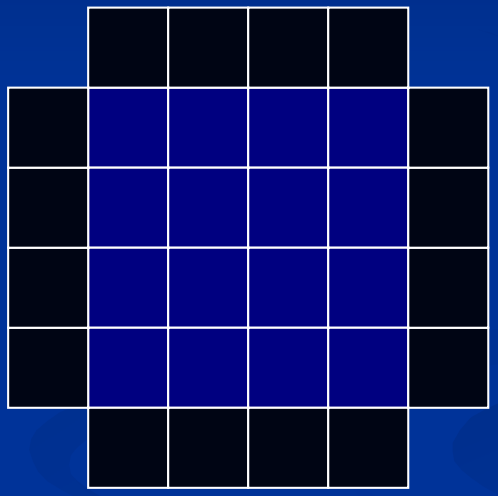


Hexagonal

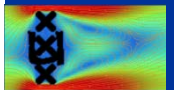
Boundary conditions



Periodic



Blocking



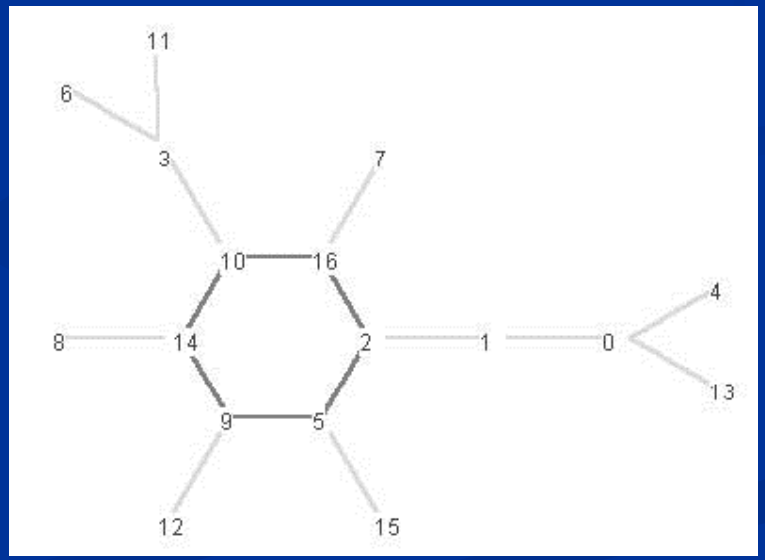
Properties on a Finite Lattice

- Garden-of-Eden states
- Cyclic States
- Transient states

Example: 1-Cell lattice

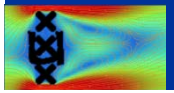
```
Tablex, Mod x^2+ 1 , 17 , x, 0, 17   TableForm
0     1
1     2
2     5
3     10
4     0
5     9
6     3
7     16
8     14
9     14
10    16
11    3
12    9
13    0
14    10
15    5
16    2
17    1
```

$$X_{i+1} = \left(X_i^{\,2} + 1\right) \bmod 17$$



Behavioral Classes of CA

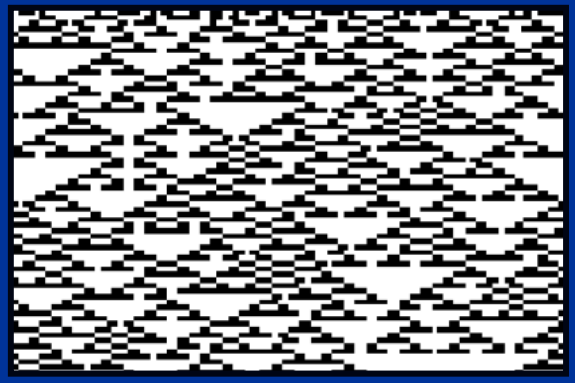
- **Class 1:**
  - Evolution leads to a homogeneous state, in which all cells eventually attain the same value.
- **Class 2**:
  - Evolution leads to inhomogeneous state: either simple stable states or periodic and separated structures.
- **Class 3**:
  - Evolution leads to chaotic nonperiodic patterns.
- **Class 4**:
  - Evolution leads to complex, localized propagating structures.



Examples

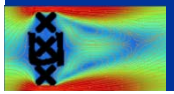
Class 1

Class 2



Class 3

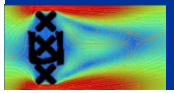
Class 4



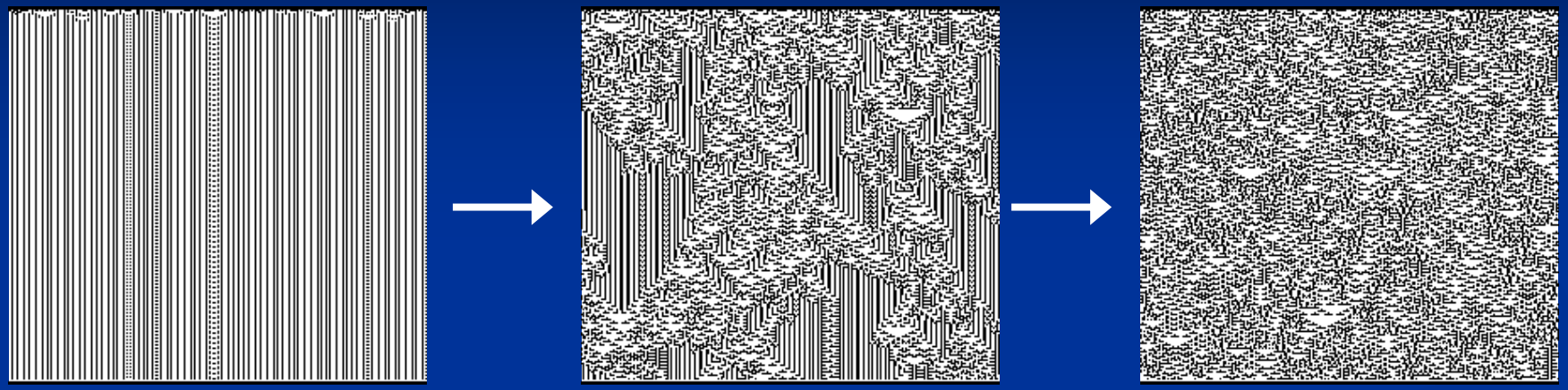
Langton's λ-parameter

- Define an arbitrary **quiescent state** $s_q \in \Sigma$.
- Let there be n_q transitions to s_q in Δ.
- Let the remaining $(k^N - n_q)$ transitions in Δ be filled at random.
- Define:

$$\lambda = (k^N - n_q)/k^N$$



Variation in λ



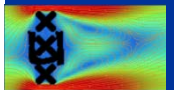
λ = 10/32 λ = 12/32 λ = 14/32

- Dynamical behavior a function of increasing λ:

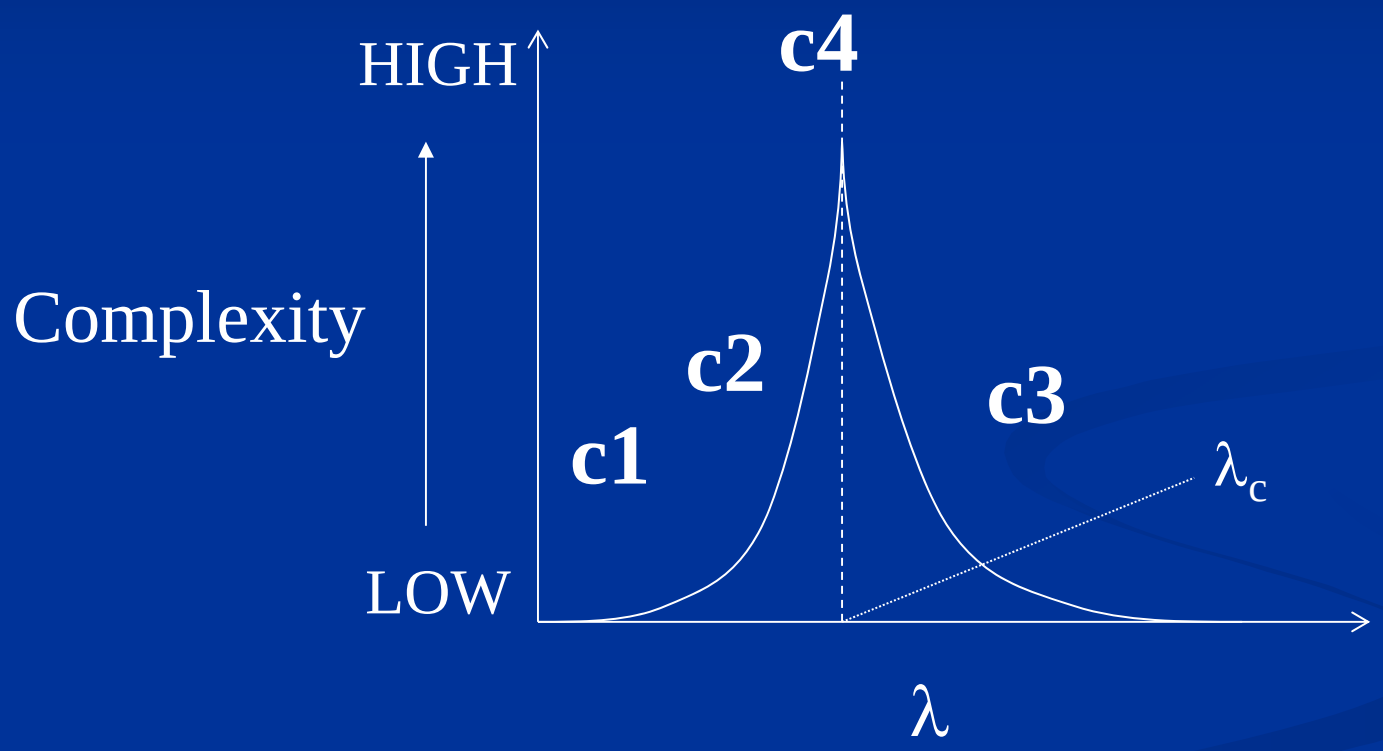
  fixed-point → periodic → "complex" → chaotic

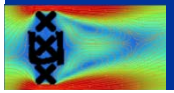
- Analogous to Wolfram's classes:

  c1 → c2 → c4 → c3



“Edge of chaos”

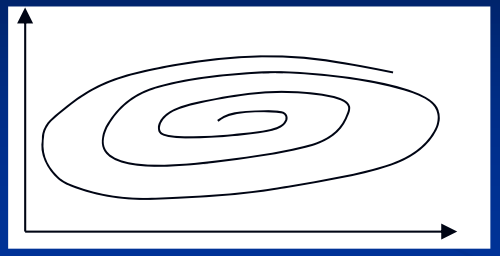




Analogy to Continuous Systems

t

Homogeneous state (**c1**)



Attractive Fixed Point

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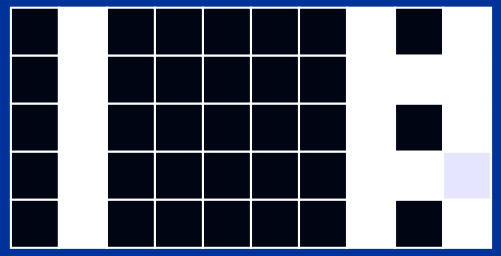
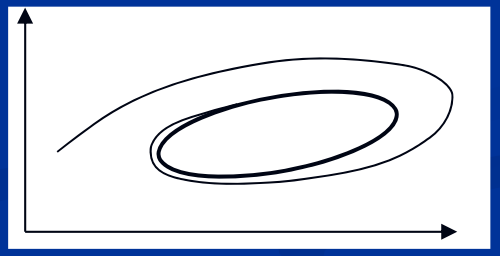
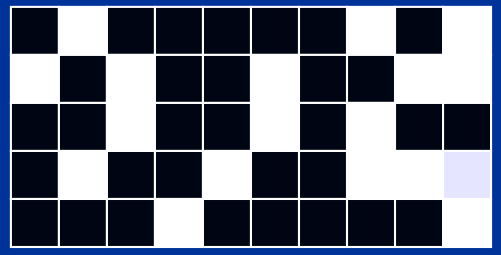


Periodic structures (**c2**)

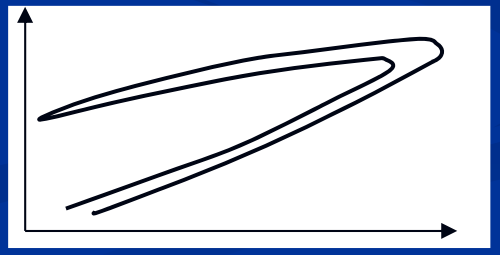


Limit Cycle

t



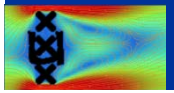
Chaotic nonperiodic patterns (**c3**)



Strange Attractor

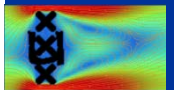
Observations on c4 rules

- No obvious continuous analogue.
- Soliton-like in appearance.
- Dynamic behaviour is *irreducible*.
- *Undecidable* question:
  - “Will a rule operating on an initial seed lead to a quiescent final state?” (CA analog of Turing’s *Halting Theorem*)



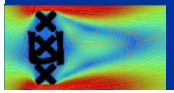
Qualities of CA

- Simple local rules ➔ Parallelism (!)
- Association with universal computing automata
- Alternative to differential equations
- Models of complex systems with emergent behavior
- And bridging the gap between microscopic rules and macroscopic observables.



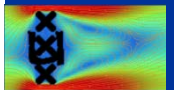
CA and Universal Computation

- It is speculated that all CA's with **c4** behaviour are capable of *universal computation*.
- Examples:
  - Game of Life (Conway)
  - Billiard-ball (Tuffoli)
  - Range-1 1D CA (Lindgren & Nordahl)
  - **R110** is also a good *elementary* candidate.



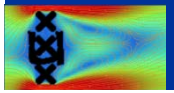
Lindgren & Nordahl (1990)

- Discovered computation-universal 1D cellular automata for:
  - $r = 1$, $k = 7$
  - $r = 2$, $k = 4$
- Proved:
  - A Turing Machine with m tape symbols and n internal states can be simulated by a CA with $r = 1$ and $k = m + n + 2$.



CA as Modeling Device

- Differential equations are usually discretized when modeled on a computer.
- Using CA-based models, we can start directly from a discrete system.
- Advantages of CA:
  - More convenient for simulations.
  - No numerical “approximations”.
- Disadvantage:
  - Finding a CA for a particular DE is not easy.



Example: Wave Equation in 1D

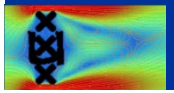
- Wave eq. in 1D: $$\frac{\partial^2 f}{\partial t^2} = c^2 \frac{\partial^2 f}{\partial x^2}$$

- Solution: $$f = \sum A_k \exp(ikx - w_k t) + B_k \exp(ikx + iw_k t)$$

- Particular solution:

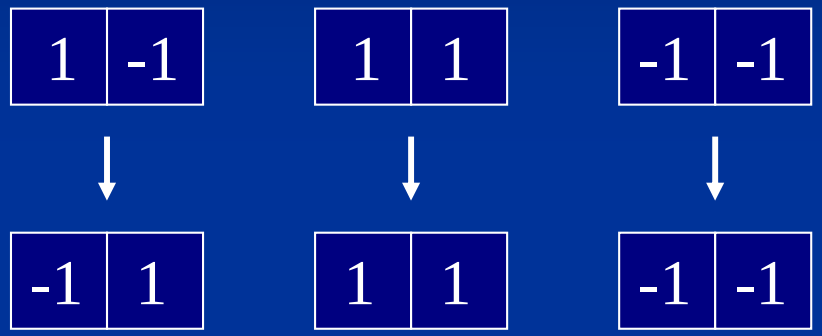
$$f = A(x - ct) + B(x + ct)$$

$$A(x) = \sum_k A_k \exp(ikx) \qquad B(x) = \sum_k B_k \exp(ikx)$$

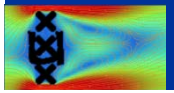


Wave Equation as CA

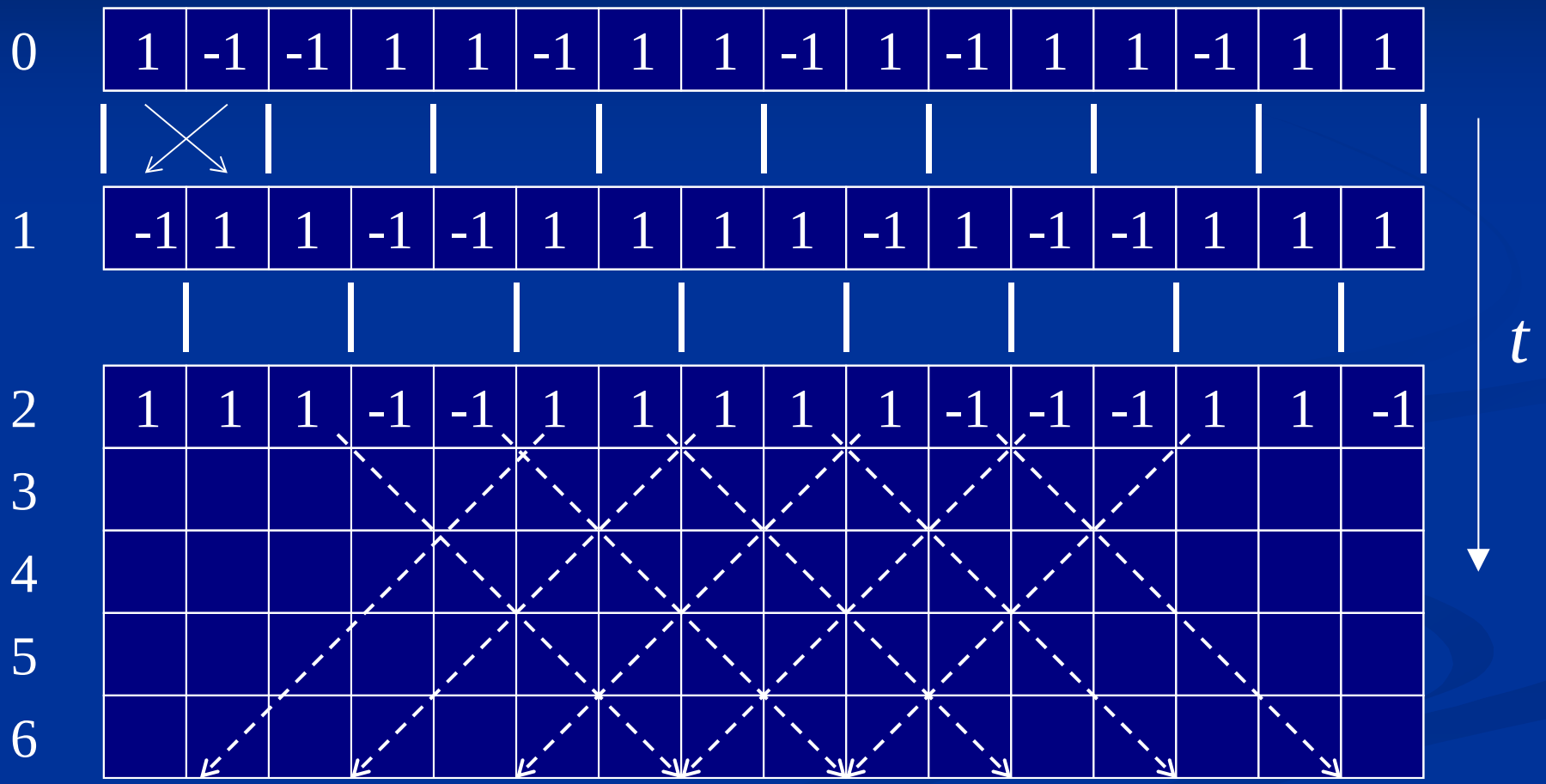
- 1D partitioned-space dynamics (Margolus rule):



- Constant velocity of c = 1 cell/update:
  - Odd cells: rightward traveling wave
  - Even cells: leftward travelling wave.
- Wave equation arises only as long-wave limit.

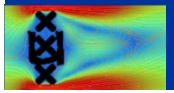


1D Margolus rule



Applications of CA

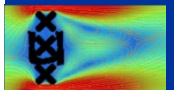
- Simple Examples
  - Traffic Flow
- Growth and Form



Approach

- Look for Occam's razor: Find simple computational models that simulate processes within the same universality class as the real phenomena.

- Use Cellular Automata as a mesoscopic model system:
  - Simple local interaction
  - Support for real physics *and* heuristics
  - Computational efficient

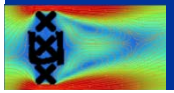


The Lattice Gas model

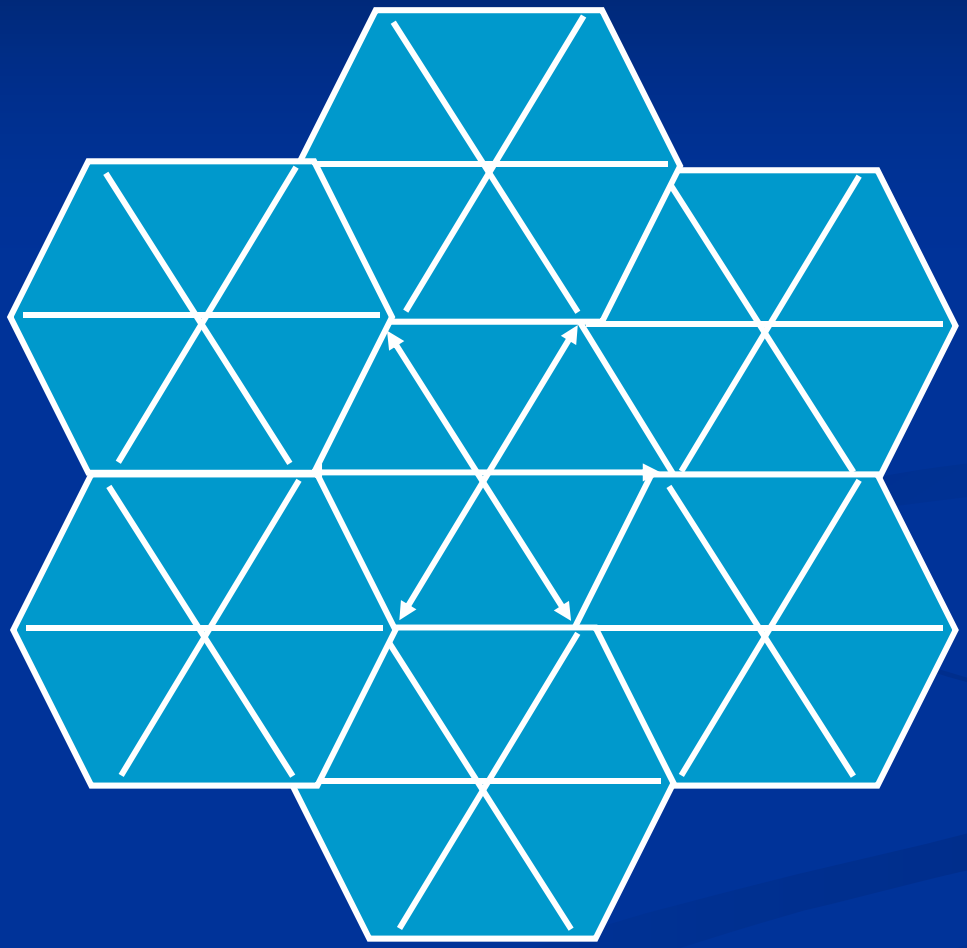
- Fluid model with Cellular Automata rules

$$n_i(\mathbf{x}+c_i, t+1) = n_i(\mathbf{x}, t) + \varpi_i(n_i(\mathbf{x}, t))$$

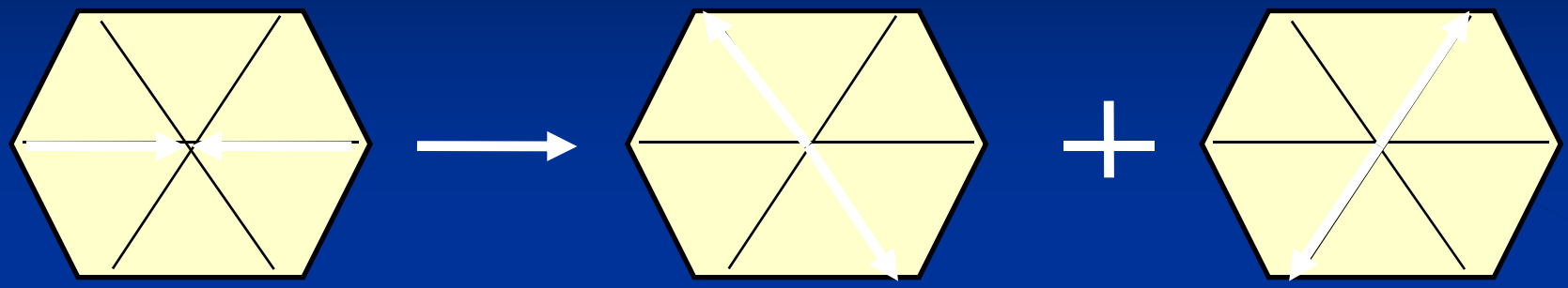
- Collision: particles reshuffle velocities
- Imposed Constraints
  - Conservation of mass
  - Conservation of momentum
  - Isotropy



The Hexagonal Lattice

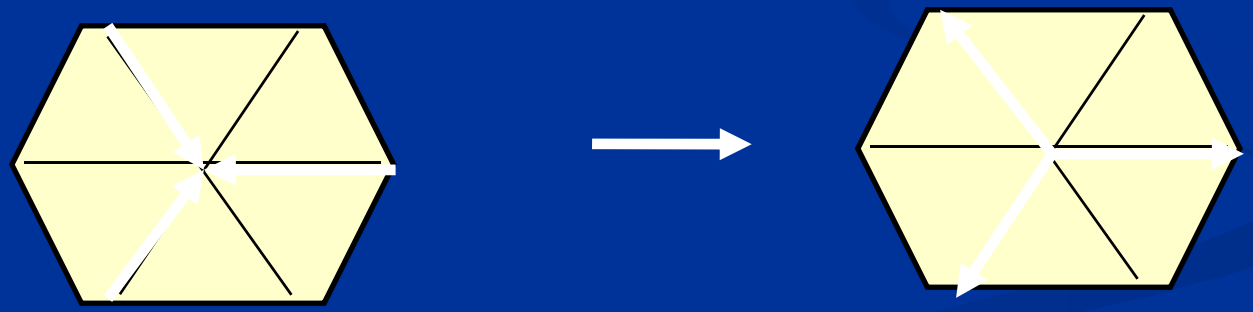


Collision rules examples



Two body collision

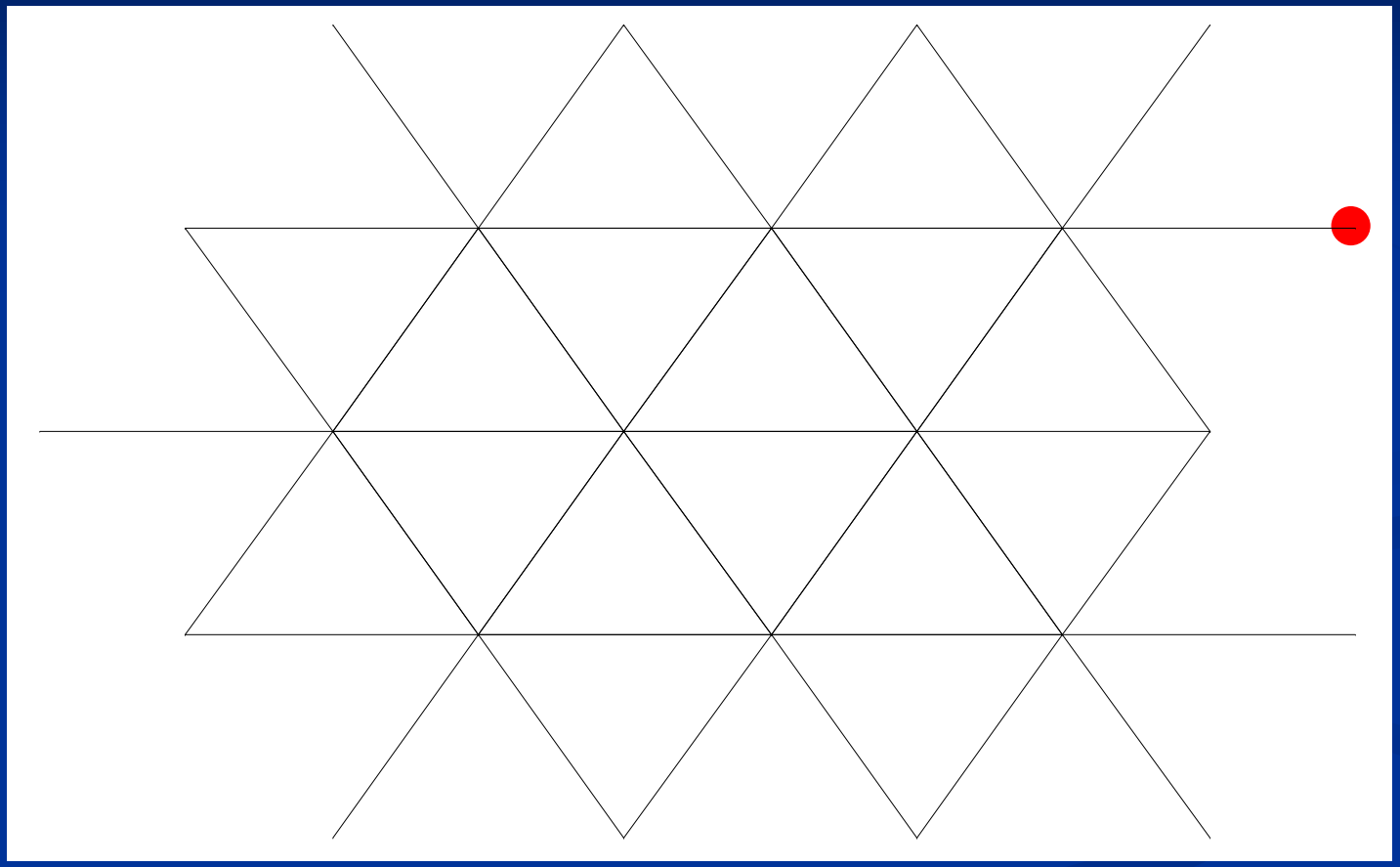
N1 AND N4 => N2 AND N5 && N3 AND N6



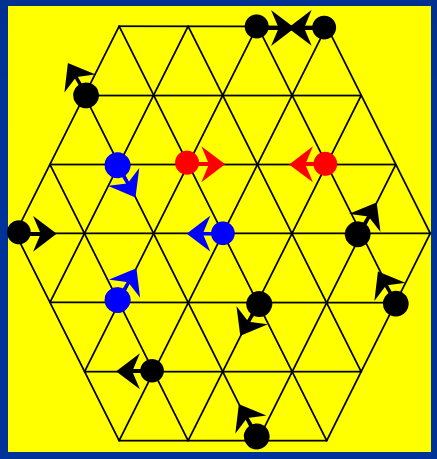
Three body collision

N2 AND N4 AND N6 => N1 AND N3 AND N5

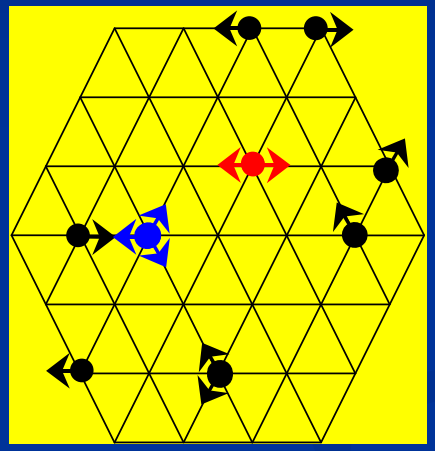
Streaming and Colliding



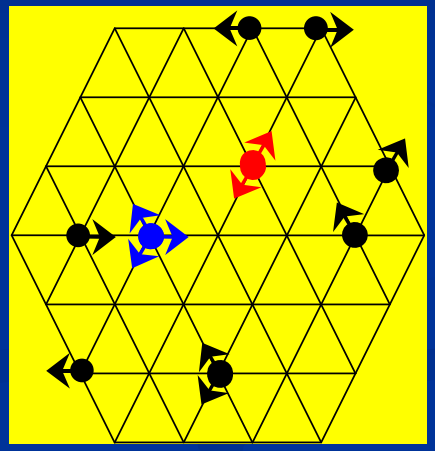
Lattice Gas Cellular Automata



Start

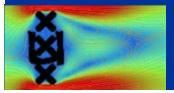


Streaming



Collision

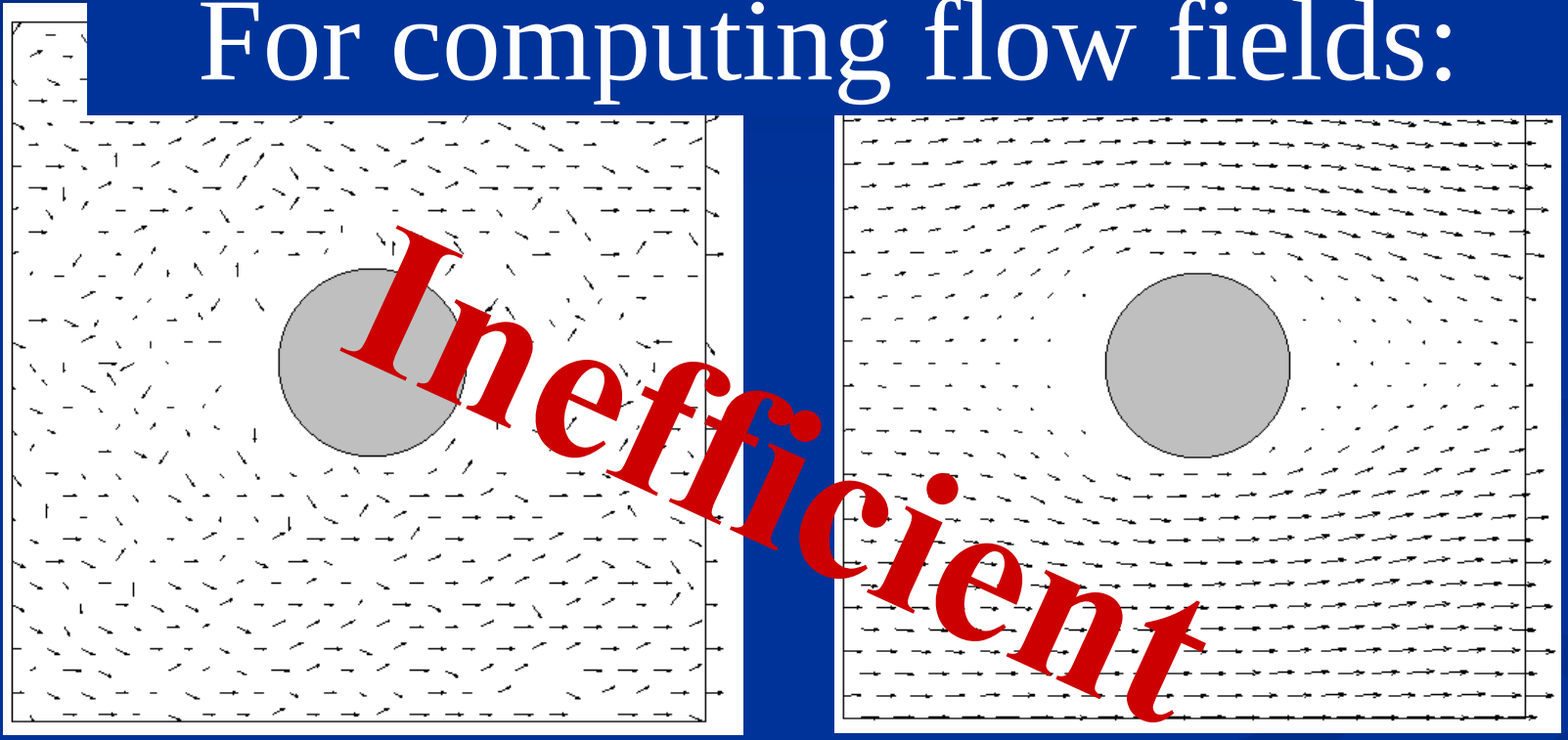
Conservation of mass, momentum, energy



Lattice Gas Cellular Automata

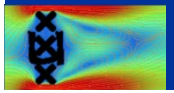
Need for averaging

For computing flow fields:



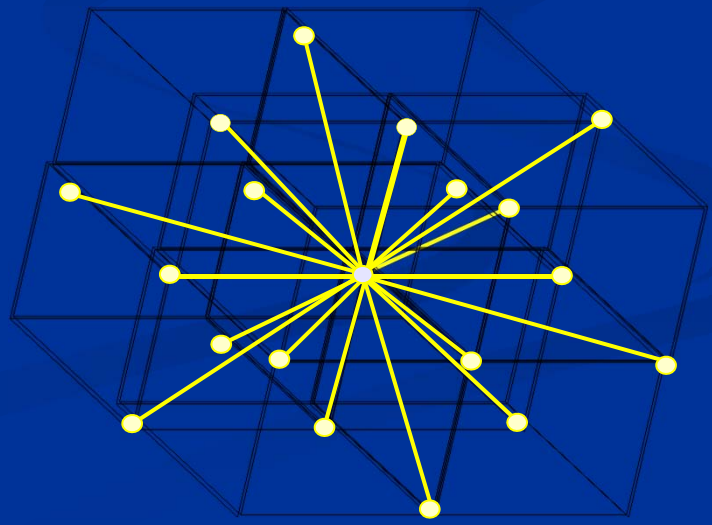
One time step

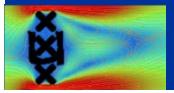
After averaging



Solution: pre-averaging
Lattice Boltzmann BGK

- Describe particle densities f_i, one density for each lattice velocity, rather than individual particles
- Propagation: propagate densities
- Collision: relax to equilibrium distribution f_i^{eq}
- On cubic lattice
  18 velocities +
  rest particle

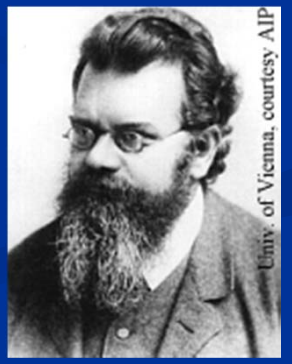




From LGA to LBM

- Average LGA equation to get continuous values instead of boolean values
- Boltzmann molecular chaos assumption to factorize products in collision operator:

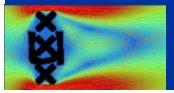
$$f_i = \langle N_i \rangle \text{ and } \langle N_i N_{i+3} \rangle \approx \langle N_i \rangle \langle N_{i+3} \rangle$$



From Micro Dynamics to Macro Dynamics (1)

- Taylor expansion to get continuous differential operators:

$$\Omega_i = \partial_t f_i + (\mathbf{e}_i \cdot \nabla) f_i + \frac{1}{2}\partial_t^2 f_i + \frac{1}{2}(\mathbf{e}_i \cdot \nabla)^2 f_i + (\mathbf{e}_i \cdot \nabla)\partial_t f_i$$



From Micro Dynamics to Macro Dynamics

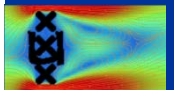
- Chapman Enskog expansion of equilibrium Distribution Function:

$$f_i = f_i^{eq} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots$$

- With imposed constraints:

$$\rho = \sum_{i=1}^{6} f_i^{eq} \quad \text{and} \quad \rho \mathbf{u} = \sum_{i=1}^{6} f_i^{eq} \mathbf{e}_i$$

$$0 = \sum_{i=1}^{6} f_i^{(j)} \quad \text{and} \quad 0 = \sum_{i=1}^{6} f_i^{(j)} \mathbf{e}_i \ , \ j \geq 1$$



From Micro Dynamics to Macro Dynamics

- Multi-scale expansion of time and space derivatives:

$$\partial_t = \varepsilon \partial_{t_1} + \varepsilon^2 \partial_{t_2} \text{ and } \partial_{r_\alpha} = \varepsilon \partial 1_\alpha$$

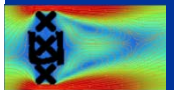
- Solve collision/flow equation for different order of ε:

$$(1\text{-st order balance}):$$

$$\partial_t \rho + \partial_{\bar{r}} \rho \mathbf{u} = 0.$$

$$(2\text{-nd order balance}):$$

$$\partial_t \rho u_\alpha + \partial_{r_\beta} \left[\Pi_{\alpha\beta} + \frac{1}{2} \tau \left(\varepsilon \partial_{t_1} \Pi^{(0)}_{\alpha\beta} + \partial_{r_\gamma} S^{(0)}_{\alpha\beta\gamma} \right) \right] = 0$$

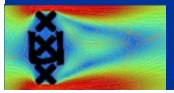


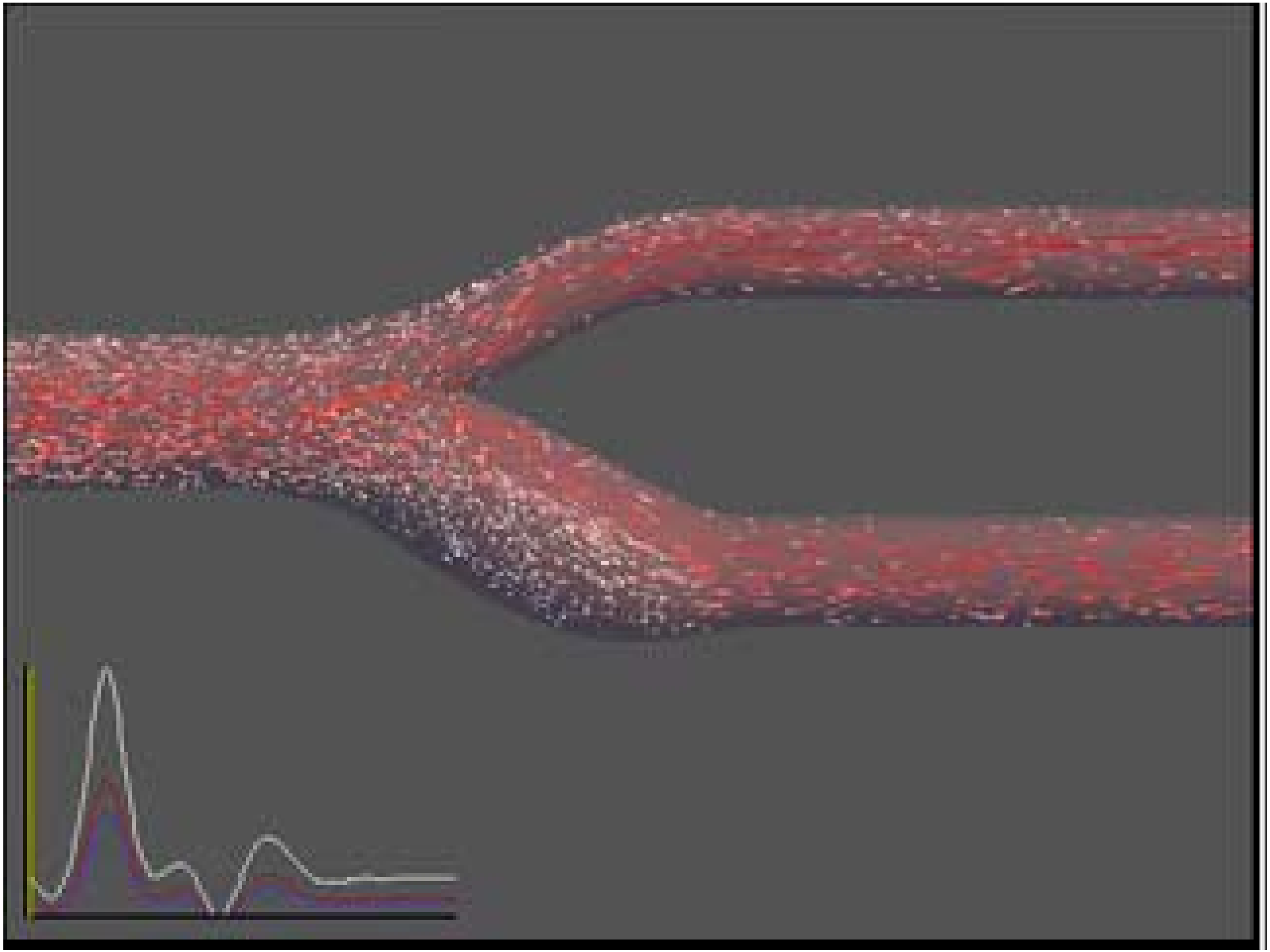
Equivalence with NS

- For lattice with enough symmetry: equivalent to the continuous incompressible Navier-Stokes equations:

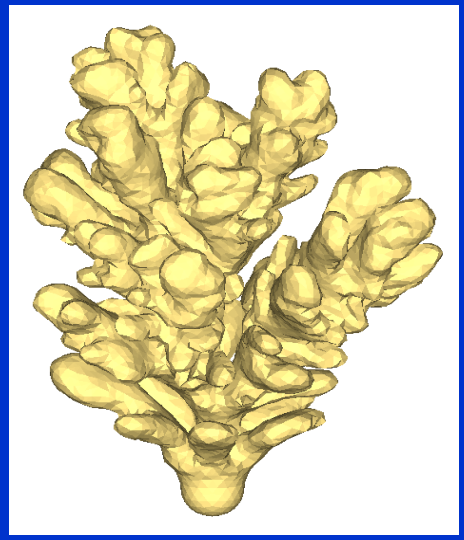
$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial u}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla P + \upsilon \nabla^2 \mathbf{u}$$

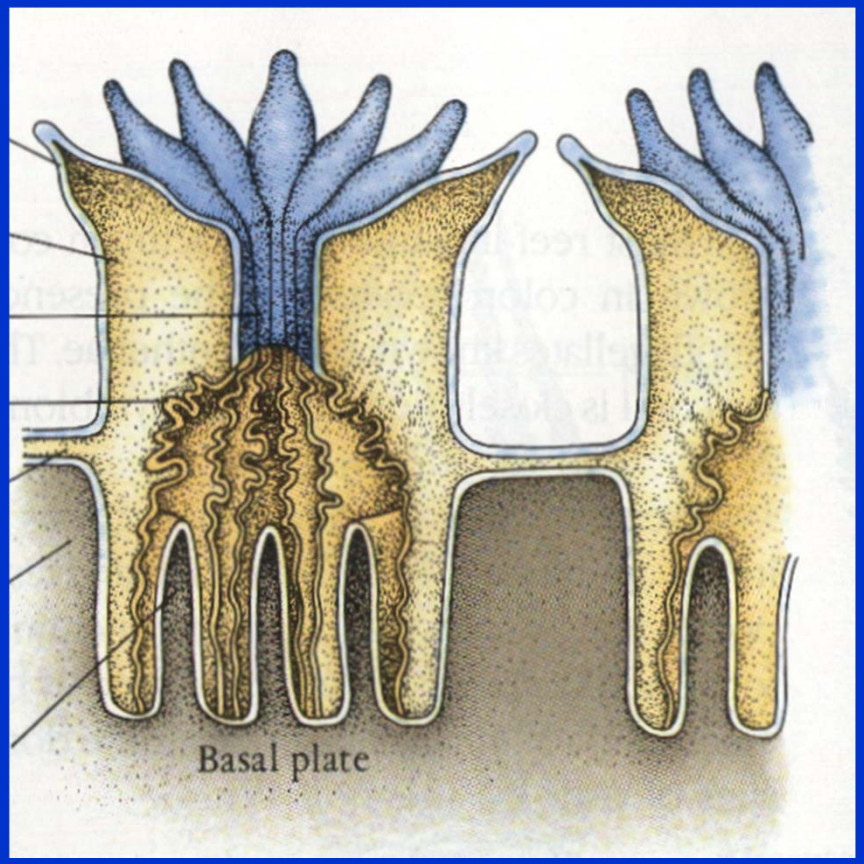




Coral Growth and Form

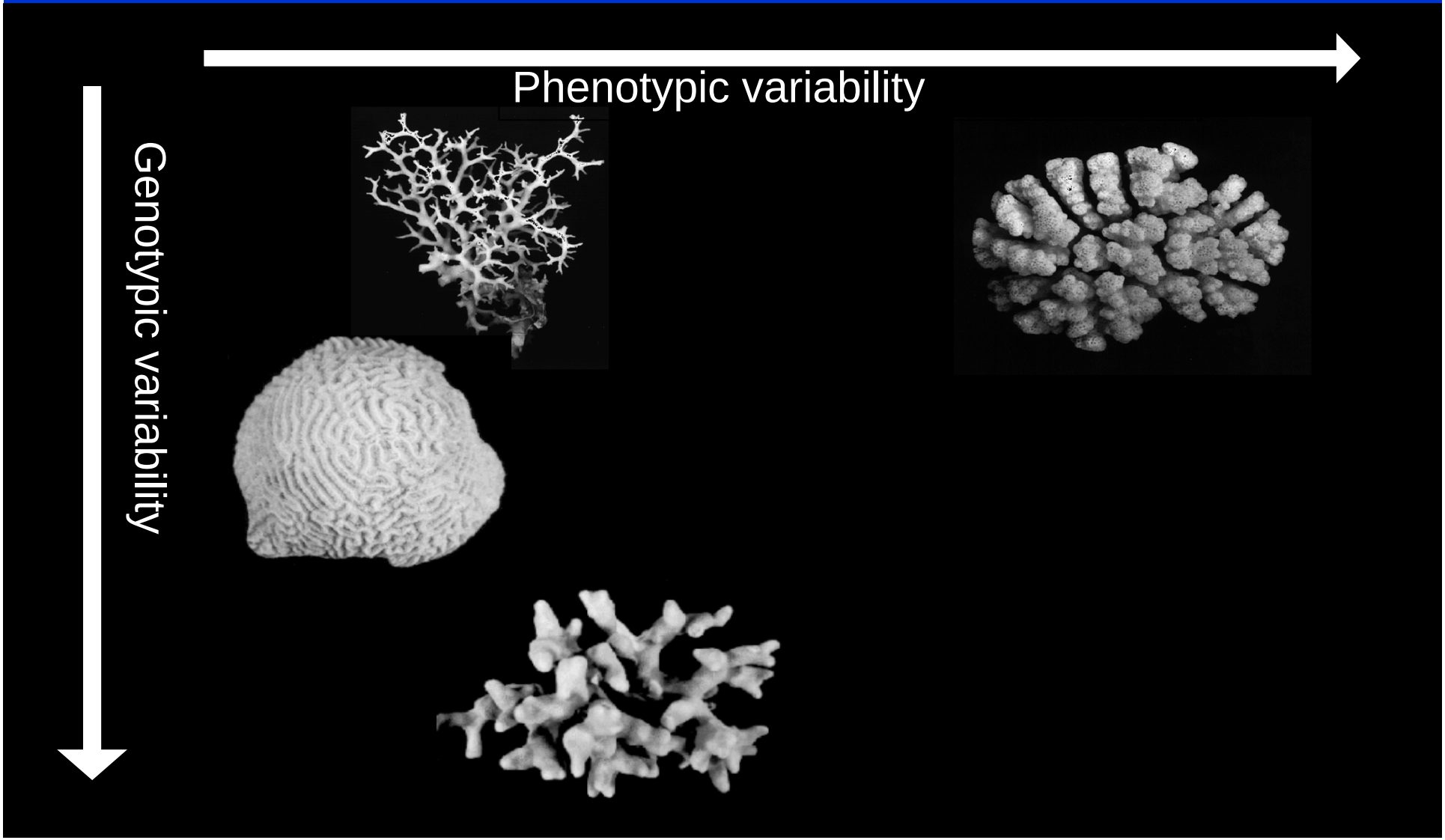


Coral Growth: Structure of coral colony



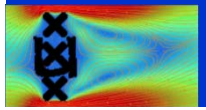
Outcome of growth process

wide range of morphologies!



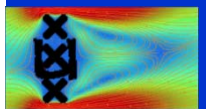
Need for multi-physics concepts

- Diffusion & gradient of Morphogenes
- Mechanical structure of polyps in corals
- Internal transport (e.g. sponge channels)
- Passive and active absorption
- Erosion
- Fluid-flow and diffusion
- Underwater light models
- ...



Approach to Physical Models

- We want to *understand* the underlying physical processes
  - Realistic (3D, correct conservation laws …)
  - No Artificial Live …$%^&*(…
- We observe *Macro-scale* phenomena emerging from *Micro-scale* processes, which we model by *Meso-scale* physics.



The Scale of things

Example: Material Properties
Micro molecules
Meso single-crystal grains with dislocations and impurities
Macro material properties

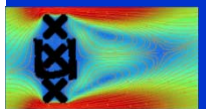
Example: Coral
Micro Genes & Bio-molecules
Meso Polyps
Macro Branches

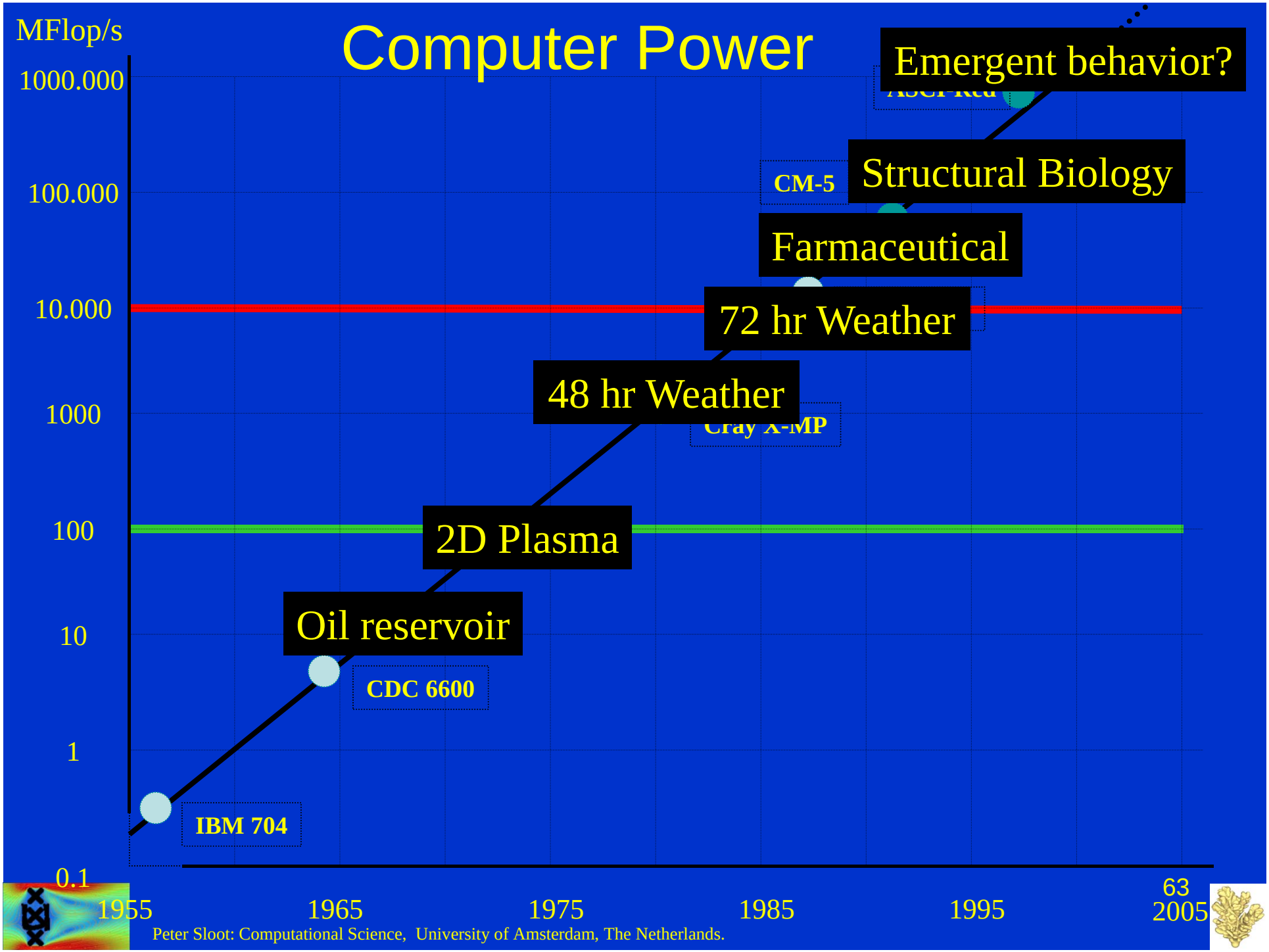
	Length (meters)	Time (seconds)
Microscale	$10^{-8} – 10^{-10}$	$10^{-14} – 10^{-12}$
Mesoscale	$10^{-6} – 10^{-2}$	$10^{-10} – 10^{-2}$
Macroscale	10^{-3} - 10^{+4}	10^{-6} - 10^{+7}

Implications for computational Requirements…

- To represent mesoscale on a microscale mesh requires > 10^{12} points
- To evolve time we need > 10^5 time steps

  => if algorithms linear in space: > 10^{17} operations == a few days on a teraflop system
- To make life worse: *Infrequent events like diffusion necessitate evolution to macroscale > 10^{20} operations*

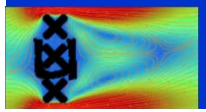



MFlop/s
Computer Power
1000.000
100.000
10.000
1000
100
10
1
0.1
Emergent behavior?
Structural Biology
CM-5
Farmaceutical
72 hr Weather
48 hr Weather
Cray X-MP
2D Plasma
Oil reservoir
CDC 6600
IBM 704
1955
1965
1975
1985
1995
2005

Approach

- Look for Occam's razor: Find simple computational models that simulate processes within the same universality class as the real phenomena.

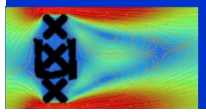
- Use Cellular Automata as a mesoscopic model system:
  - Simple local interaction
  - Support for real physics *and* heuristics
  - Computational efficient



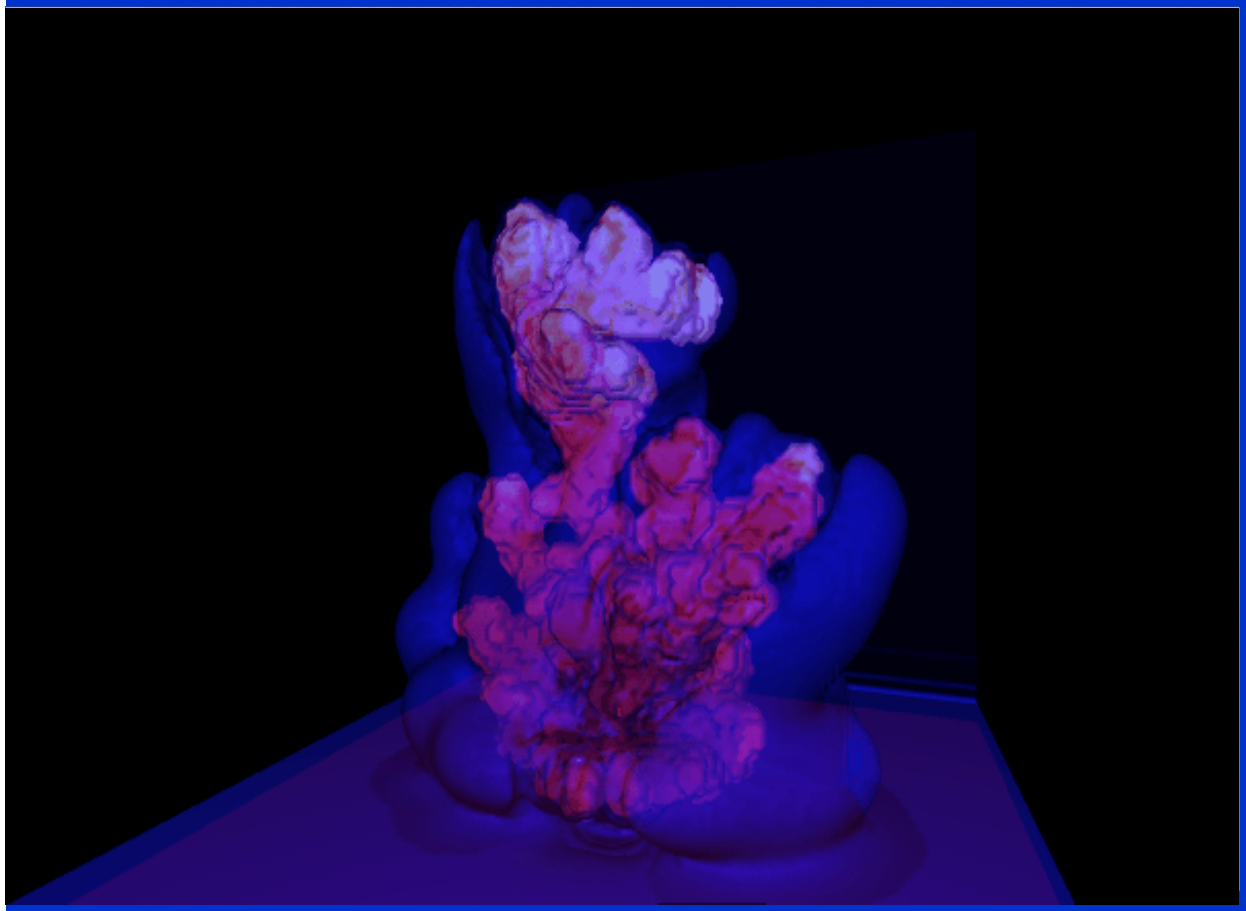
Universality

- Abstraction where essential behavior is controlled by very few parameters.
- Physics near critical points independent of microscopic details.
- Universallity classes characterize the critical properties that depend only on dimensionality and symmetry properties.
- Usually supporting renormalization (as in Ising Spin models).

Back

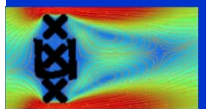


Simulation of Coral Growth



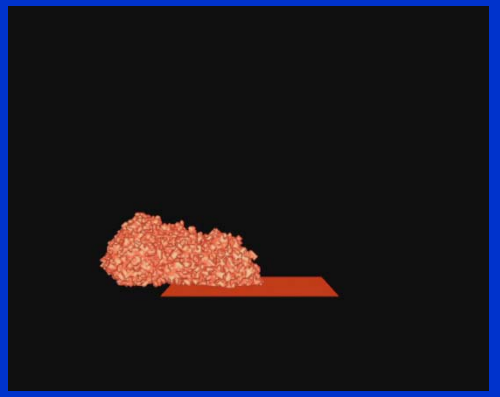
- Apply solid boundary conditions
- Propagation step
- Post collision distribution
- Curvature rule

72 hrs on 10 GigaFlop/s Supercomputer



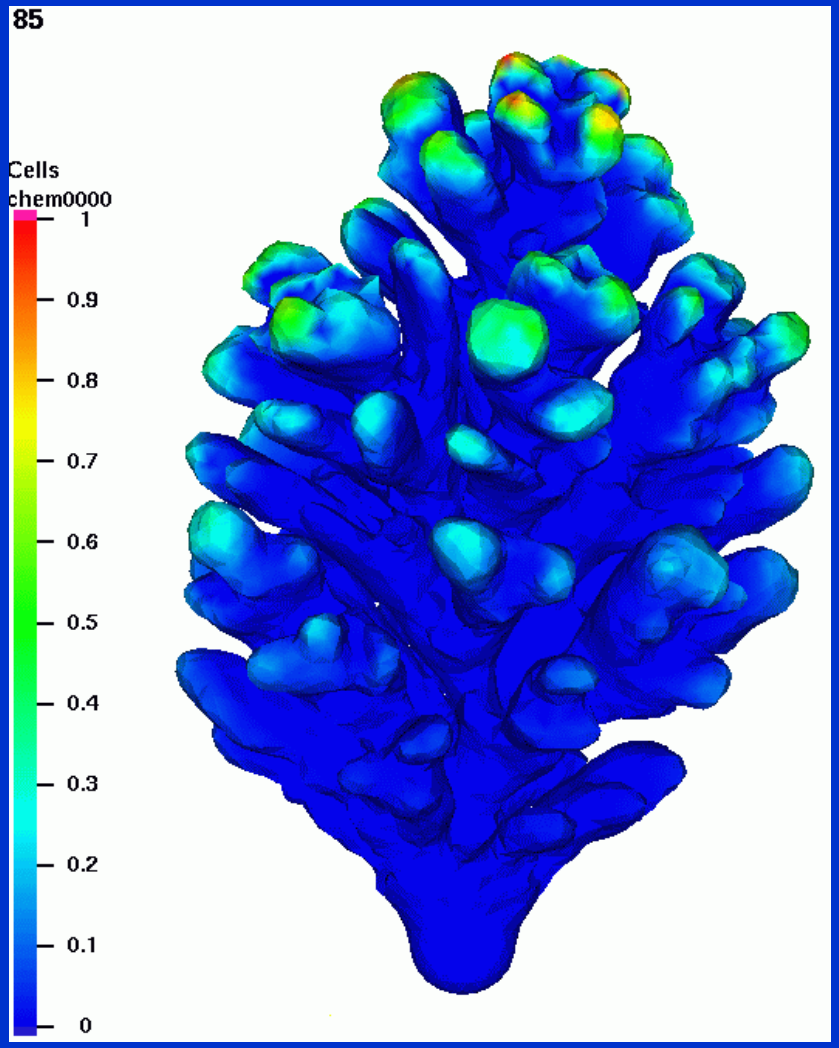
Results for different Peclet numbers

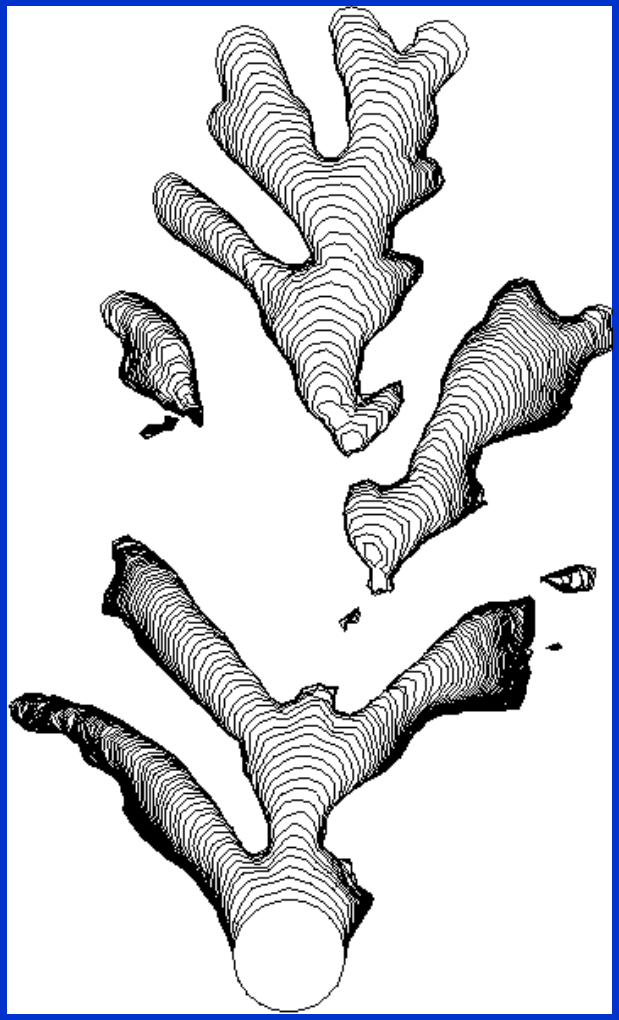
Diffusion Limited
Pe ~ 0
Fractal Dimension: 2.27 ± 0.05



Flow Dominated
Pe ~ 3
Fractal Dimension: 2.05 ± 0.05

Results: Branching without curvature rule

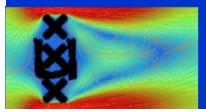




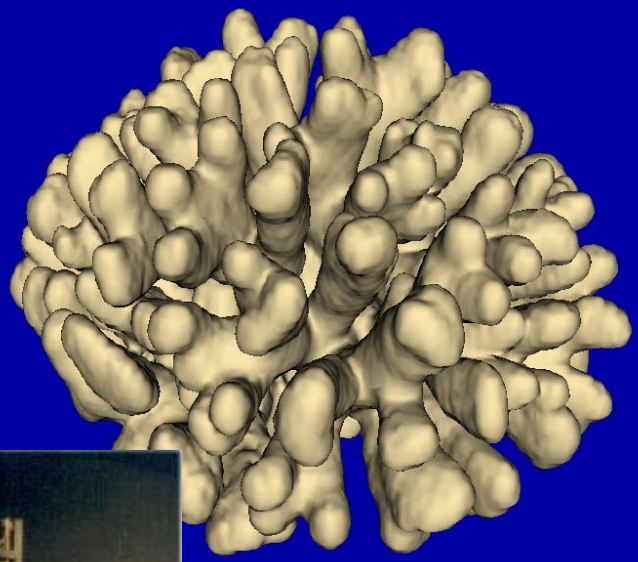
Combined Results

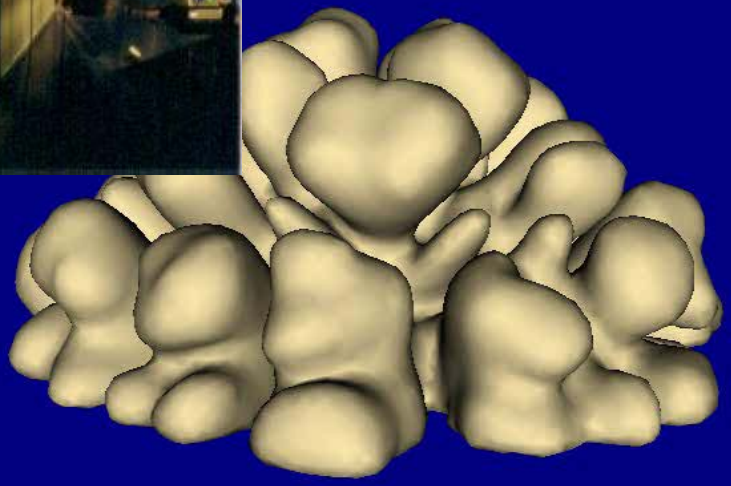
Madracis Mirabilis Scan

Madracis Mirabilis Sim

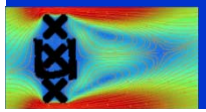


Turing test
Accretive growth model (diffusion limited conditions)
(Kaandorp, Sloot et al., Proc. Roy. Soc. Lond. B, 2004)





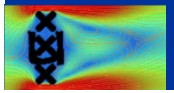
End



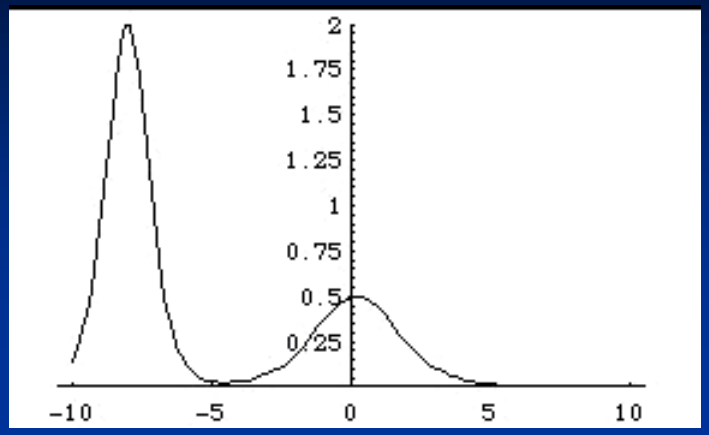
Solitons

- Localized waves
- Solutions to nonlinear PDE's
- Example: KdV: $u_t + u_{xxx} + 6uu_x = 0$

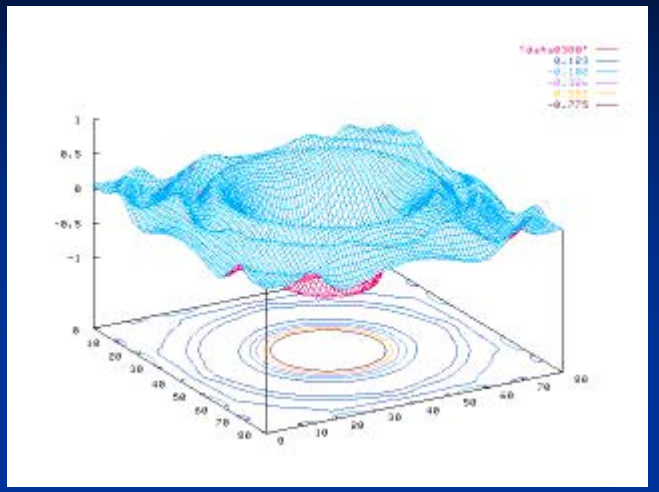
- Mma code solution two 1-D KdV



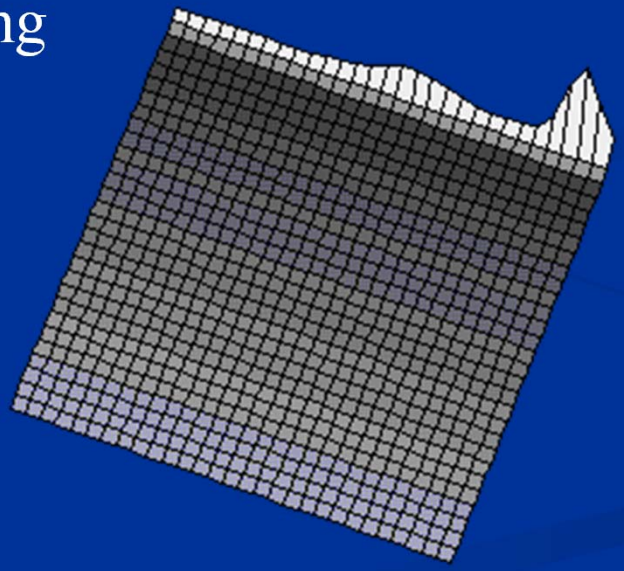
Soliton Animations



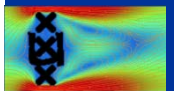
Two 1D Colliding

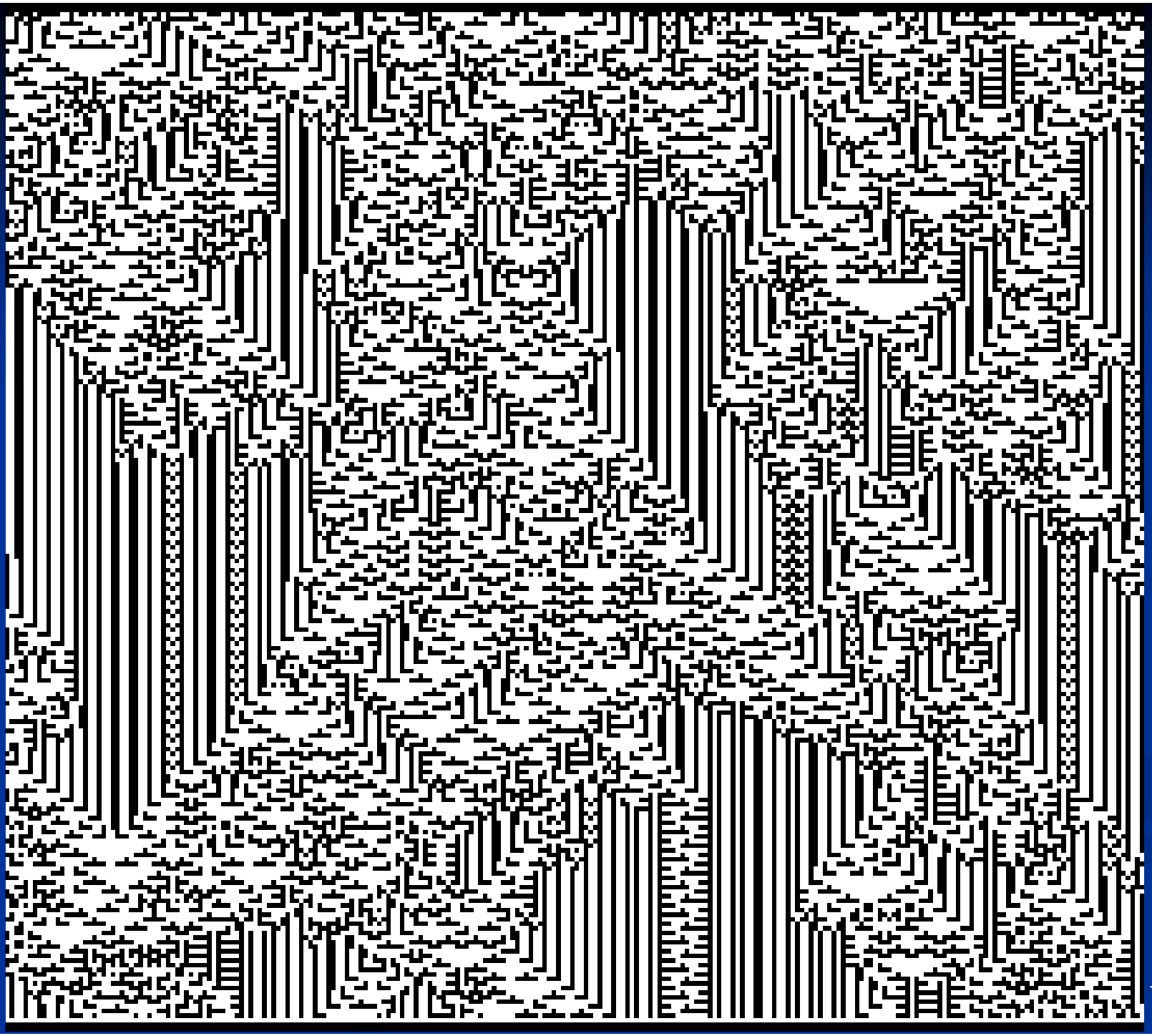


One 2-D



Two 2-D Colliding





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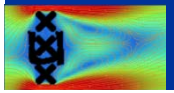

CA as Modeling Device

- Differential equations are usually discretized when modeled on a computer.
- Using CA-based models, we can start directly from a discrete system.
- Advantages of CA:
  - More convenient for simulations.
  - No numerical “approximations”.
- Disadvantage:
  - Finding a CA for a particular DE is not easy.