Application portfolio

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Outline

1. **Overview**
2. **Cellular automata in practice**
   - The Game of Life
   - Sharks and fishes
   - Soil-water flow
   - Thermodynamics
   - Epidemic modeling
   - Biological competition
   - Biofilm dynamics
   - Fish migration
   - Fungal growth
   - Chemical engineering
3. **References**

The Game of Life

- Conquest for a CA simulating life-like behavior
- Postulated by Conway in 1971
- 2D outer-totalistic CA based upon a square tessellation of $\mathbb{R}^2$
- $S = \{\text{alive, death}\}$

Transition function

- survival: if c_i surrounded by two or three living neighbors
- birth: death cell surrounded by 3 living neighboring cells
- death: as a consequence of isolation , if at most 1 neighbor is alive, or by competition if surrounded by at least four living neighboring cells

The Game of Life

- Conquest for a CA simulating life-like behavior
- Postulated by Conway in 1971
- Bio-inspired mathematical game
- 2D outer-totalistic CA based upon a square tessellation of $\mathbb{R}^2$
- $S = \{\text{alive, death}\}$

Transition function: mathematically

$$s\left(c_i, t+1\right) = \begin{cases} 1 & \text{, if } |\{c_j \in N(c_i) \mid s(c_j, t) = 1\}| = 3\,, \\ 0 & \text{, if } |\{c_j \in N(c_i) \mid s(c_j, t) = 1\}| \leq 1 \vee \\ & \quad |\{c_j \in N(c_i) \mid s(c_j, t) = 1\}| \geq 4\,, \\ s\left(c_i, t\right) & \text{, else}\,. \end{cases}$$

The Game of Life

Exemplary simulation

Simulation starting from a random initial condition on a 100×100 grid

Wa-Tor

- Developed by Dewdney in 1984
- Mimics the interplay between sharks and fishes
- See demo

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CA approach

- 2D outer-totalistic irregular CA
- rule representing gravitational displacement of water

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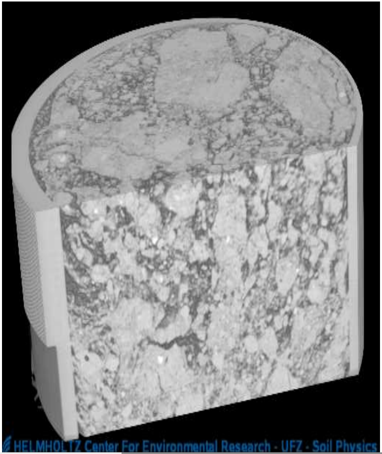


CCA for 2D heat flow

$$T(c_i, t+1) = \sum_{c_j \in N(c_i)^*} \frac{T(c_j, t)}{w_{ij}},$$

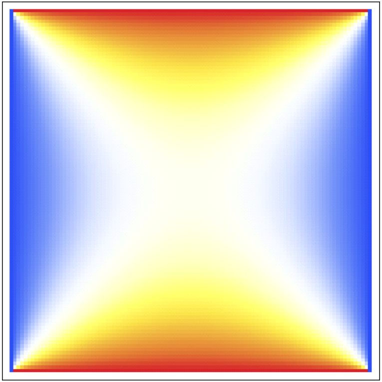
where $N(c_i)^* = N(c_i) \setminus \{c_i\}$ and

- $T(c_i, t)$: temperature in cell c_i a the t-th time step
- w_{ij}: proportion of c_i's circumference shared with c_j

- steady-state solution approaches the solution of the Laplace equation
- differences in material properties such as thermal conductivity can be incorporated
- irregular tessellations can be employed
- see demonstration

CCA for 2D heat flow

Heating a room



CML

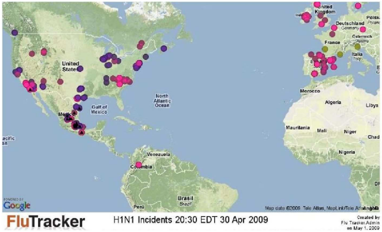
PDE

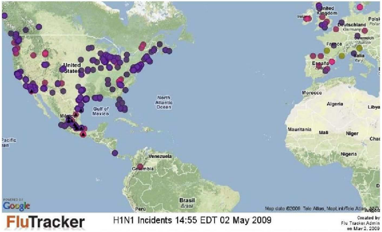
Justification

- throughout history epidemics have played an important role
- epidemics have led to
  - millions of casualties
  - increased health care expenses
  - panic
- not restricted to humans
  - cattle: blue tongue, foot-and-mouth disease
  - plants: Dutch elm disease
  - insects

Epidemic dynamics

- Mainly focus on temporal dynamics in a well-mixed population
- Though, also intriguing spatial dynamics
  - populations are not well-mixed
  - in a globalized world: individuals are highly mobile
  - factors influencing disease spread are spatially heterogeneous





A CCA for epidemic spread (CASIR)

$$
\begin{cases}
S_i^{t+1} = S_i^t - S_i^t \sum_{c_j \in N(c_i)} w_{ij}\, H\left(\mathbf{E}_i, d_{ij}\right)\, U_j^t \\
U_i^{t+1} = I_i^t + S_i^t \sum_{c_j \in N(c_i)} w_{ij}\, H\left(\mathbf{E}_i, d_{ij}\right)\, U_j^t - r\, U_i^t \\
R_i^{t+1} = R_i^t + r\, U_i^t
\end{cases}
$$

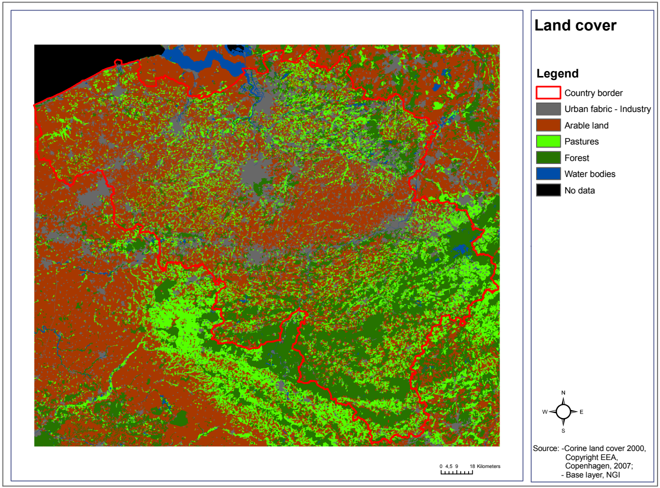
- population subdivided into three groups
  - S: susceptible
  - U: infected
  - R: recovered
- no population growth, nor decline, thus $S_i^t + U_i^t + R_i^t = \text{Cte}\,, \forall i, t$
- S, U and R are expressed as proportions of the total population in c_i
- $N(c_i)$: c_i's neighborhood
- w_{ij}: weighting coefficients

A CCA for epidemic spread (CASIR)

- $\mathbf{E}_i$: spatial information on c_i, *i.e.* 5 land cover classes
- d_{ij}: graph distance between c_i and c_j

A CCA for epidemic spread (CASIR)

- $\mathbf{E}_i$: spatial information on c_i, *i.e.* 5 land cover classes



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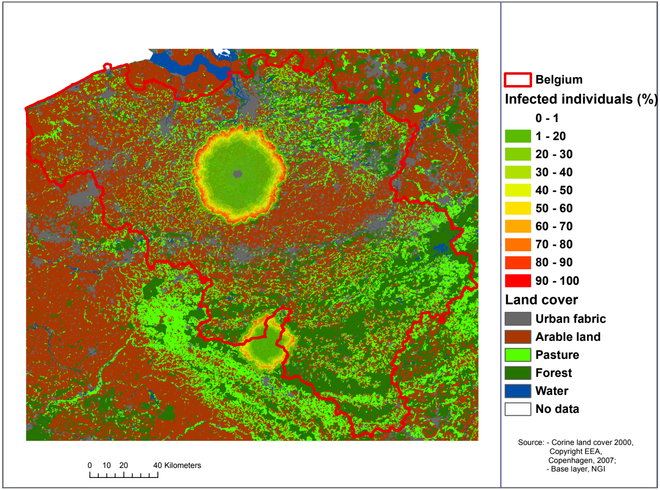
- $\mathbf{E}_i$: spatial information on c_i, *i.e.* 5 land cover classes
- d_{ij}: graph distance between c_i and c_j

$$H(\mathbf{E}_i, d_{ij}) = H(\mathcal{C}_i, d_{ij})$$

land cover	d_{ij}	
	0	1
urban	$\nu_{u,0}$	$\nu_{u,1}$
arable land	$\nu_{a,0}$	$\nu_{a,1}$
pasture	$\nu_{p,0}$	$\nu_{p,1}$
forest	$\nu_{f,0}$	$\nu_{f,1}$
water body	$\nu_{w,0}$	$\nu_{w,1}$

Model simulations

Model simulations



Dealing with uncertainty

impreciseness in

- severity initial outbreak
- transmittability

thus S , U and R are intervals in $[0, 1]$

- does not complicate the CCA simulation
- less computational demanding than a probabilistic approach, e.g. Monte Carlo

Model simulation

Vaguely known initial severity

- virulence known
- number of initially infected individuals in c_m only vaguely known:

$$U_j^0 = \begin{cases} [0.2, 0.4] & , \quad \text{if } j = m\,, \\ [0, 0] & , \quad \text{else}\,. \end{cases} \tag{1}$$

Model simulation

What about the uncertainty?

Wider applicability and perspectives

the generalized model can be used to describe several spatio-temporal diffusion phenomena

- forest fires
- biological invasion
- tumor growth
- urban growth

Perspectives

- sensitivity analysis
- model and/or parameter identification
- validation

Competition

- omnipresent in ecosystems
- evolution theory: survival of the fittest
- trade-off between
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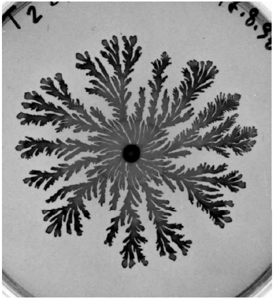

Paenibacillus dendritiformis

Competition

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- evolution theory: survival of the fittest
- trade-off between
  1. local interactions that depend on the species distribution in space: striking spatio-temporal patterns may evolve
  2. migration of micro-organisms through space: mixing effect annihilating the effect of species distribution
- biodiversity negatively correlated with the rate of migration
- critical migration threshold ϵ_{crit} above which biodiversity gets lost
- has been described through PDE, IBM and CA

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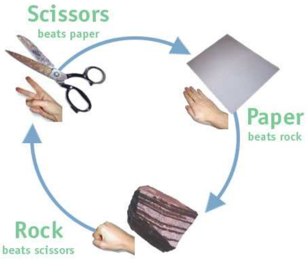
Simulating competition

- inspired on the rock-paper-scissors game
- cyclic dominance



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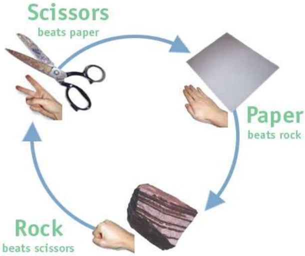

Simplifying assumptions

- three subpopulations: A, B, C
- square grid, $N \times N$ cells
- environmental conditions discarded

Mechanisms of life

- reproduction (μ)
- selection (σ)
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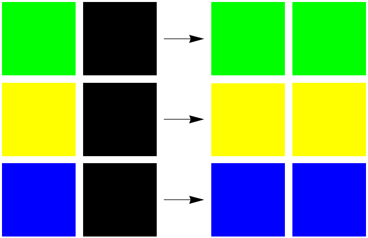

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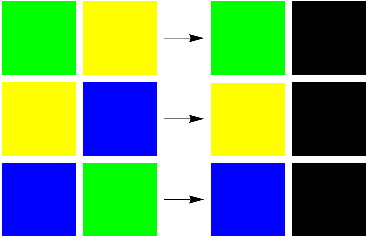

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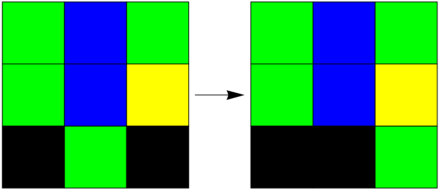

Mechanisms of life

- reproduction (μ)
- selection (σ)
- migration (ϵ)

Algorithm

initialization: individuals randomly arranged on the lattice;
foreach *time step t* **do**
  Select at random one cell c_i;
  Randomly pick one of c_i's neighbors c_{i_j};
  Perform selection, reproduction or migration conform presupposed rates;

Simulation experiments

Set-up

- $N \times N$ cells
- initial population density: 0.25 A, 0.25 B, 0.25 C, 0.25 ■, 0 □

Simulation experiments

$\epsilon < \epsilon_c$

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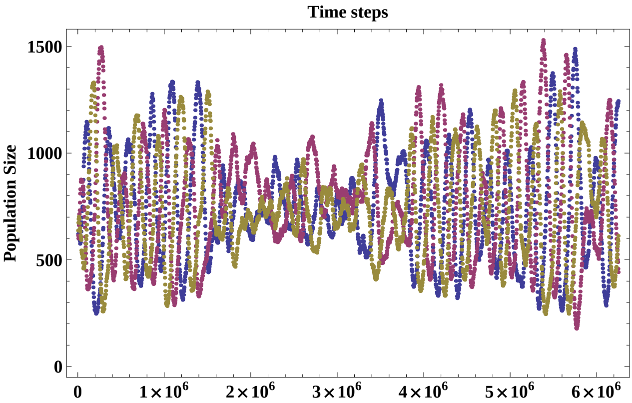

Simulation experiments

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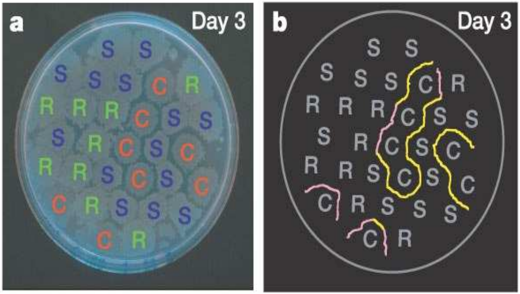

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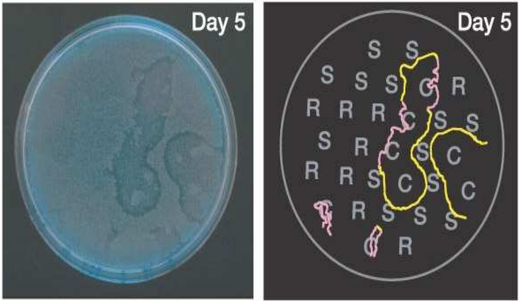

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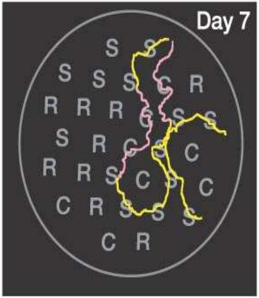

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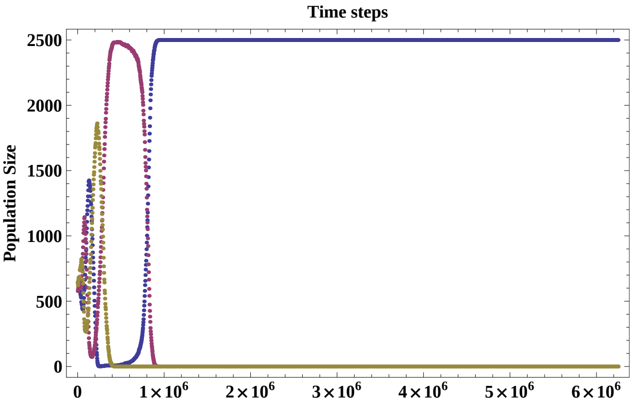

Continuum limit

- distance between cells δx decreases as $N \uparrow$
- in the continuum limit $\delta x \to 0$ as $N \to \infty$
- gives rise to a stochastic PDE

A biofilm

- a cluster of microorganisms
- adhered to each other and/or to a surface
- embedded in an extracellular polymeric substance
- omnipresent: bioreactors, hulls, pipes, soil, . . .

A biofilm

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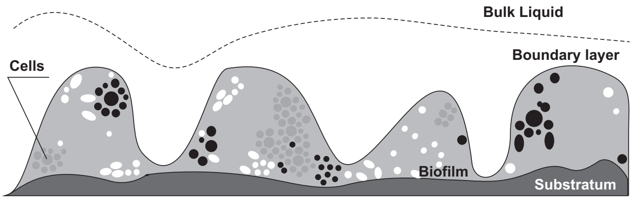
Processes of concern

- substrate diffusion
- substrate consumption
- microbial growth
- attachment and detachment



CA-Film

Historical background

- CA introduced in 1992 by Colasanti for coping with heterogeneity
- elaborated in the nineties by Wimpenny & Colasanti, Picioreanu et al. and others
- 2D or 3D, pure CA or hybrids (CA-PDE)

Model setup

- hybrid CA-CCA model
  - microbial growth: stochastic CA
  - substrate diffusion: CCA
- square or irregular tessellation
- attachment and detachment to be incorporated
- environmental conditions steer the microbial growth process
- model parameters embody environmental conditions

Substrate diffusion

- described by a CCA:

$$S(c_i, t+1) = \sum_{c_j \in N(c_i) \setminus \{c_i\}} \frac{S(c_j, t)}{w_{ij}}$$

- similar to the model for 2D heat flow (diffusion)
- steady-state solution approaches the solution of the Laplace equation

Microbial growth

in every time step

1. substrate availability in each cell c_i is checked
2. according to the substrate availability one cell is picked to split
3. new cell is placed in the neighboring lattice site which has the highest substrate availability

stochasticity involved through (2)

Substrate utilization

- growth
  - substrate originating from $N(c_i)$
  - cover biomass increase due to growth
- maintenance
  - substrate from c_i
  - cover the cell's energy consumption for maintenance

Simulation experiment

Setup

- impermeable surface at $x = 0$
- bulk fluid at $x = L$
- homogeneous substrate concentration
- initial colonization on the surface

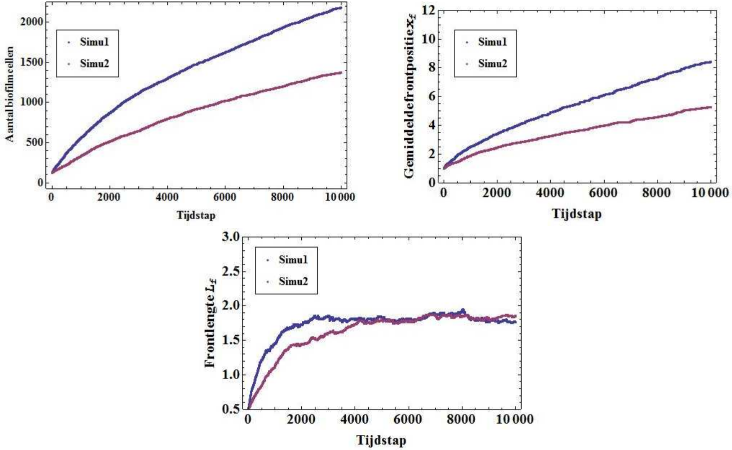
Simulation experiment

Optimal environmental conditions

Simulation experiment

Suboptimal environmental conditions

Simulation experiment



Simulation experiment

Optimal environmental conditions

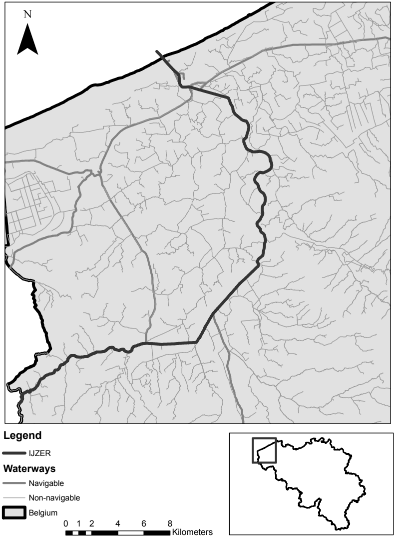
Motivation

- northern pike (*Esox lucius* L.) populations in Belgium suffer from habitat deterioration
- restoration programs not successful
- insight into the spatio-temporal distribution of pike required
- tracking of species is costly and labour-intensive
- simulation-based approach is a worthy alternative

development of a discrete model for mimicking the spatio-temporal dynamics of northern pike in the river Yser.

Northern pike

- solitary predator
- study area



northern pike

- solitary predator
- study area
- three distinct seasons during a one year's cycle
  1. spawning season: March-May
     - migration towards spawning grounds
     - not limited to territory
  2. passive sedentary season: May-December
     - sit-and-wait strategy
     - home range: 50 m
  3. active sedentary season: December-March
     - home range: 200m
     - territory

Simulation

Link to local file

Introduction

Importance of fungi

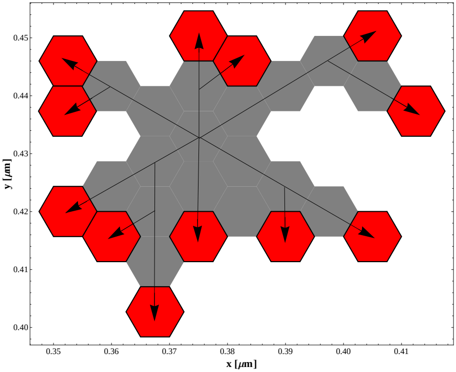
- degradation processes
- symbiosis
- crop failure
- production of antibiotics, citric acid
- ...

Model organism

- *R. solani*
- soil fungus
- develops a hyphal network

Modelling approach

- two-dimensional
- hexagonal cells
- fungus grows along the cells' diagonals
- Δt steered by CFL-condition and maximum probability
- Δx = diameter of the hyphae



Simulation

Introduction

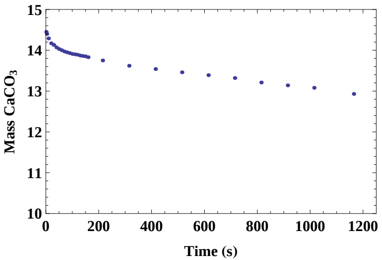
- numerous CA-based models developed
- mostly only qualitative agreement between observed and simulated process
- validity doubtful
- chemical processes of interest
  - arbitrary chemical reactions: stochastic CA
  - diffusion processes: CCA
  - clock reactions: cyclic CA

Chemical reactions

- 2D/3D CA simulating chemical reactions at molecular level
- no homogeneity assumption required
- stochastic nature: reaction probabilities
- can be traced to macroscopic reaction rates

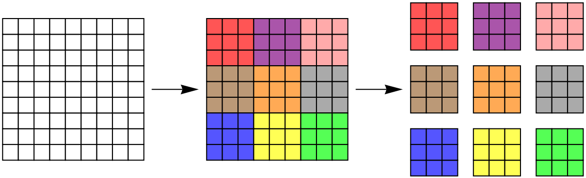
Exemplary reaction

$$CaCO_3(s) + 2\,HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$



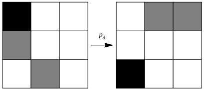
CA-based model

- stochastic CA
  - square tessellation
  - Moore neighborhood
  - states: HCl (gray), $CaCO_3$ (black) and H_2O (white)
  - initial condition: state according to the molar ratios of the reactants and water in the experiment
- block CA paradigm
  - step 0: splitting

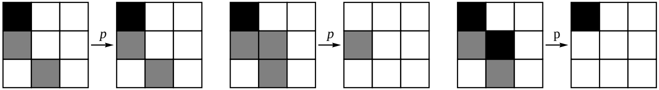


CA-based model

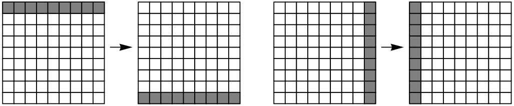
- block CA paradigm
  - step 1: diffusion



  - step 2: reaction



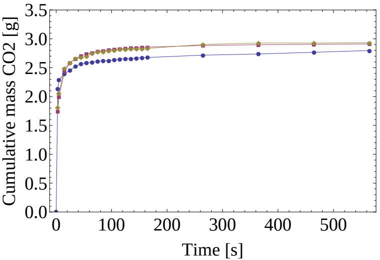
  - step 3: shuffle



Chemical reactions

Parameter optimization

- goal: tuning the model parameter(s) such that discrepancies between model output and observed data are minimized
  - model output: simulated loss of $CaC0_3$ molecules
  - observed data: time series of $CaC0_3$ loss
- particle-swarm optimization
- Pearson correlation coefficient higher than 0.95



Diffusion processes

- microscopic level: CA
  - stochastic
  - requires asynchronous updating or block CA to assure conservation of mass
  - computationally demanding
- mesoscopic level: CCA
  - formulation similar to CCA for heat flow
  - steady-state solution approaches the outcome of the Laplace equation
  - less computationally demanding

ISI papers

Baetens J. M. and B. De Baets.
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P. Van der Weeën, J. M. Baetens, J. Verwaeren, X. Van Doorslaer, P. M. Heynderickx, J. Dewulf, and B. De Baets.
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On the topological sensitivity of cellular automata.
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P. Van der Weeën, J. M. Baetens, and B. De Baets.
Design and parameterization of a stochastic cellular automaton describing a chemical reaction.
Journal of Computational Chemistry, 32:1952–1961, 2011.

J. M. Baetens and B. De Baets.
Phenomenological study of irregular cellular automata based on Lyapunov exponents and Jacobians.
Chaos, 20:033112, 2010.

Wolfram Demonstrations

- Heat flow model
  http://demonstrations.wolfram.com/ACellularAutomatonBasedH
- Greenberg-Hastings model
  http://demonstrations.wolfram.com/GreenbergHastingsModel/

More information?

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