Introduction to individual-based modelling: Spatio-temporal models

14 January 2022 FindingPheno course

Gergely Boza

Institute of Evolution, Centre for Ecological Research (CER), Hungary.

Cooperation and Transformative Governance Group, Advancing Systems Analysis (ASA) Program, IIASA.

Centre for Social Sciences, ELKH, Hungary.

Contents

- The basics of modelling.
- Components of ABMs/IBMs.
- A little history of ABMs/IBMs.
- Examples (from simple to complex models).
- Challenges and future directions.

Phenomenological (statistical) models:

The purpose is to **characterize** a pattern or a phenomena,
to demonstrate the **relationships** between the relevant variables.

Top-down

↕

Bottom-up

Mechanistic models:

The purpose is to understand the underlying **dynamics**, the **processes** and the **mechanisms** that lead to a sort of collective behavior the emergence of a studied pattern or a phenomena.

Models can be:

- Scale models: smaller versions of the target displaying reduction in size and systematic reduction in the level of detail and complexity.

- **Toy models**: some characteristics of the target are extremely simplified in order to allow a deep control of the model.

- Analogical models: based on an analogy between the target system and a better understood phenomenon.

(Gilbert 2008)

A model is „an ultimate way of asking an isolated (specific) scientific question” JNP

$$\frac{dx}{dt}$$

dx ← how a prey population...

dt ← ...changes over time

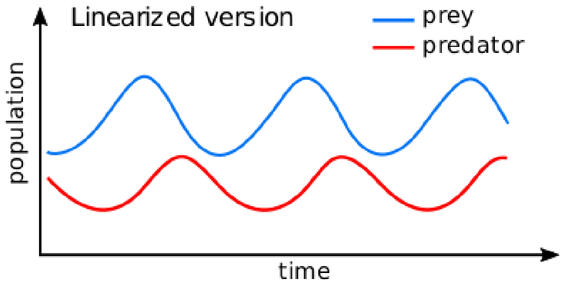
Model

Dependent variables

prey population (x)
predator population (y)

Independent variables

predation rate (β)
consumption rate (γ)
death rate (δ)
growth rate (α)



Lotka–Volterra (predator–prey) model: $\frac{dx}{dt} = \alpha x - \beta xy \qquad \frac{dy}{dt} = \gamma xy - \delta y$

Differentiating groups/ subpopulations

Model

preys ($x_1, x_2, x_3, x_4, \dots, x_N$)

predators ($y_1, y_2, \dots, y_N$)

Dependent variables

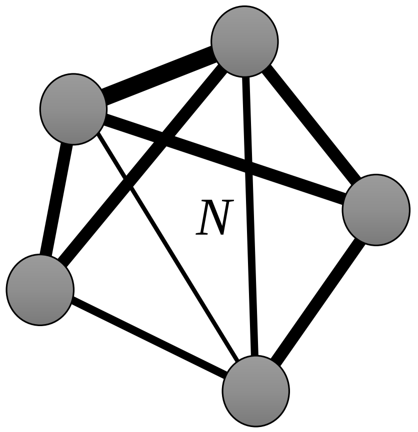
predation rate (β)

consumption rate (γ)

death rate (δ)

growth rate (α)

Independent variables



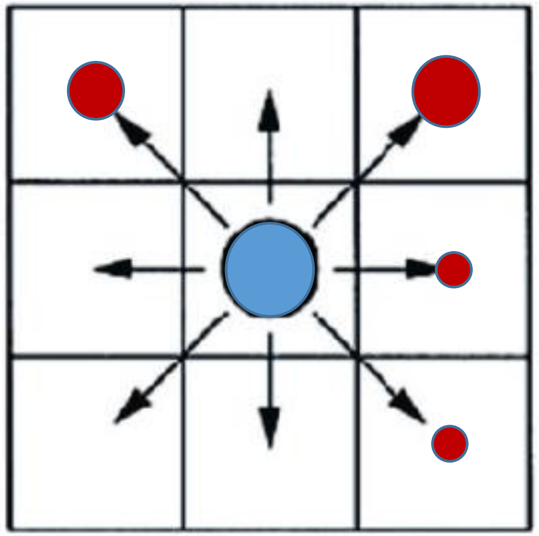
dispersal rate

Differentiating individuals **OR** adding complex population structure

Model

Prey 1; α_1
Prey 2 ; α_2
Prey 3 ; α_3
Prey 4 ; α_4

Predator 1; δ_1; γ_1
Predator 2; δ_2; γ_2
Predator 3; δ_3; γ_3
Predator 4; δ_4; γ_4



A(I)BM

Agent-based models

Agent-based modeling is a computational method that enables a researcher to **create**, **analyze**, and **experiment** with models composed of agents that interact within an environment.

A form of computational science aiming to capture the essence of the studied system by retaining the fundamental ingredients built in a simplified system with which we can study the specific questions and problems.

(Gilbert 2008; Macan 2010)

A quick terminology

- Humans, banks, companies, countries → **agent**-based models
- Biological entities → **individual**-based models
- Molecules, compounds, cells → **particle**-based models

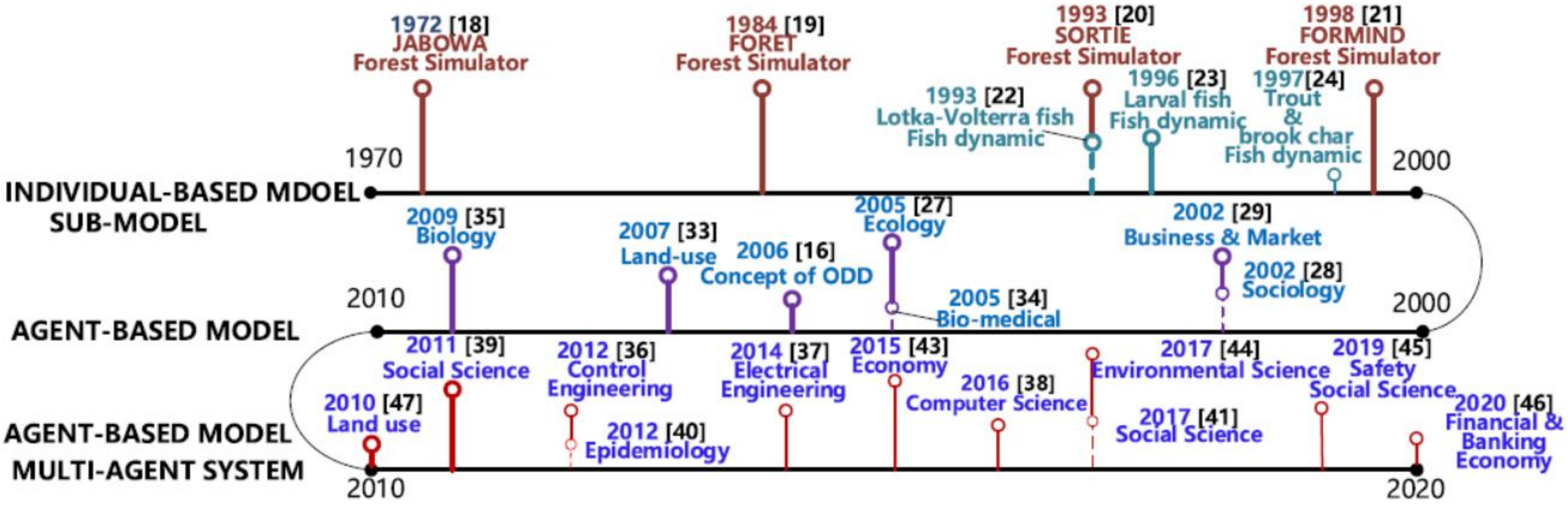
\+ Multi-agent models (interactions) ↔ Individual-based models (development)

\+ Multi-agent systems (complex adaptive systems)

\+ Intelligent agents (AI)

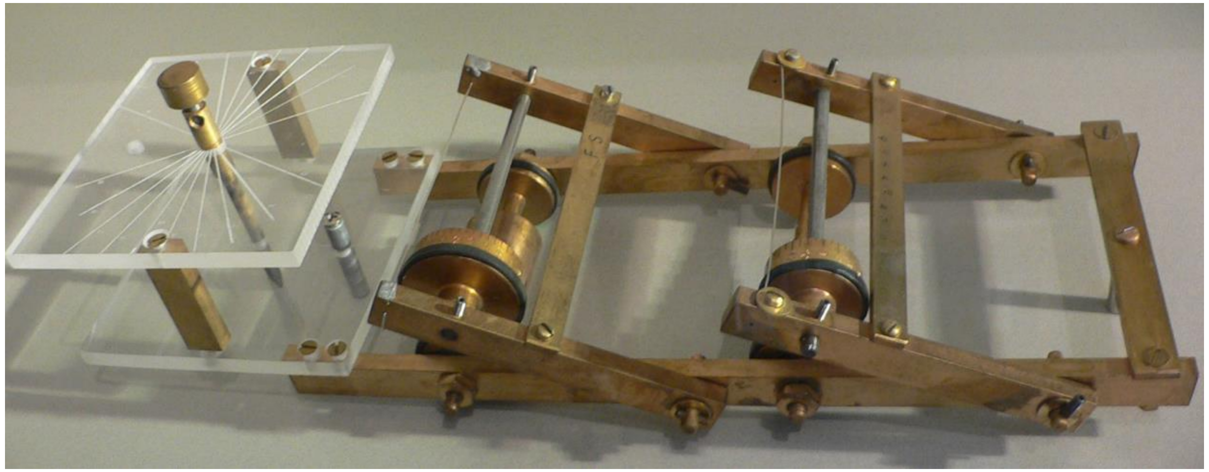
\+ Cellular Automaton (spatial)

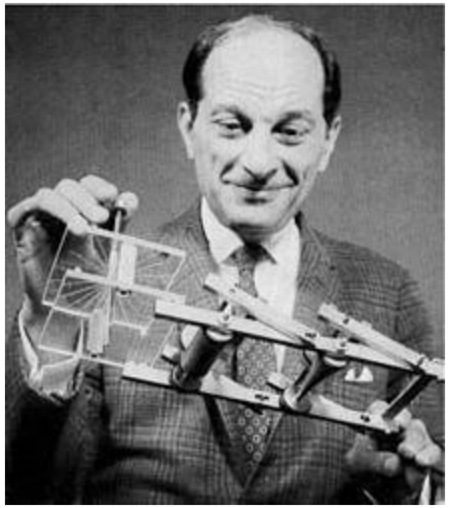
History of IBMs and ABMs

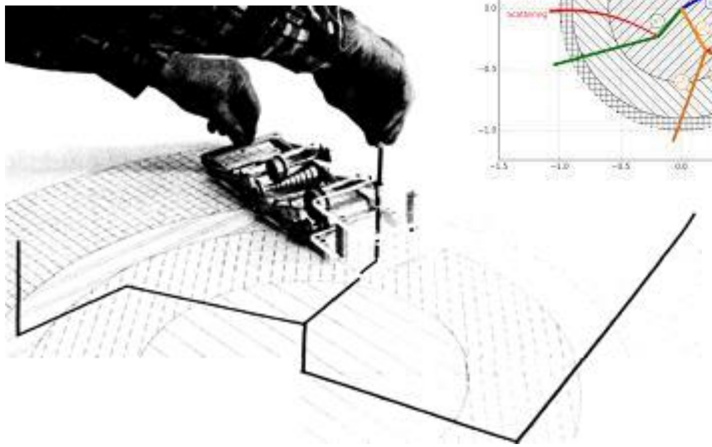


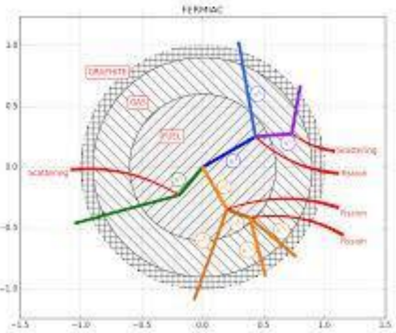
(Zhang et al. 2021)

ABM history: the first ABM and the Monte Carlo Method









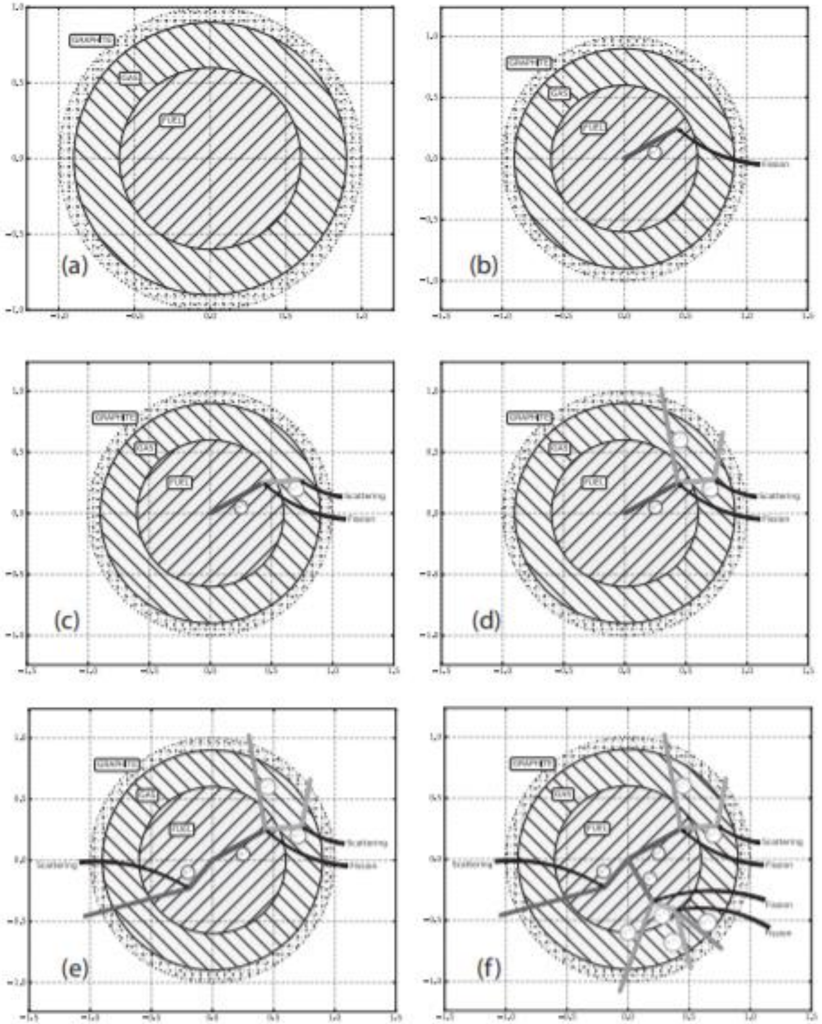
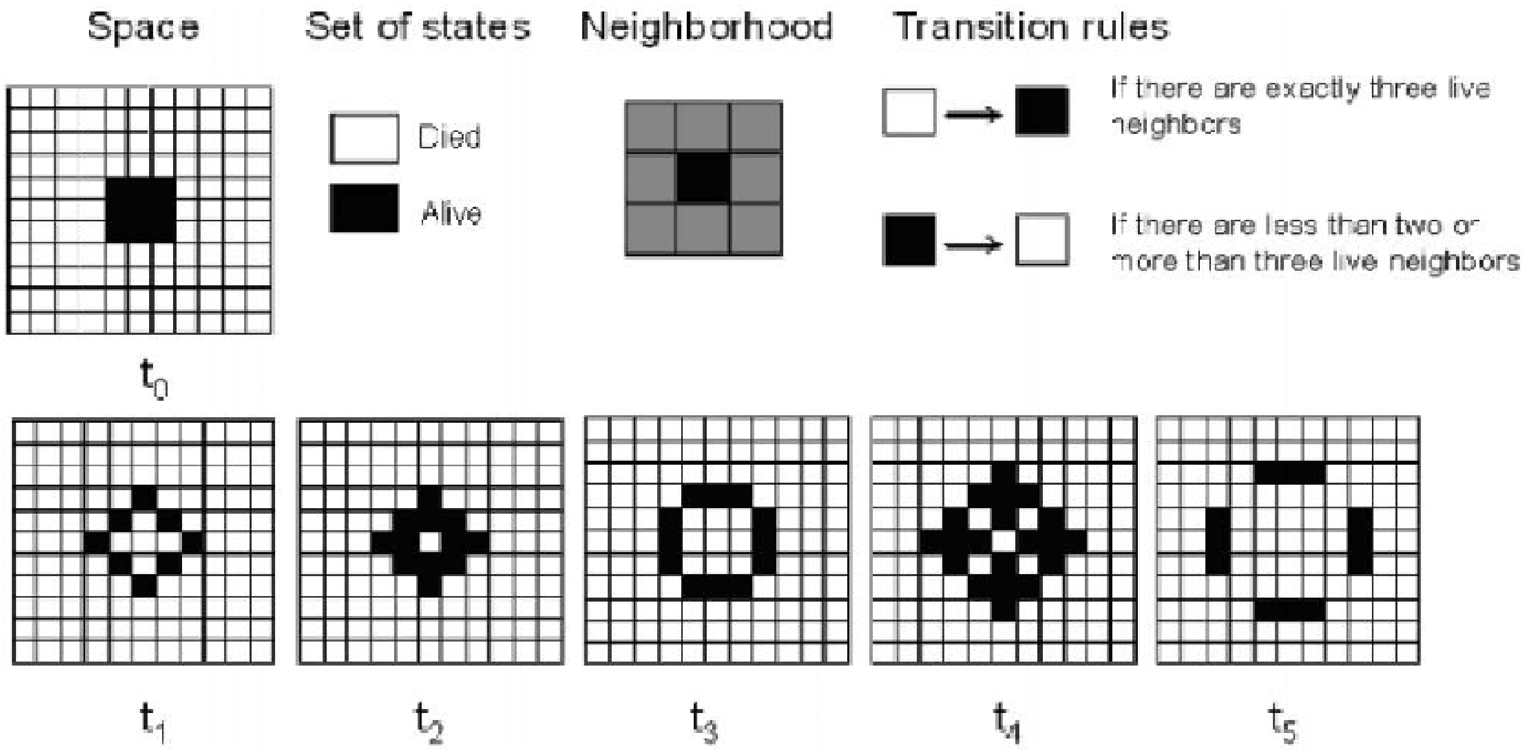


Fig. 6. – An example of the Fermiac used to follow the fate of the genealogy of source neutrons n^1, n^2, n^3 in a cell of a nuclear reactor.

(Coccetti 2016; Zhang 2021; wikipedia)

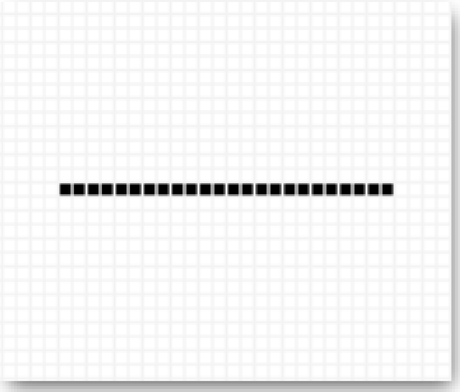
ABM history: The cellular automaton & Game of Life

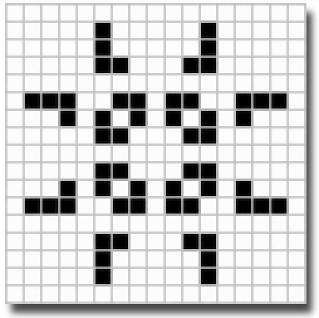
A cellular automaton is a collection of "colored" cells on a grid of specified shape that evolves through a number of discrete time steps according to a set of rules based on the states of neighboring cells.

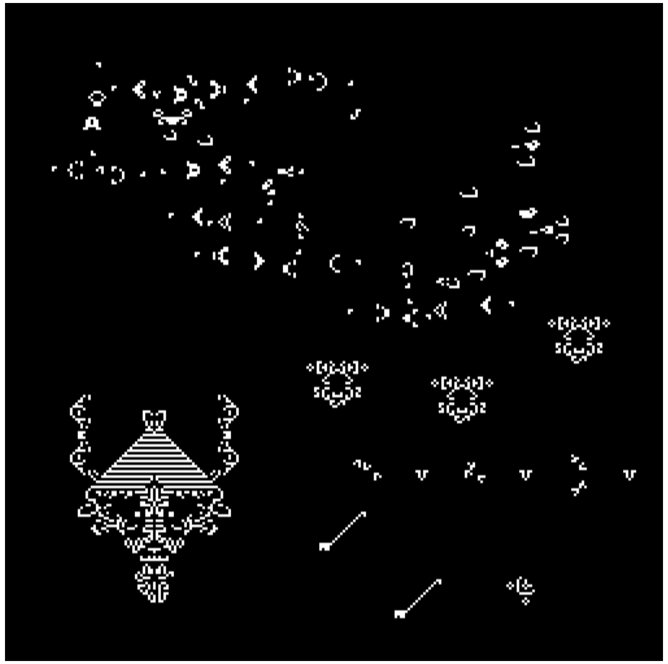


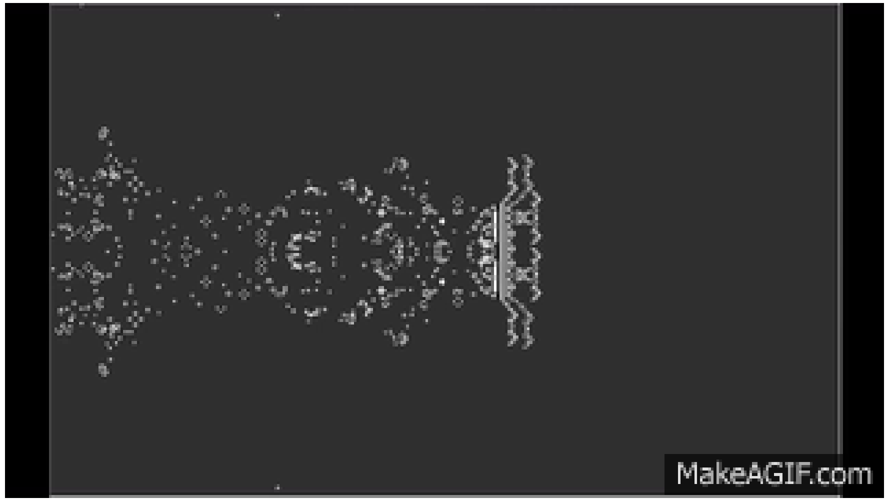
(Turing 1950; von Neumann 1951,1956; Conway 1970; Wolfram 1983; Wahyudi et al. 2015; macleans.ca)

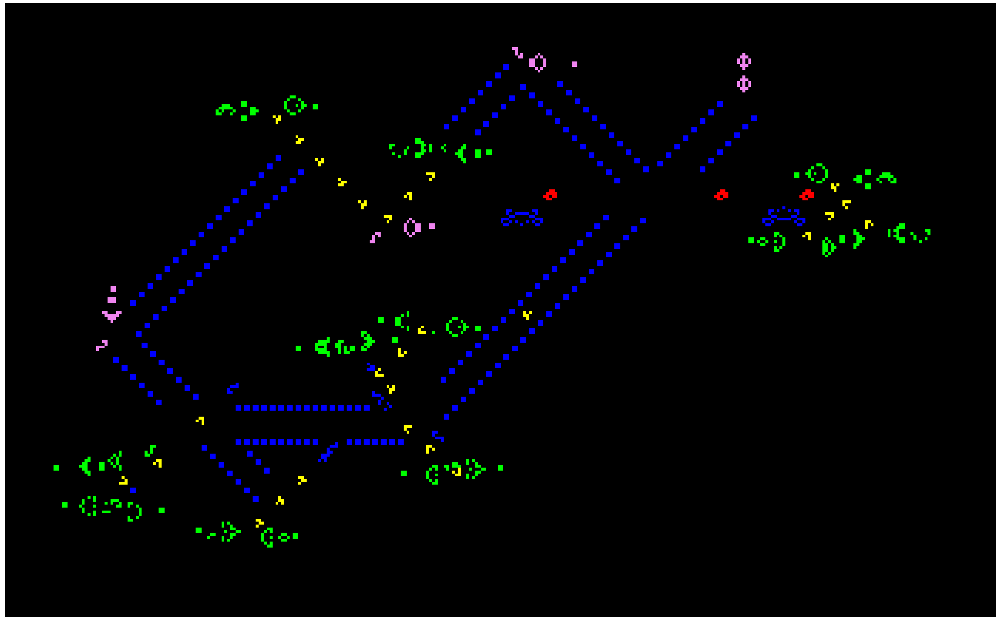
ABM history: CA & Game of life



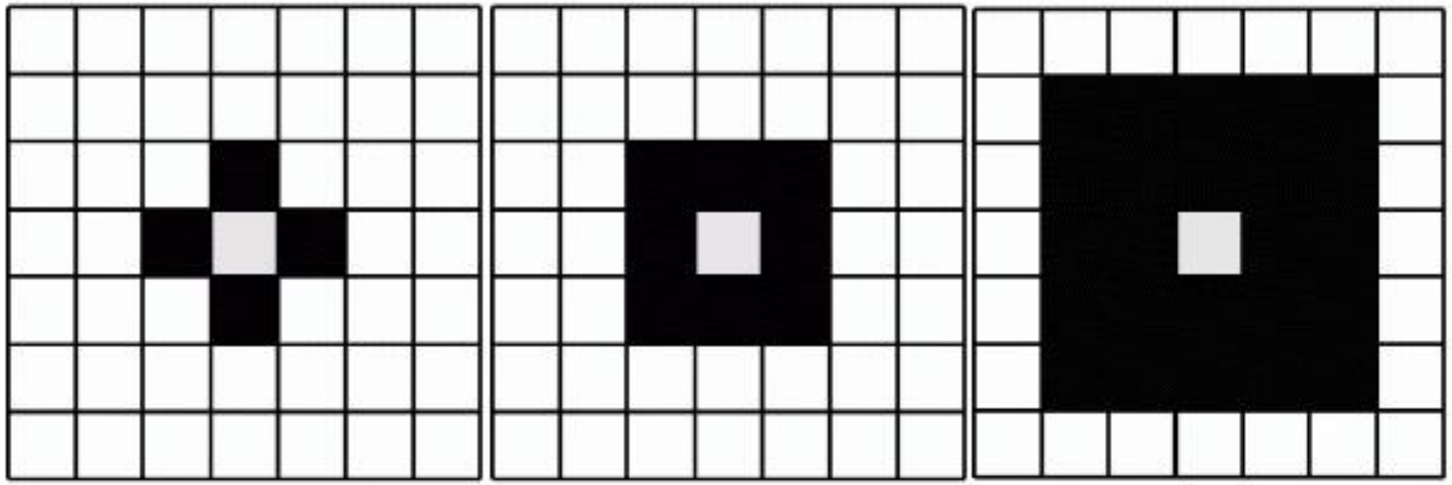






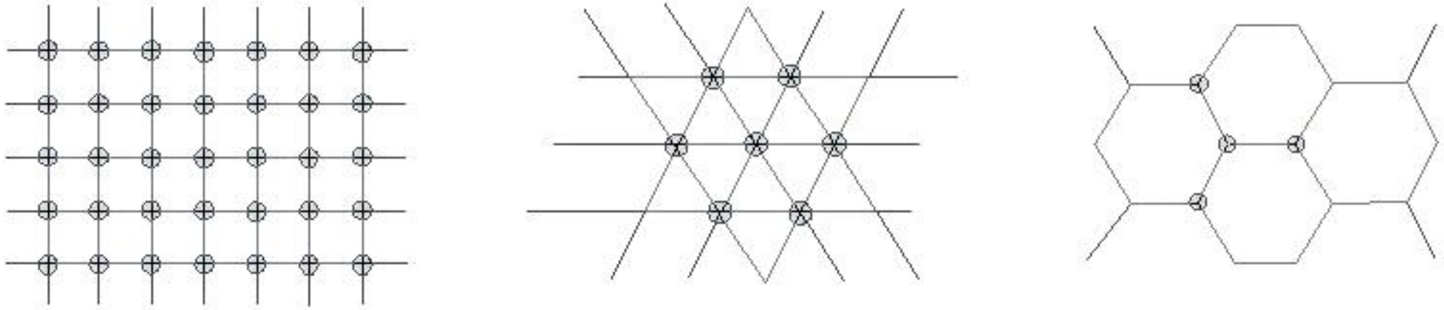


(commons.wikimedia.org; mathoverflow.net)



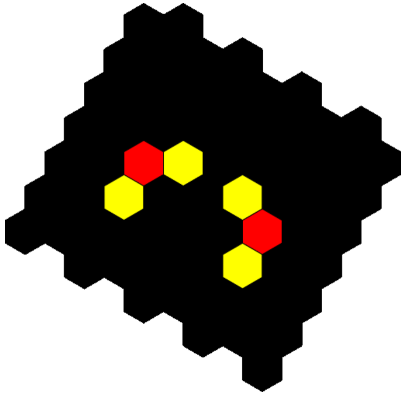
von Neumann Neighborhood | Moore Neighborhood | Extended Moore Neighborhood

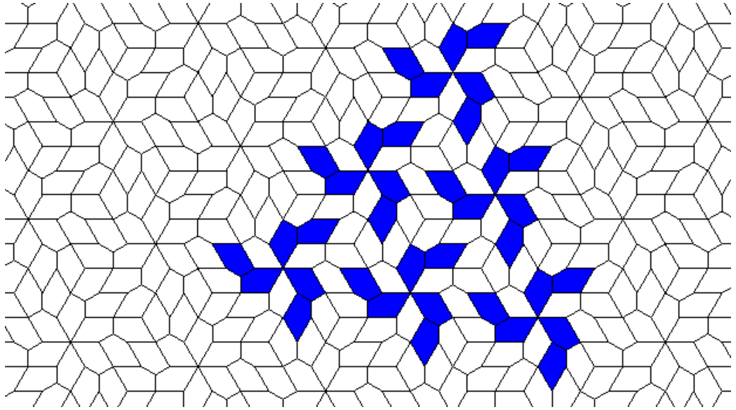
Two-dimensional Lattice Configurations

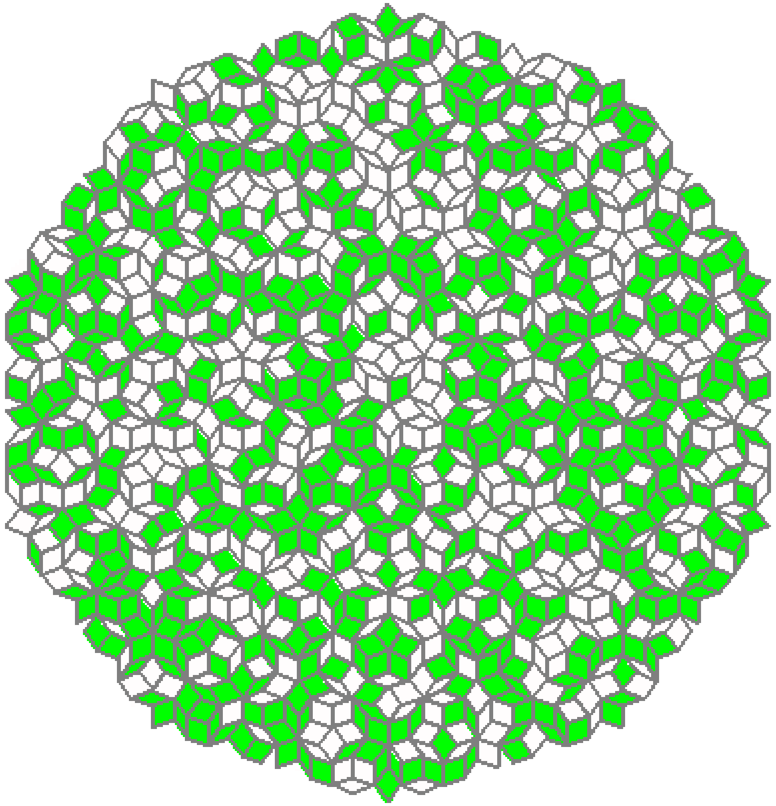


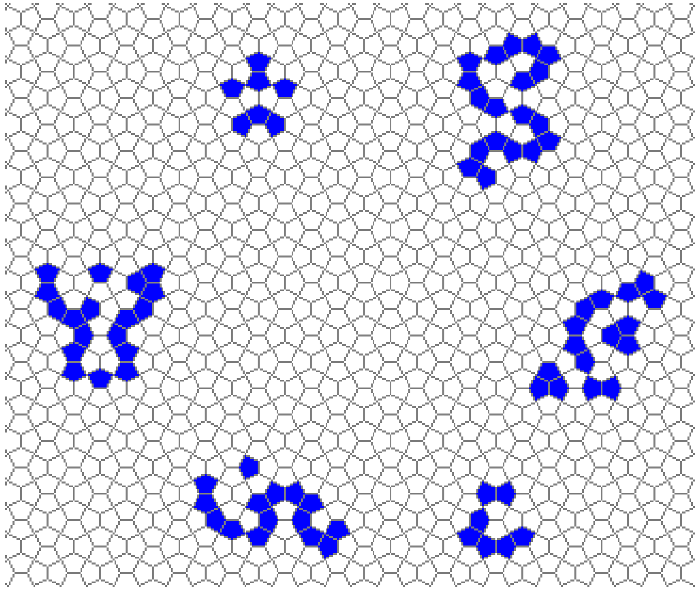
Rectangular | Triangular | Hexagonal

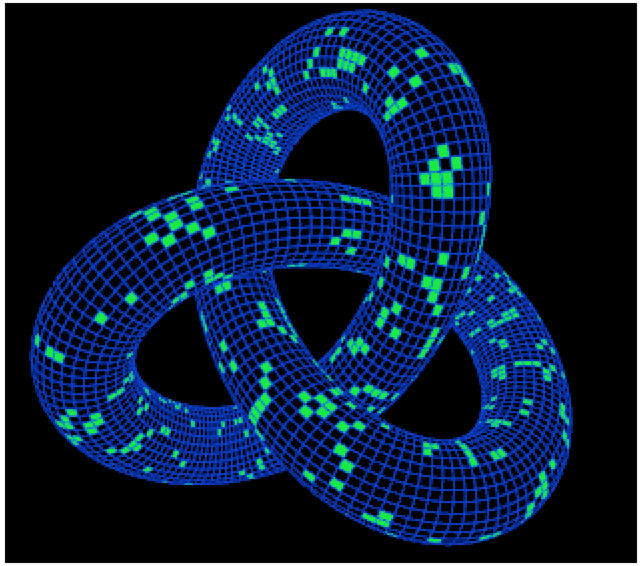
ABM history: CA & Game of life





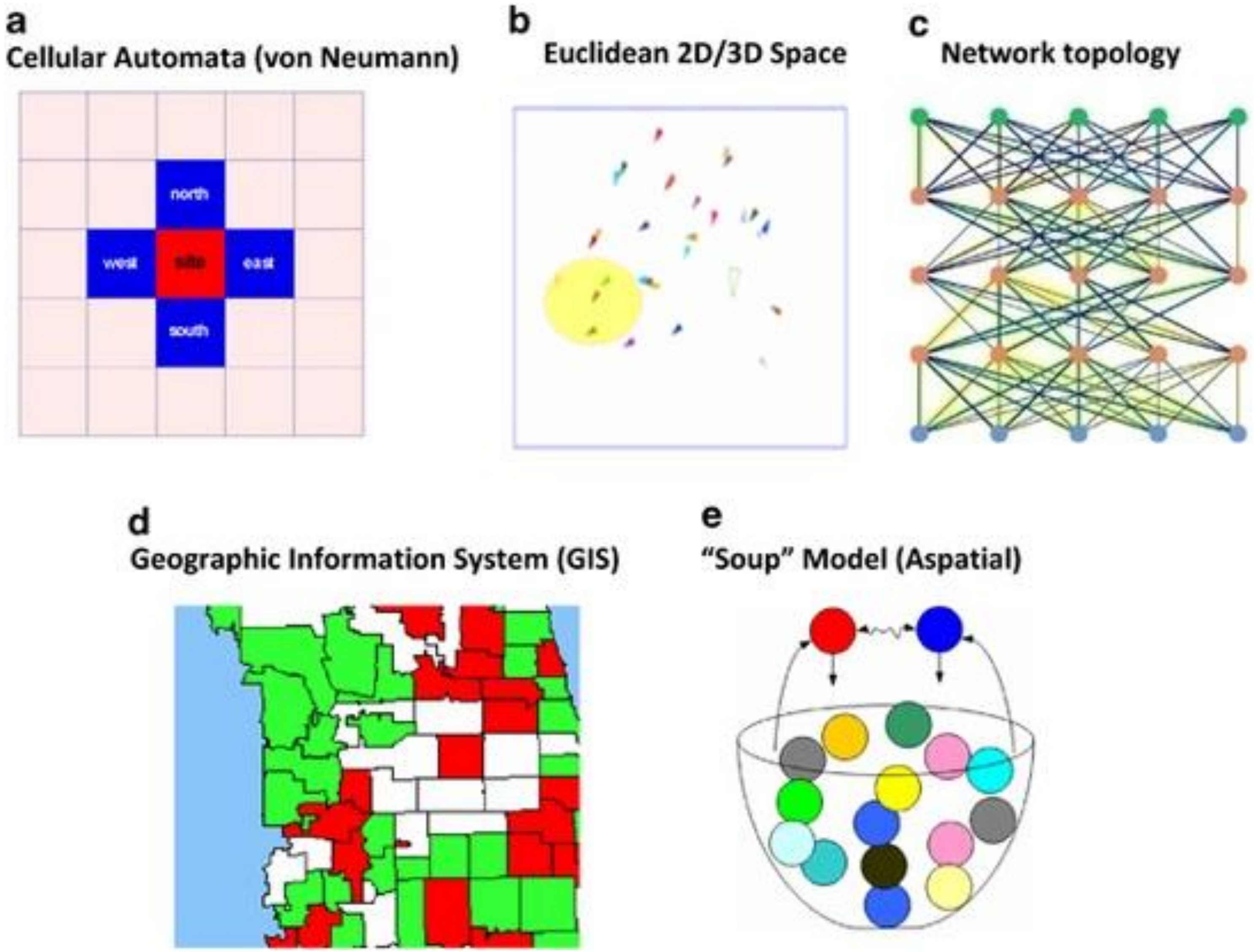






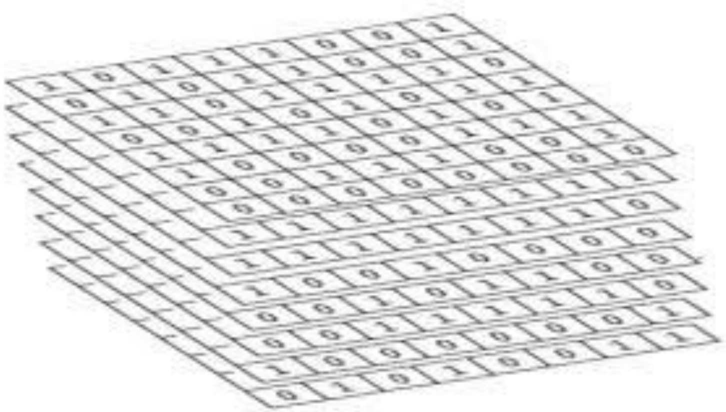
(commons.wikimedia.org; codegolf.stackexchange.com; newbedev.com)

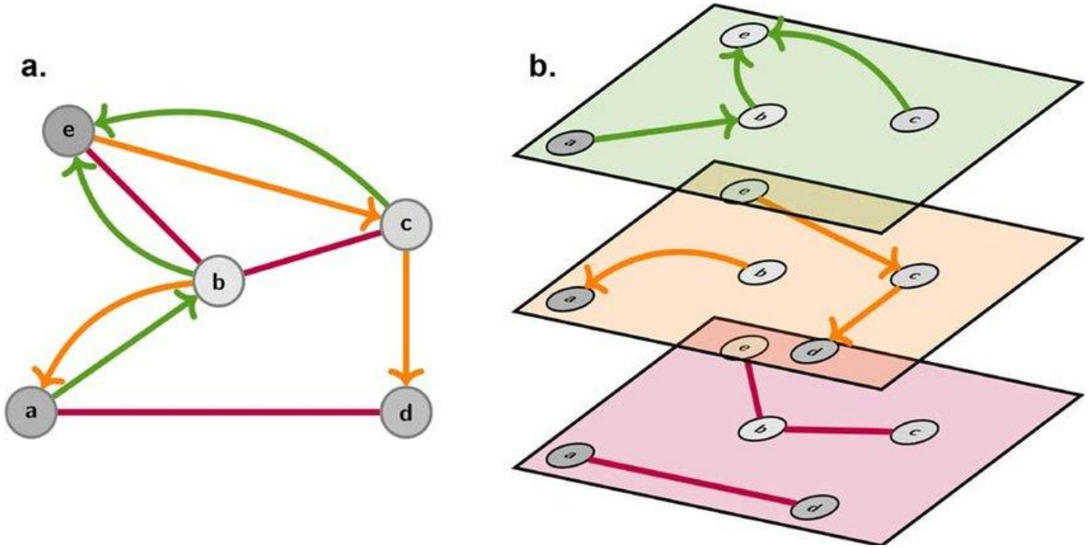
ABM fundamentals: topology, population structure

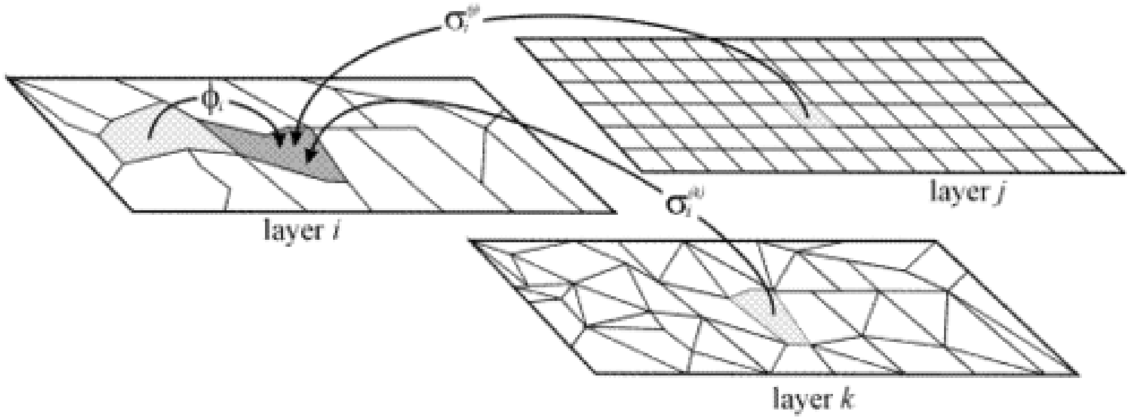


(Macan 2010)

Multi-layer ABM & heterogeneous layers

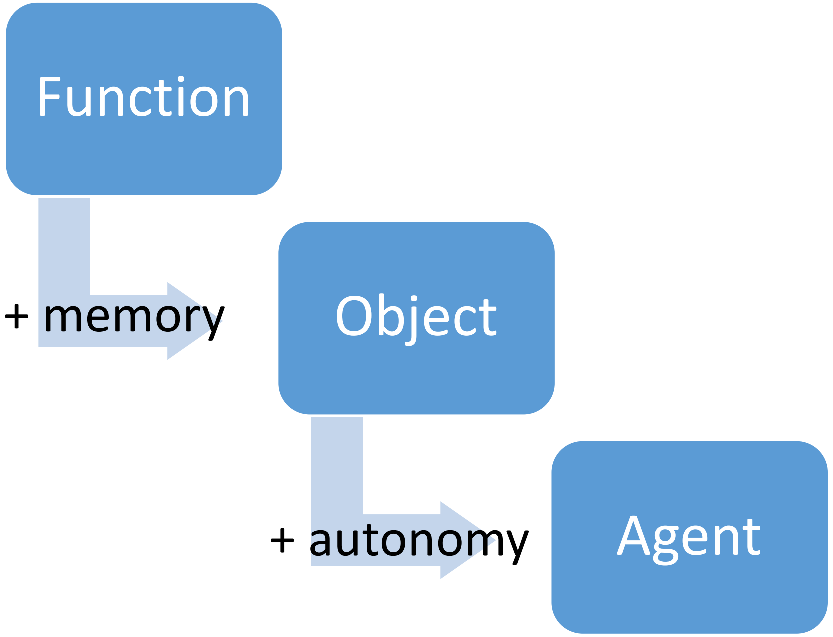






(Gaudlet 2021)

What is an *agent*?

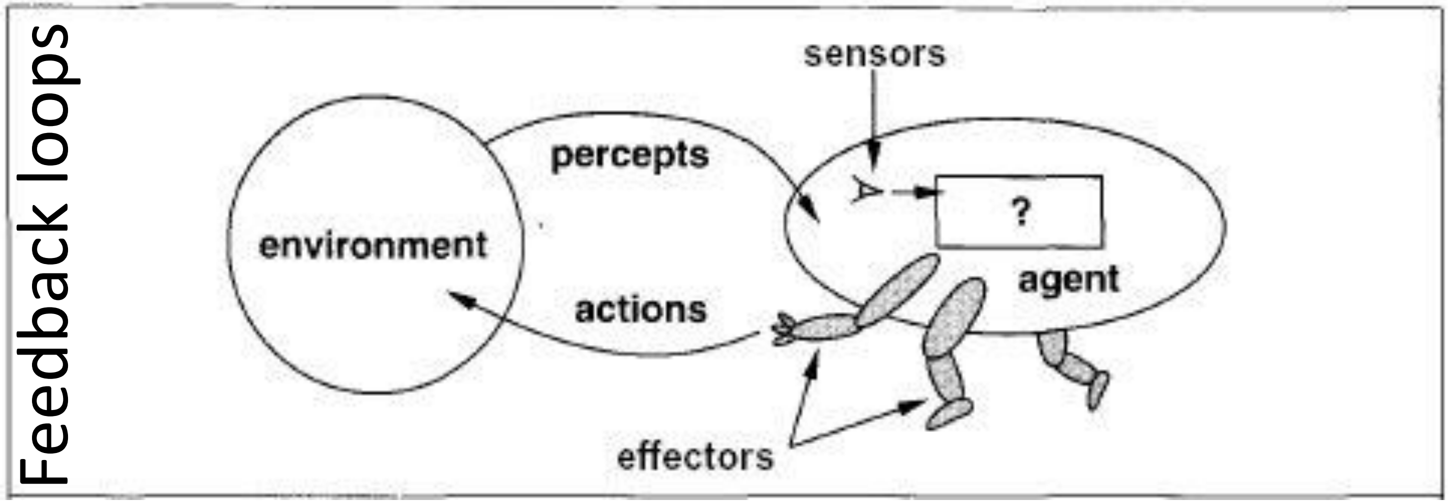


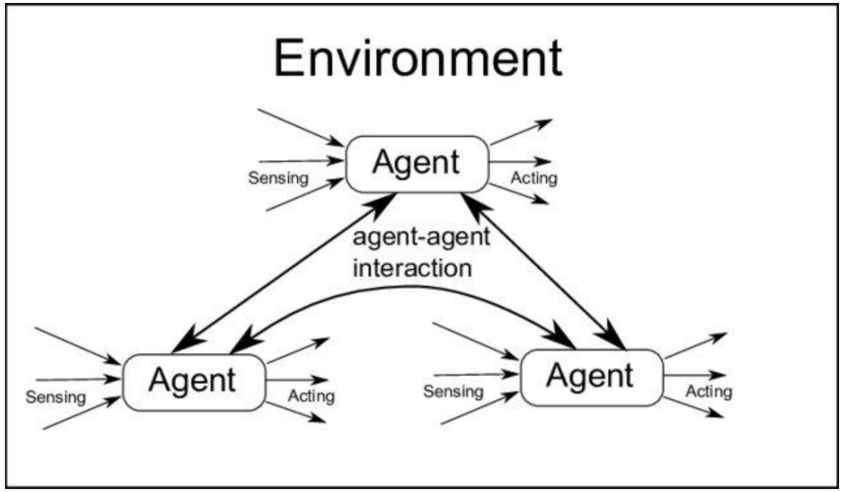
An agent:

- is **self-contained** and unique,
- is **autonomous** and self-directed, has behaviors,
- has a **state** that changes over time,
- is **social** having dynamic interactions;

They can also be:

- adaptive,
- goal-directed
- heterogeneous





(Bodea 2007; Macan 2010; Telgen 2017)

Main features of Agents

- Autonomy: simple decision rules
- Social ability: interaction between agents
- Reactivity: perceive stimuli from others or from the environment
- Proactivity: agents have goals

Main characteristics of Agents

- Perception: observe the environment and closeby agents
- Performance: react according to a set of behaviors
- Memory: storing information about a number of past states, actions
- Policy: a set of rules, heuristics, or strategies controlling their response based on the present situation also taking into account their past

More (potential) features for ABMs

- Large, closed systems
- Flexibility
- Modularity
- Tracking the behavior of each unit through time
- Dynamic system (dep. variables)
- Simple, mechanistic rules
- Agent heterogeneity (no representative agent)
- Bounded rationality, limited knowledge
- Agents have aims, objectives
- Interactions between the agents
- Shared environment
- Interaction/ population / environment structure
- Feed-back between the environment and the agents
- Adaptation, learning (evolutionary, individual, social, imitation)
- Linking different organizational levels
- Scale separation
- Stochasticity, randomness

ABM fundamentals: state (S) –rule (R) –input (I) architecture

$$A \sim (S,R);\ S = \{S^1, S^2, \ldots, S^k\};\ R: (S_t, I_t) \rightarrow S_{t+1}$$

The dynamics of ABM simulations

- Complex systems
- Stochastic symmetry breaking
- Emergent properties
- Non-equilibrium dynamics and outcomes
- Multi-stable systems, dependency of initial conditions, hysteresis effect
- Phase transitions, tipping points, self-organized criticality, critical phenomena, fat tail events

- Cheap experimenting, *in silico* labs

Designing an ABM

1 - What specific problem should be solved by the model? What specific questions should the model answer? What value-added would agent-based modelling bring to the problem that other modelling approaches cannot bring?

2 - What should the agents be in the model? Who are the decision makers in the system? What are the entities that have behaviours? What data on agents are simply descriptive (static attributes)? What agent attributes would be calculated endogenously by the model and updated in the agents (dynamic attributes)?

3 - What is the agents' environment? How do the agents interact with the environment? Is an agent's mobility through space an important consideration?

4 - What agent behaviours are of interest? What decisions do the agents make? What behaviours are being acted upon? What actions are being taken by the agents?

5 - How do the agents interact with each other? With the environment? How expansive or focused are agent interactions?

6 - Where might the data come from, especially on agent behaviours, for such a model?

7 - How might you validate the model, especially the agent behaviours?

(Macan 2010)

Create an environment in which the agents may interact and make the environment sensitive to actions by the agent.

Create a virtual space where agents interact according to the defined rules and patterns.

Define the feedback loops between the agent and its environment.

Create a population of autonomous **agents** (run-time objects) capable of **making simple decisions in a domain**.

Create a population of autonomous agents that encapsulate functions, internal memory, and a strategy.

Agents can follow different (heterogeneous) or the same (homogeneous) strategy.

Set-up agent **relationships** and the modes of interaction.

Define the underlying topology of connectedness> who interacts with whom, and driven by what rules?

Define the **update rules**. Define the algorithm by which the different components (functions) of your model will be evaluated.

Determine the mode and sequence of updating the population of agents and the environment.

Define what rules apply for the elementary processes in the system, such as death, survival, proliferation, reproduction, migration, production, consumption/feeding, etc.

Determine the **dependent** and **independent variables** of the system, the **static** and the **dynamic** attributes.

Independent → the cause: input (controlled, explanatory) – Dependent → the effect: output (response).

What can change and what is kept constant, unchanged during a simulation run and what changes?

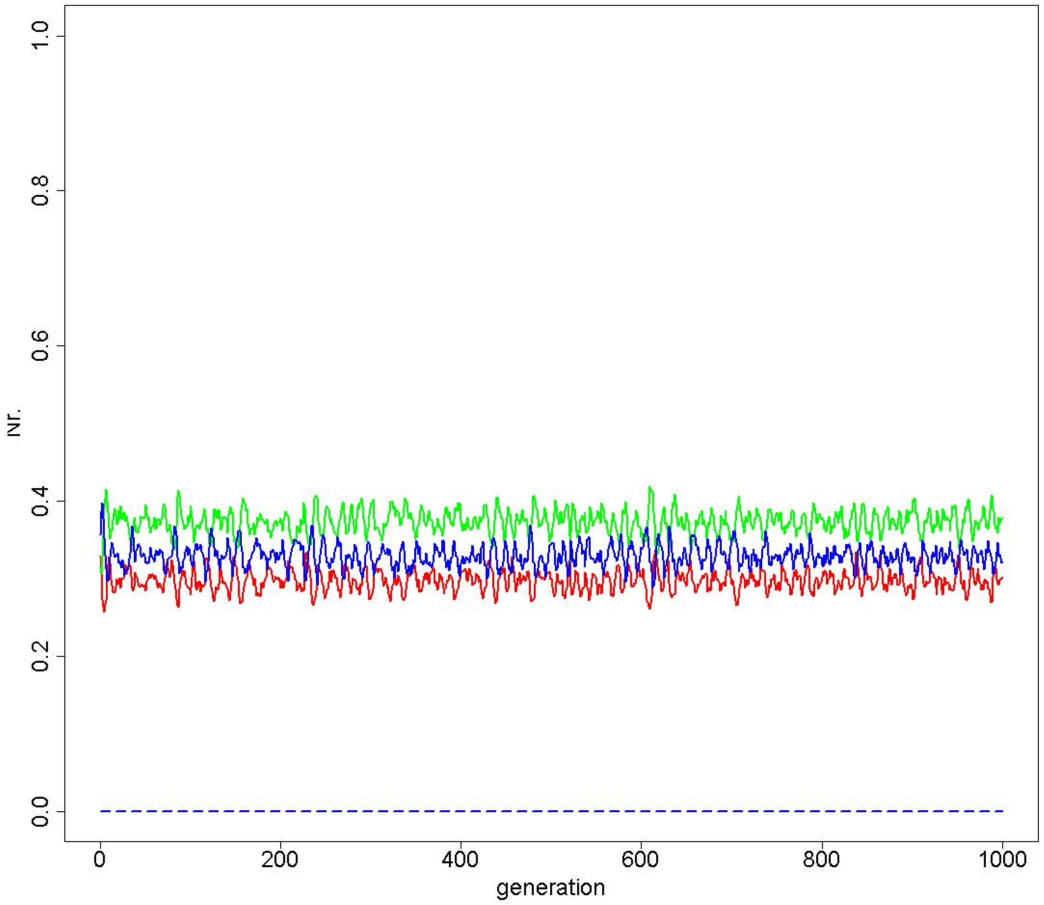
Initialize the model, allow the agents to operate autonomously, and observe for emergent complex phenomena.

Run the simulation. Allow the agents to **act** and to **adapt** to their changing („abiotic", „biotic", „social") environment through mechanisms such as evolutionary, learning or optimization algorithms.

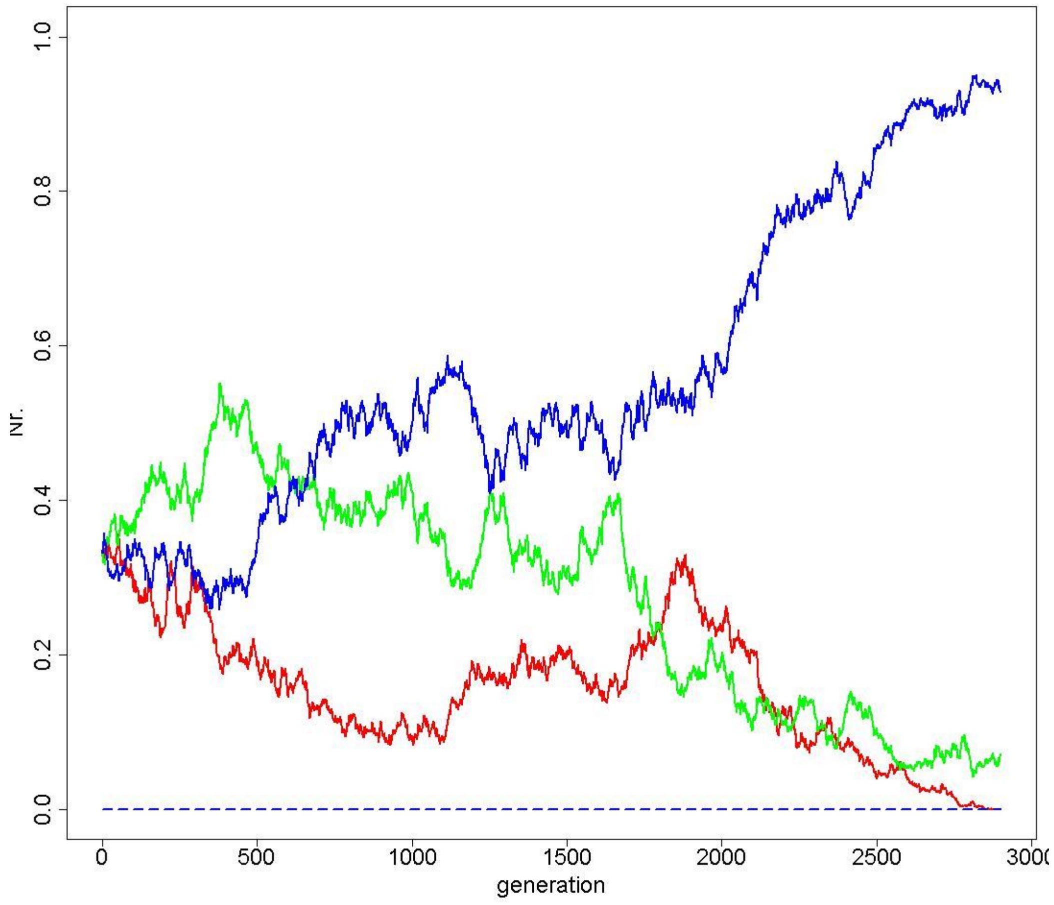
(Macal et al. 2010; turingfinance.com/perfect-imperfection-agent-based-models-abm)

Update

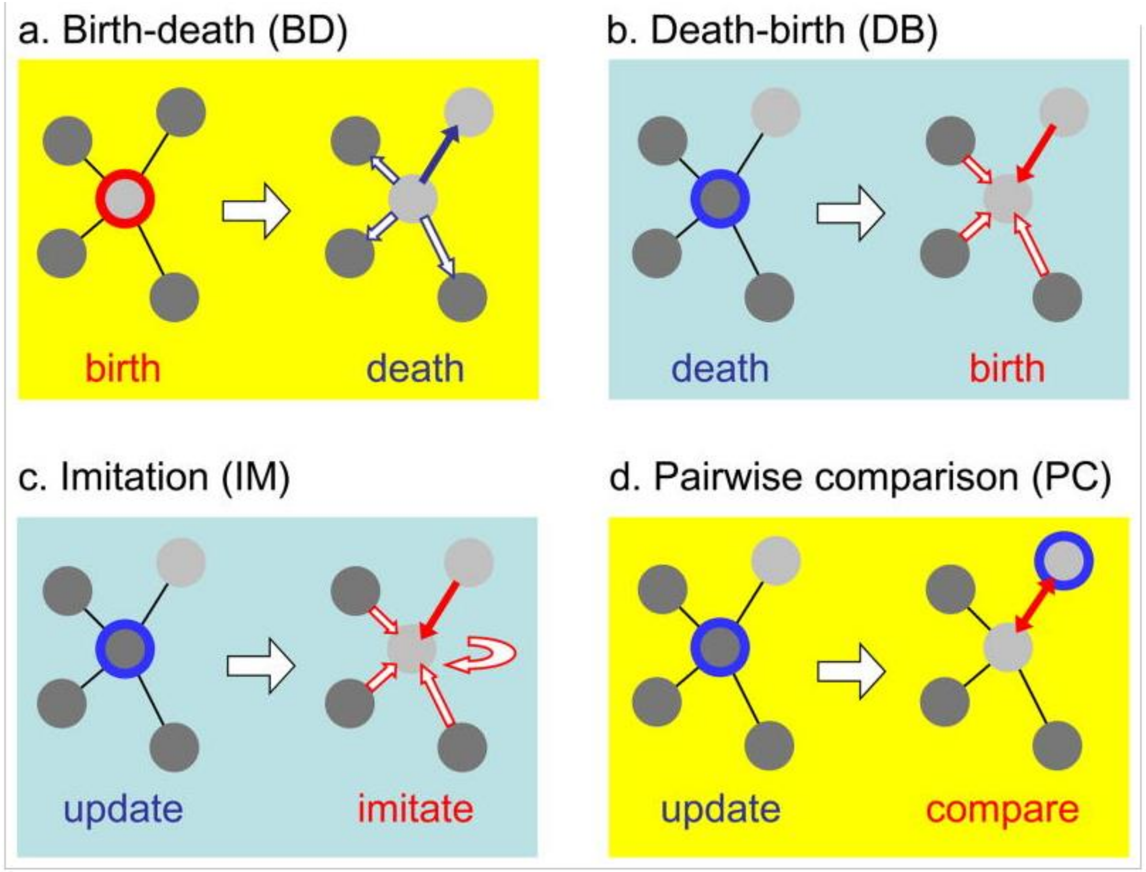
Synchronous

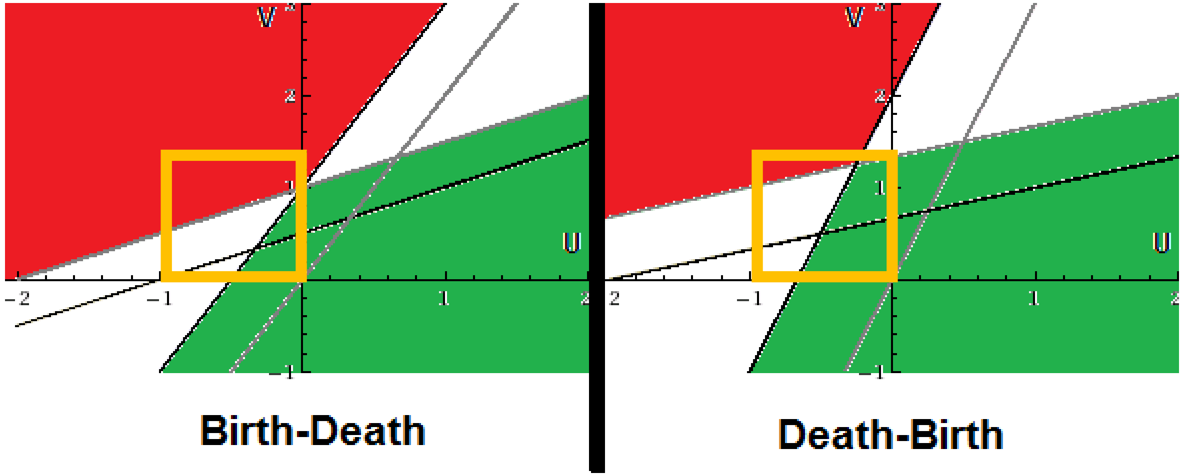


Asynchronous



Update rules



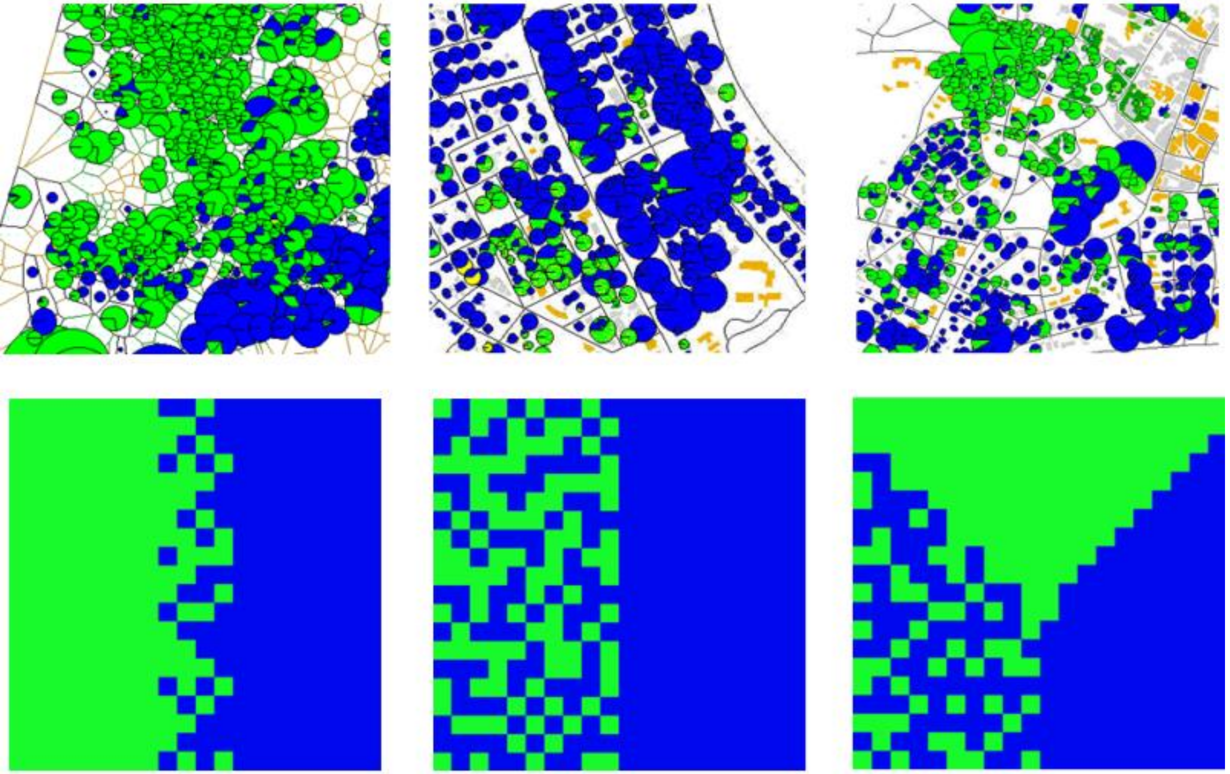


BD and PC updates promote defection
DB and IM updates promote cooperation

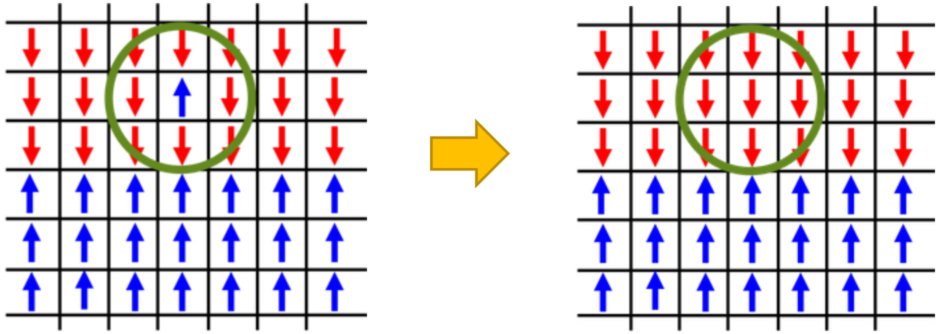
(Ohtsuki 2006)

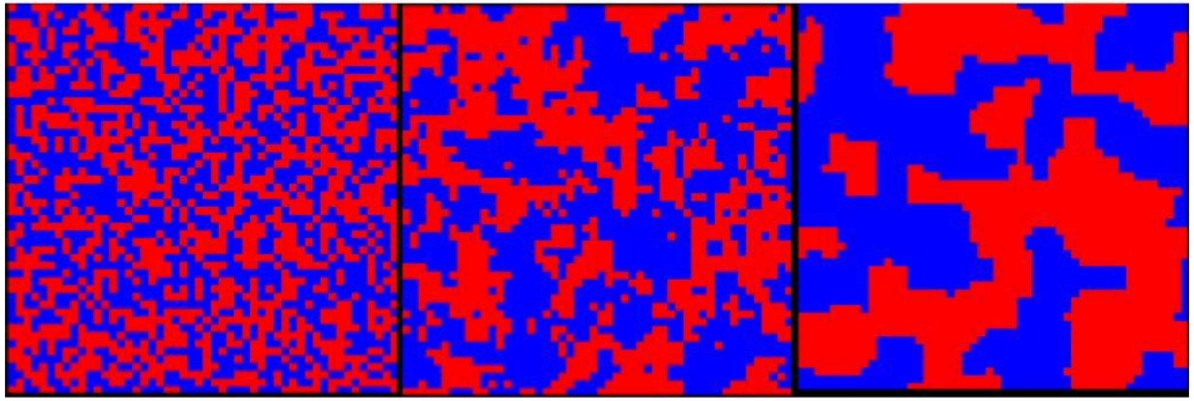
A few examples

ABM history- Socio-economic systems:
A model of segregation (Schelling 1969)
& 2D Ising model



(a) (b) (c)

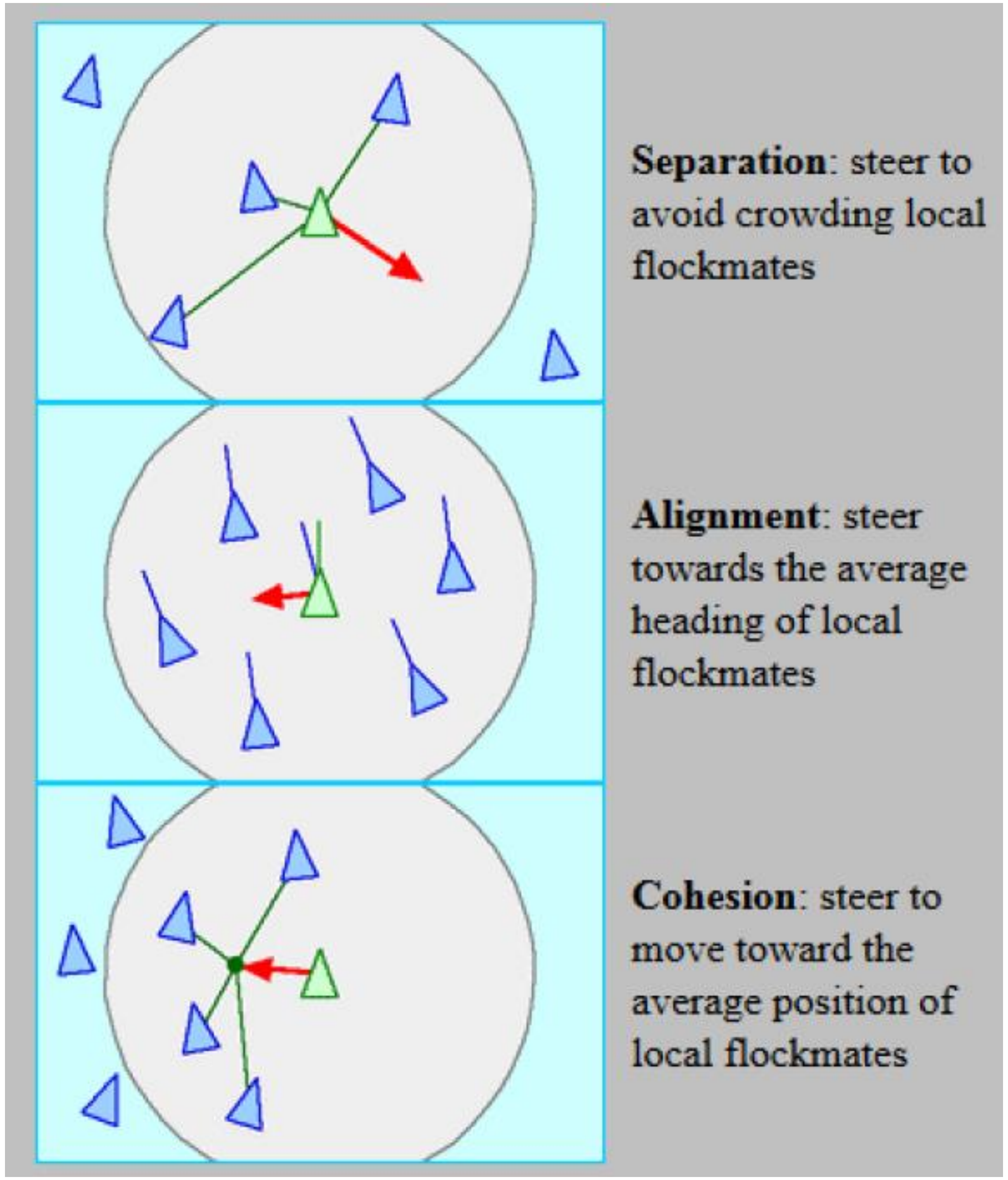




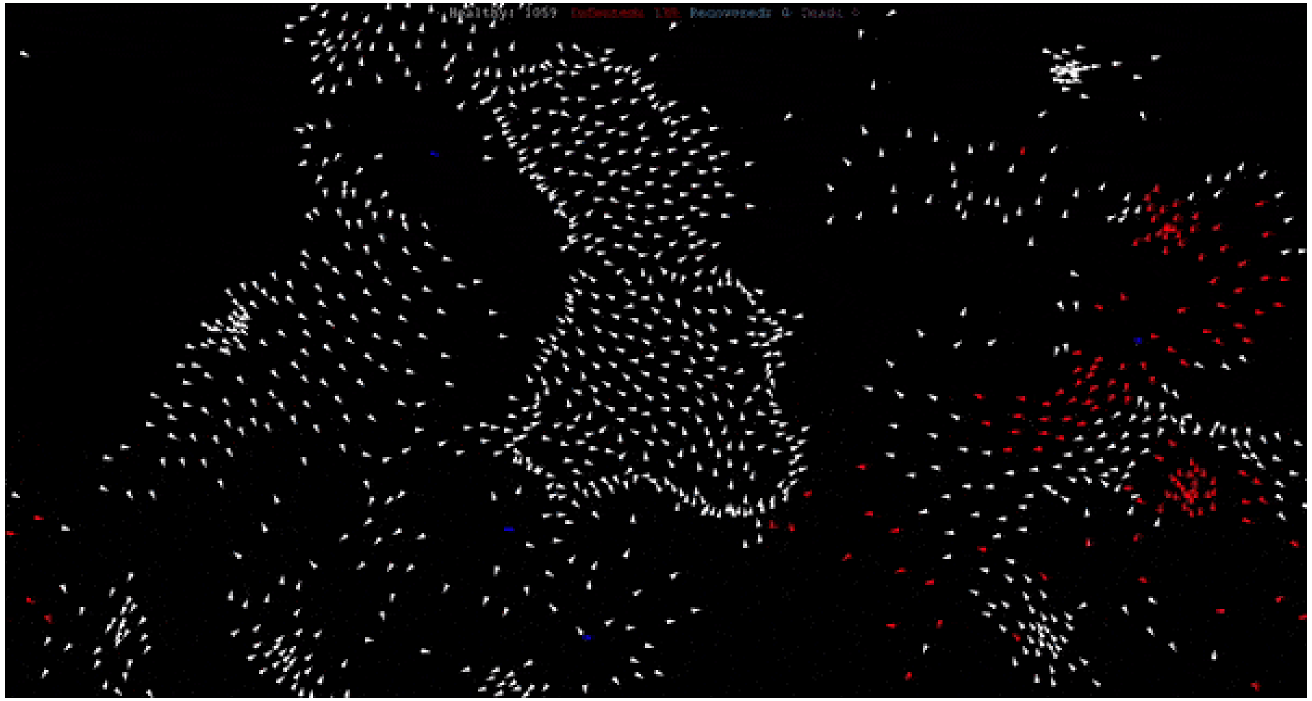
Simple rules:
- look around
- relocate if not satisfied (many other types are around).

Yet, can explain observed, real-life patterns

ABM history – Biology: The flocking model

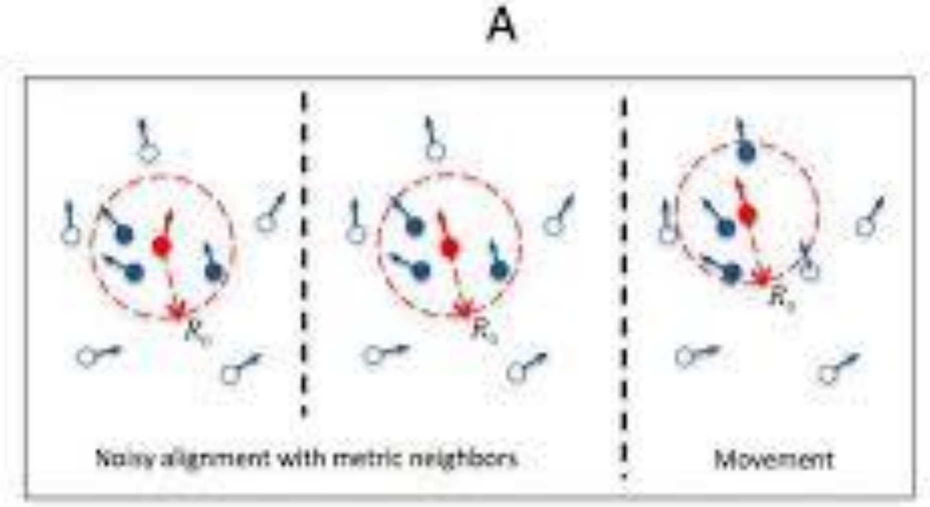


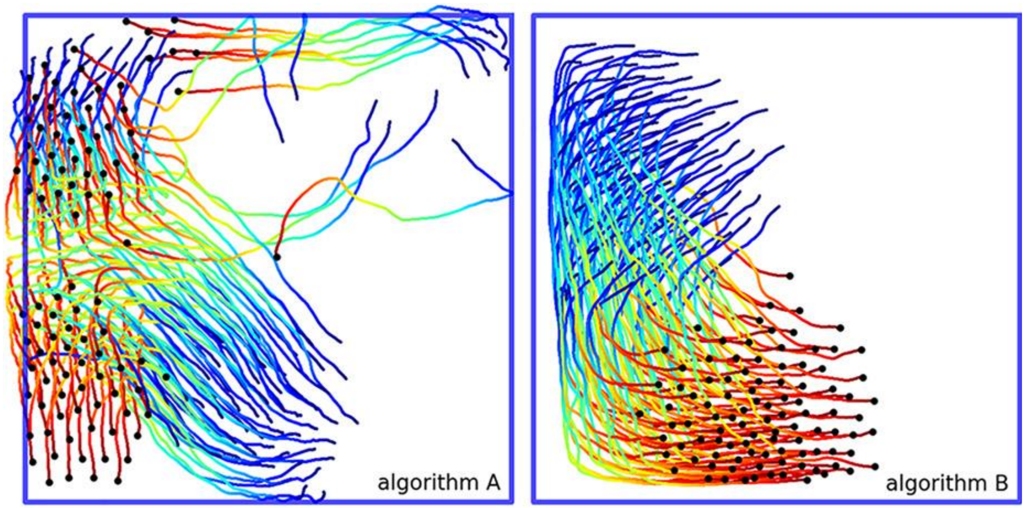
ABM history – Biology: The flocking model



(github.com/IvanHornung)

ABM history - Biology
The flocking model & real-life use

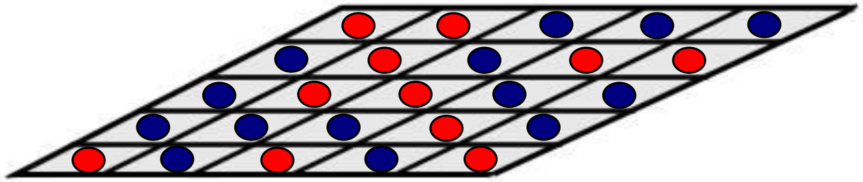


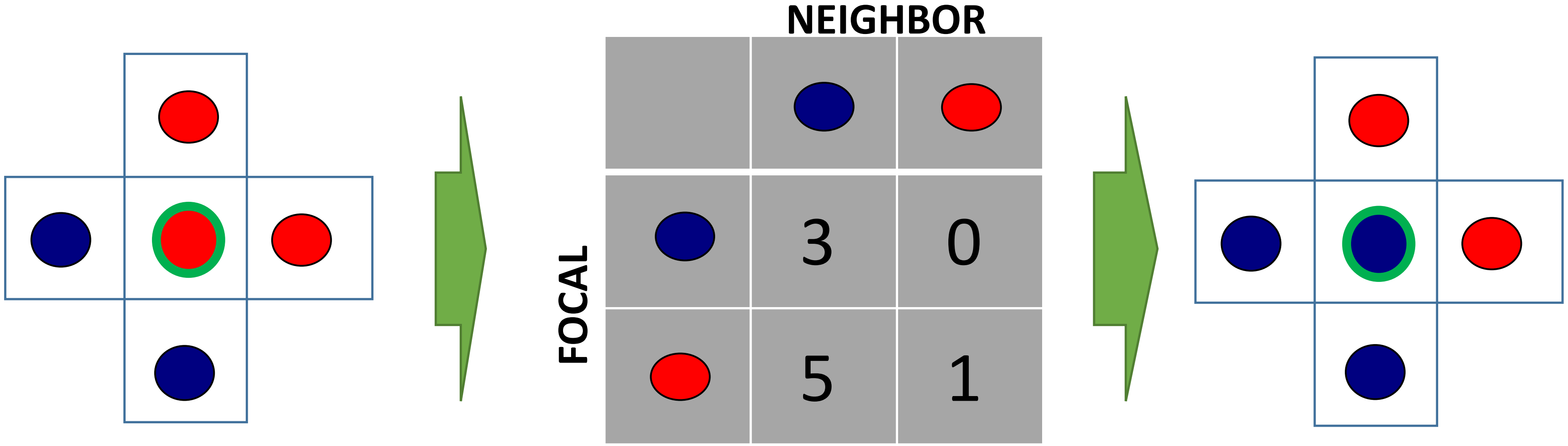


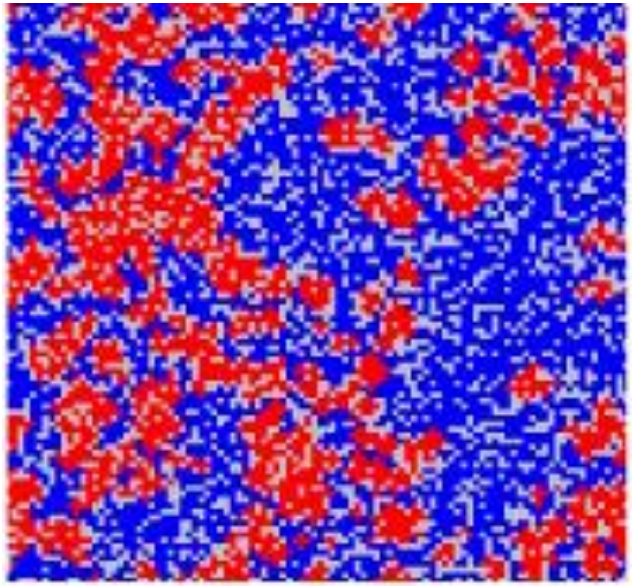
ABM & Game theory

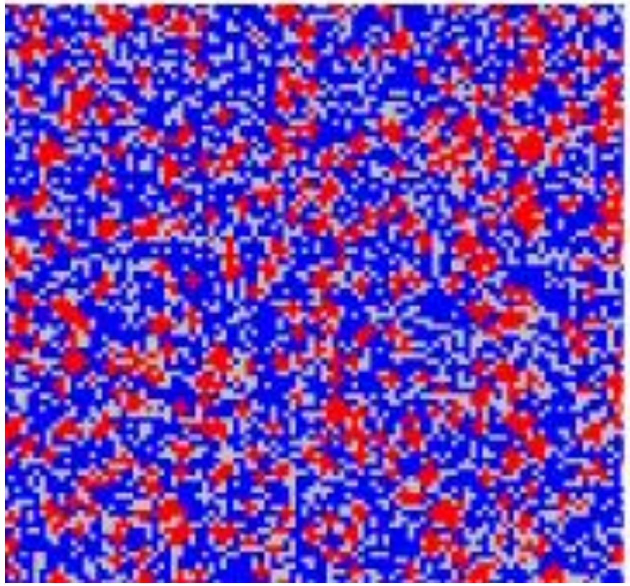
= cooperators / producers

= defectors / free-riders

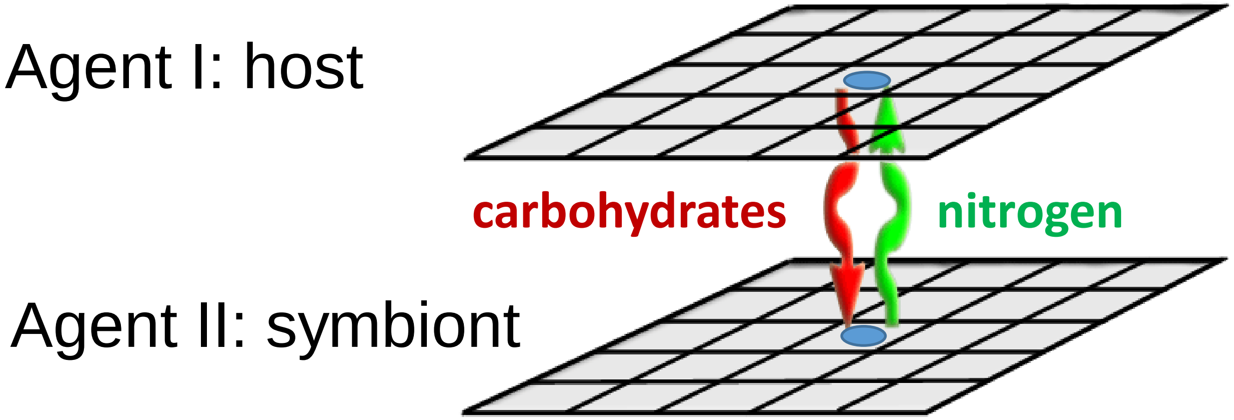


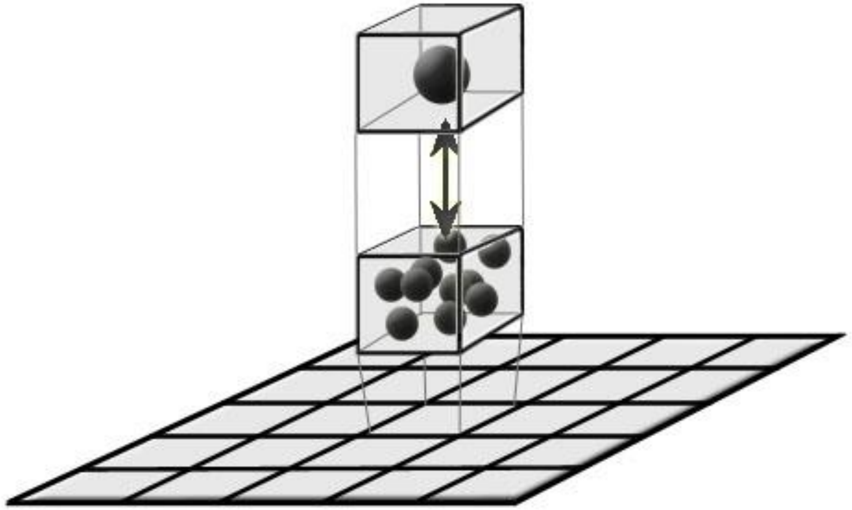






IBM & Inter-species mutualism

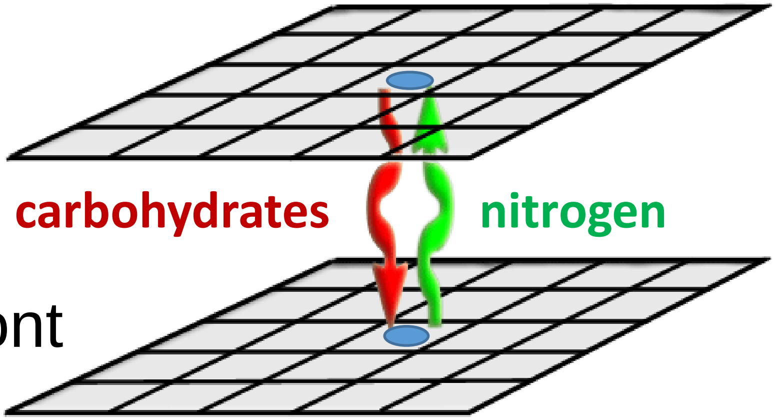


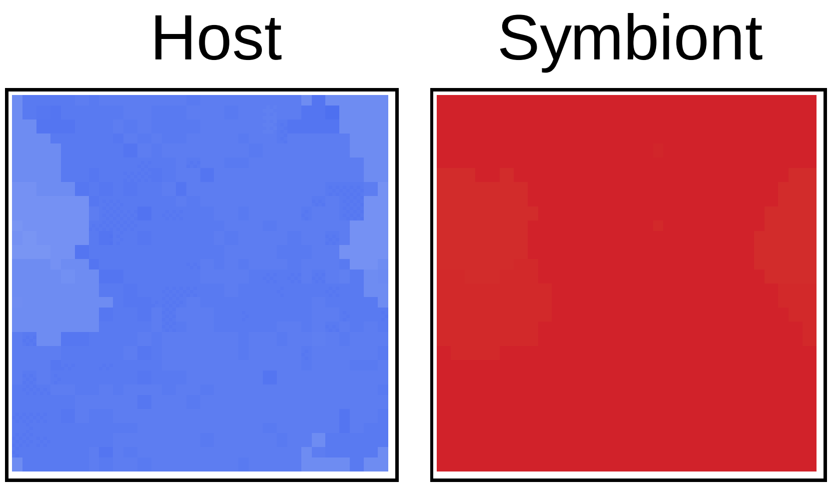


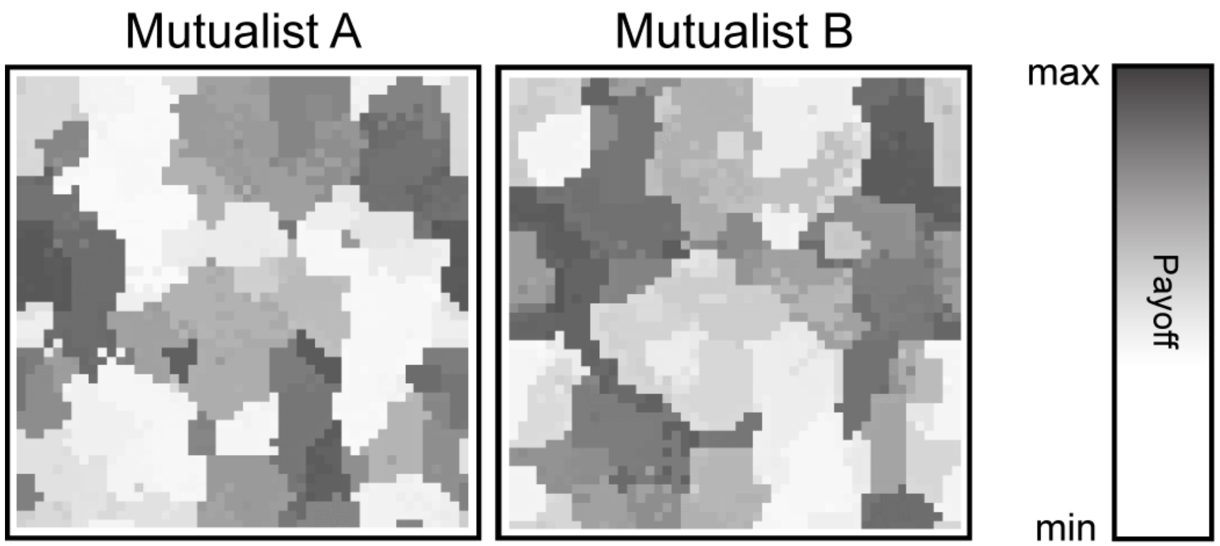
IBM & Game theory with two types of agents

Agent I: host

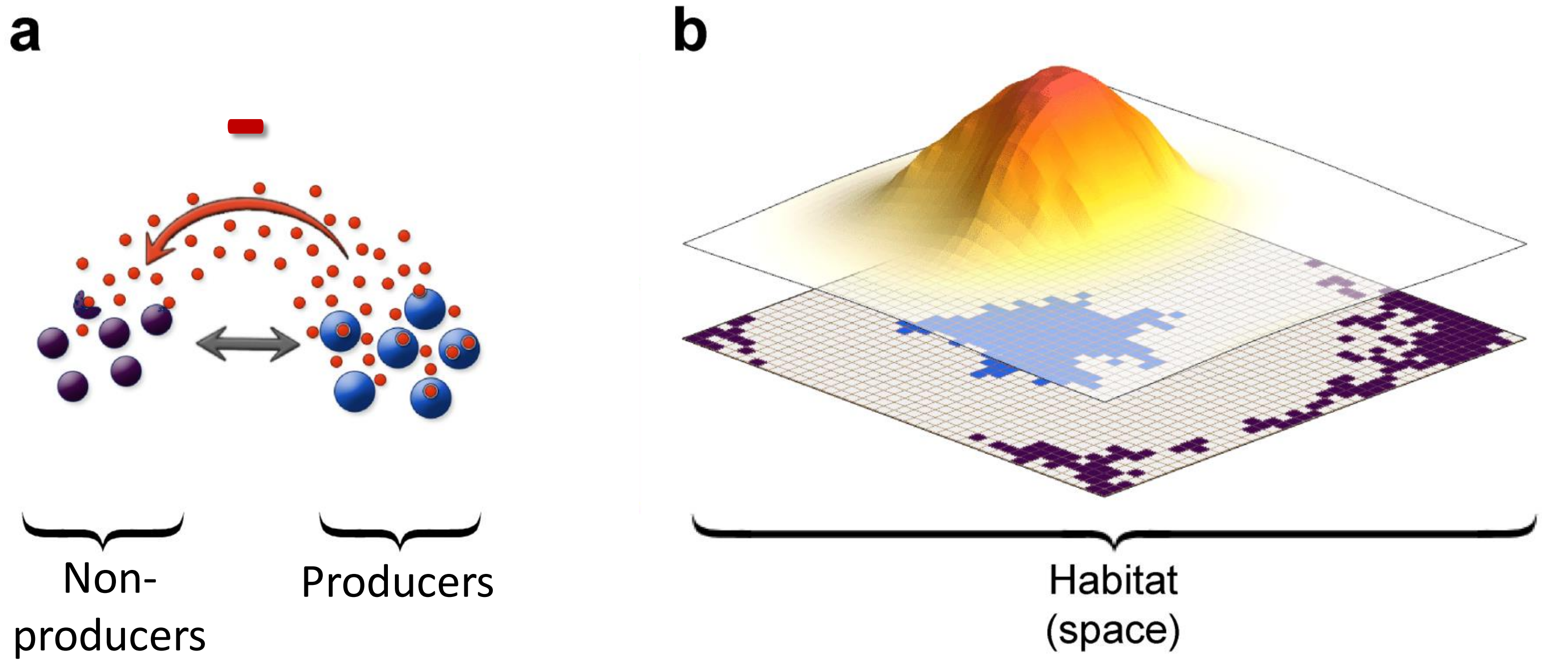
Agent II: symbiont







IBM & particle-based modelling



IBM & particle-based modelling

Dynamics of the antibiotics in the environment

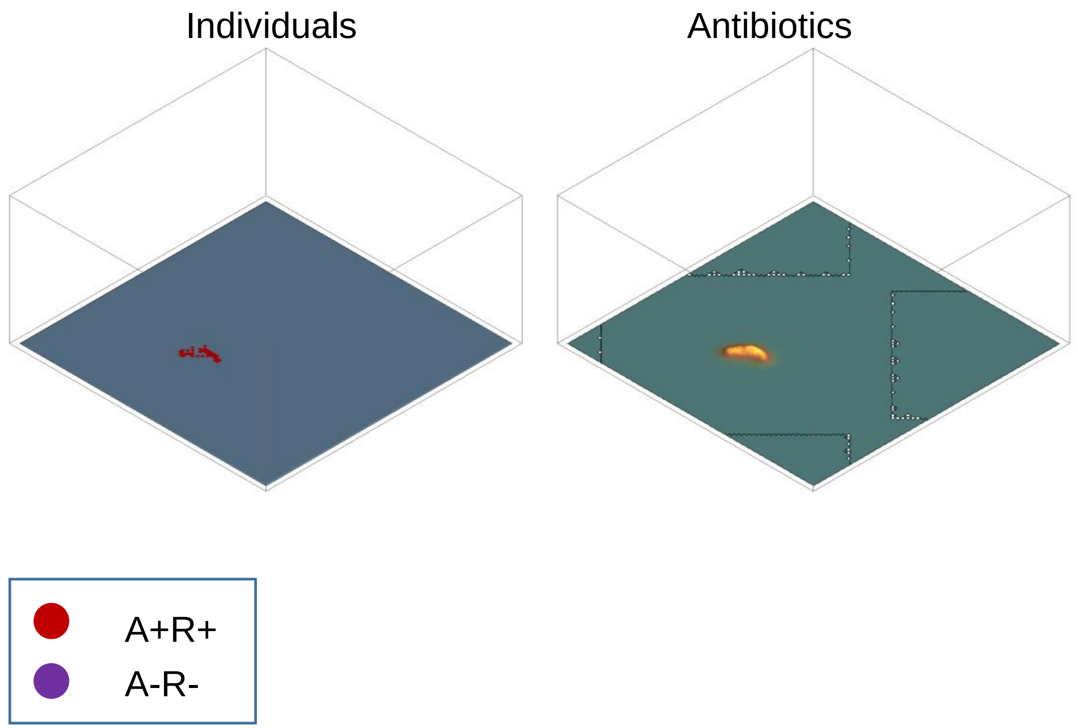
$$A^{\mathrm{Ext}}(i,t+\Delta t) = A^{\mathrm{Ext}}(i,t)$$

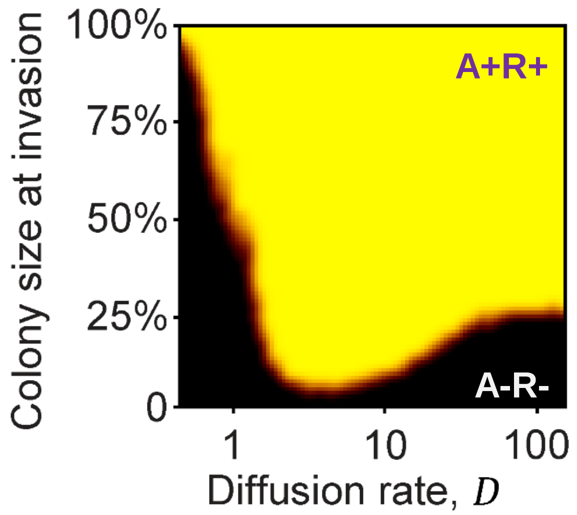
$$+\left[\underbrace{\frac{D}{\Delta x^2}\left(\sum_{j=1}^{v} A^{\mathrm{Ext}}(j,t) - vA^{\mathrm{Ext}}(i,t)\right)}_{\text{diffusion}} + \underbrace{\boxed{\left(\rho_*(t)\right.}}_{\text{production}} + \underbrace{\boxed{\beta_* A^{\mathrm{Int}}(i,t)}}_{\text{cellular efflux}} - \underbrace{\boxed{\alpha_* A^{\mathrm{Ext}}(i,t)}}_{\text{cellular uptake}} - \underbrace{\boxed{\left.\varphi A^{\mathrm{Ext}}(i,t)\right)}}_{\text{decay}}\theta(i)\right]\Delta t$$

Intracellular dynamics of the antibiotics

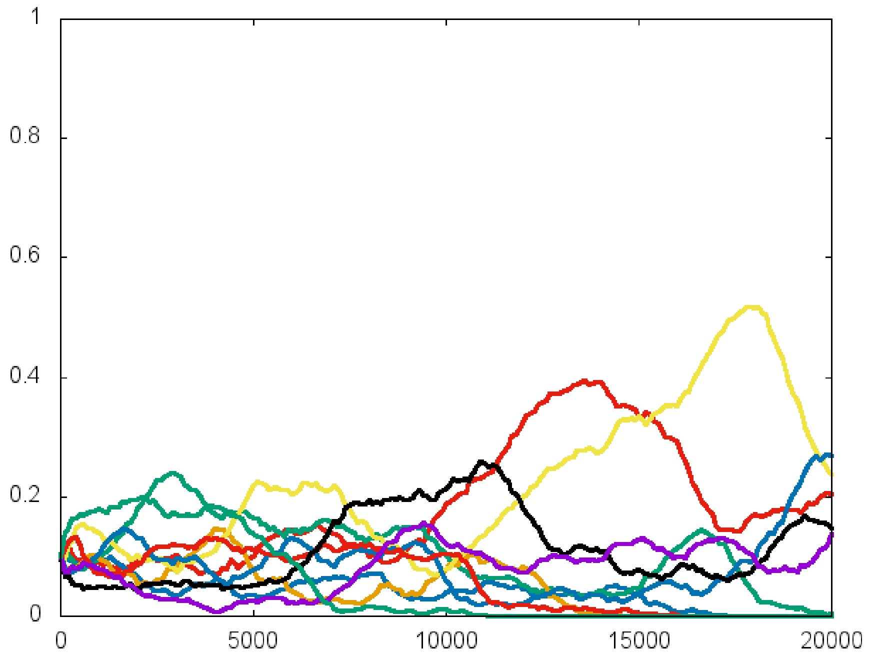
$$A^{\mathrm{Int}}(i,t+\Delta t) = A^{\mathrm{Int}}(i,t) + \left(\underbrace{\boxed{\alpha_* A^{\mathrm{Ext}}(i,t)}}_{\text{cellular uptake}} - \underbrace{\boxed{\beta_* A^{\mathrm{Int}}(i,t)}}_{\text{cellular efflux}} - \underbrace{\boxed{\gamma_* A^{\mathrm{Int}}(i,t)}}_{\text{decomposition}}\right)\Delta t$$

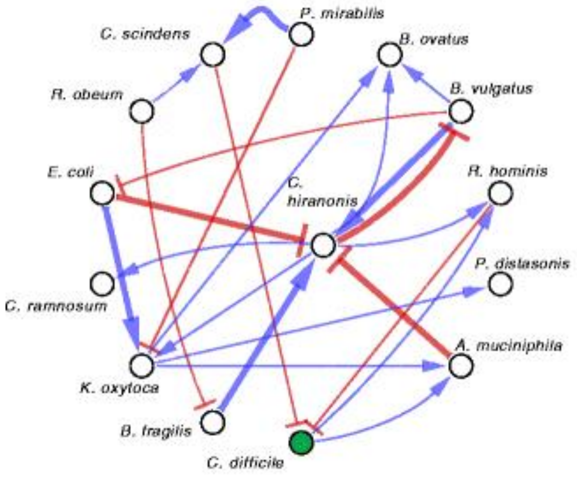
IBM & particle-based modelling



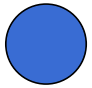
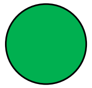
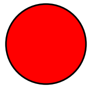
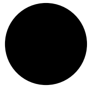


IBM & interaction networks & particle-based modelling

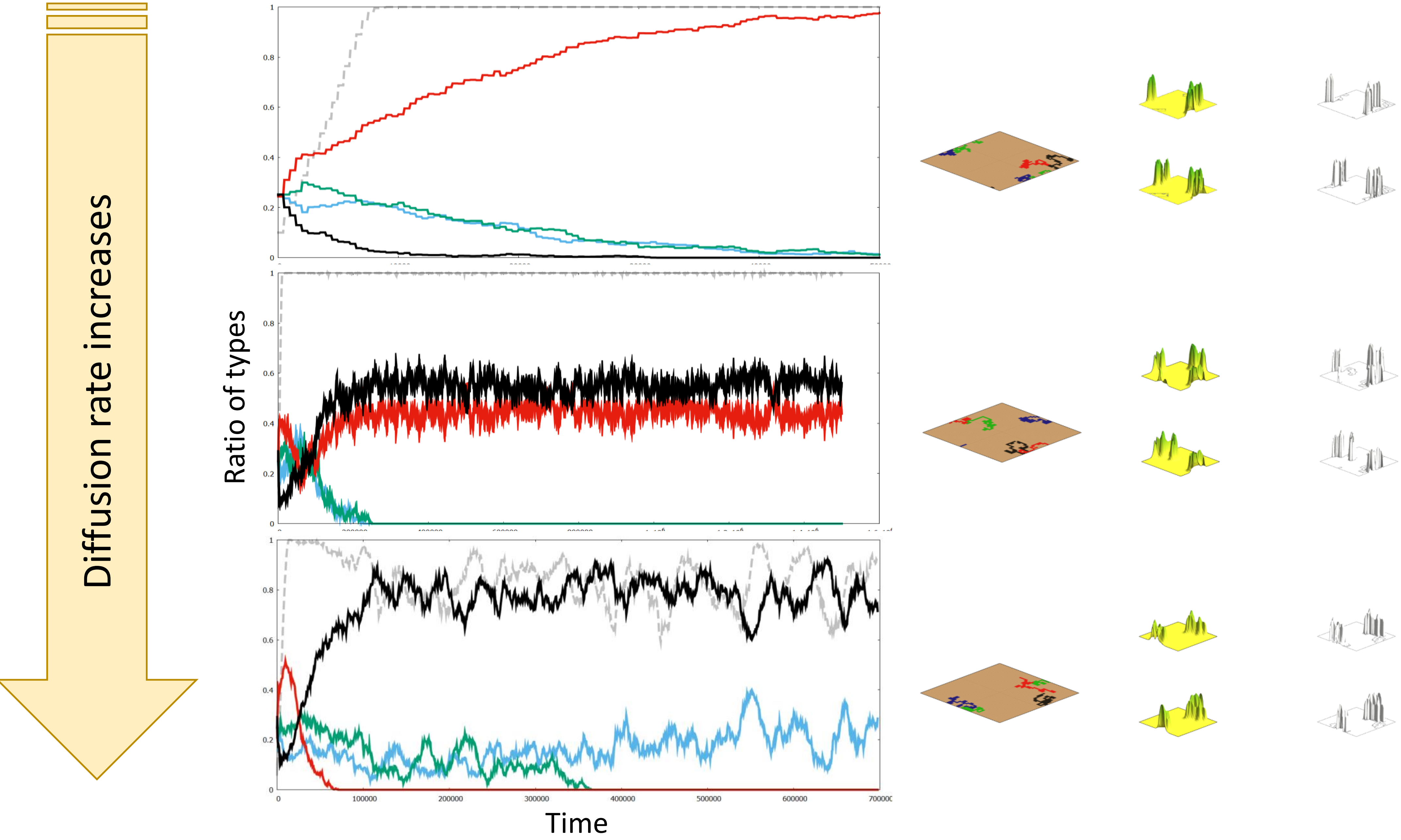




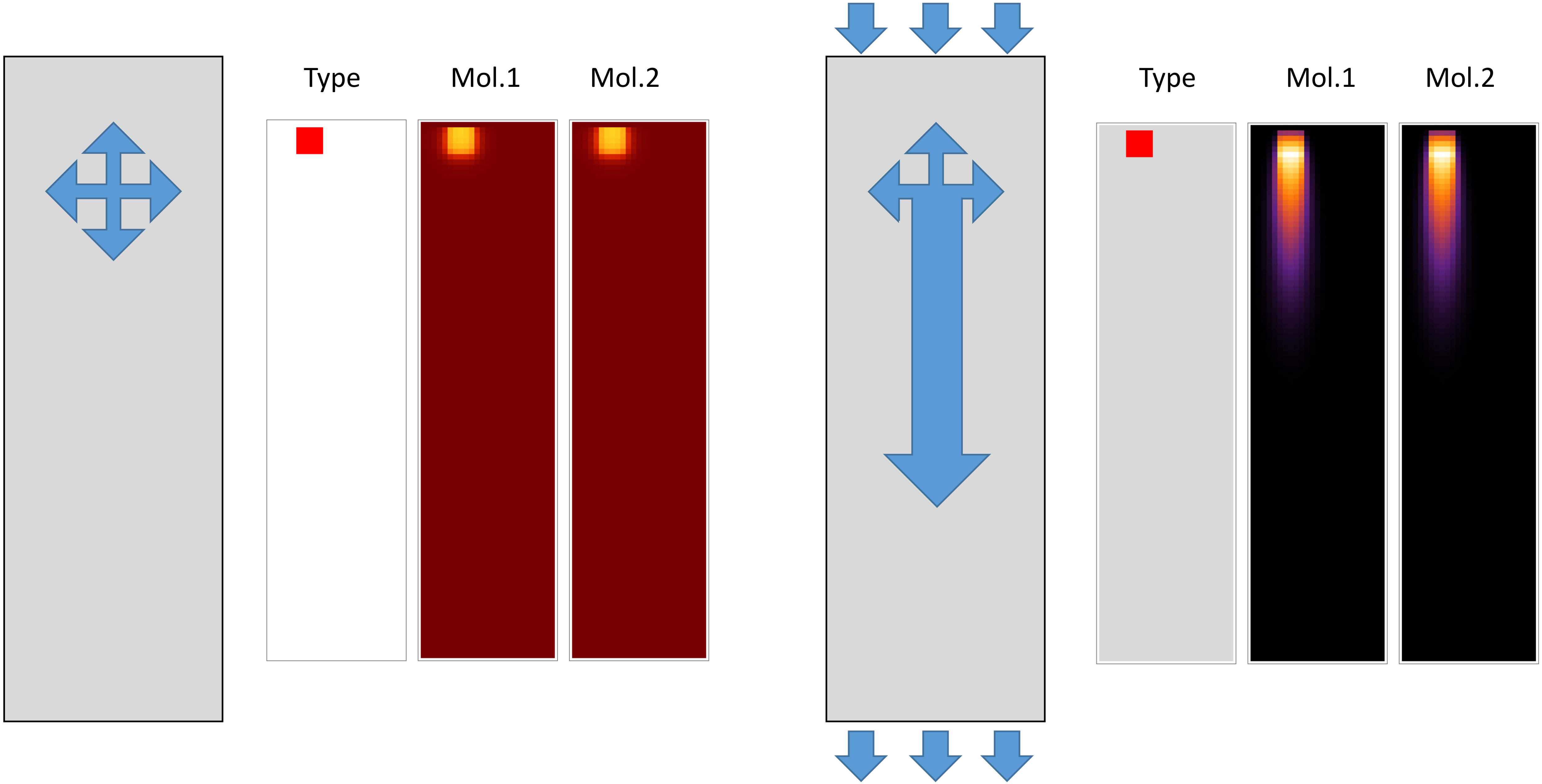
IBM & Cross-feeding: **Specialists** – **Generalist** – **Free-rider** population dynamics

Species		Diffusible resource produced (Public good) PG 1	PG 2	Cost of producing	Growth effect of the resource: Mutualism (1)
	→	✗	✓	-c	**1**
	→	✓	✗	-c	**1**
	→	✓	✓	-2c	**1**
	→	✗	✗	0	**1**

IBM & Cross-feeding: **Specialists** – **Generalist** – **Free-rider** population dynamics

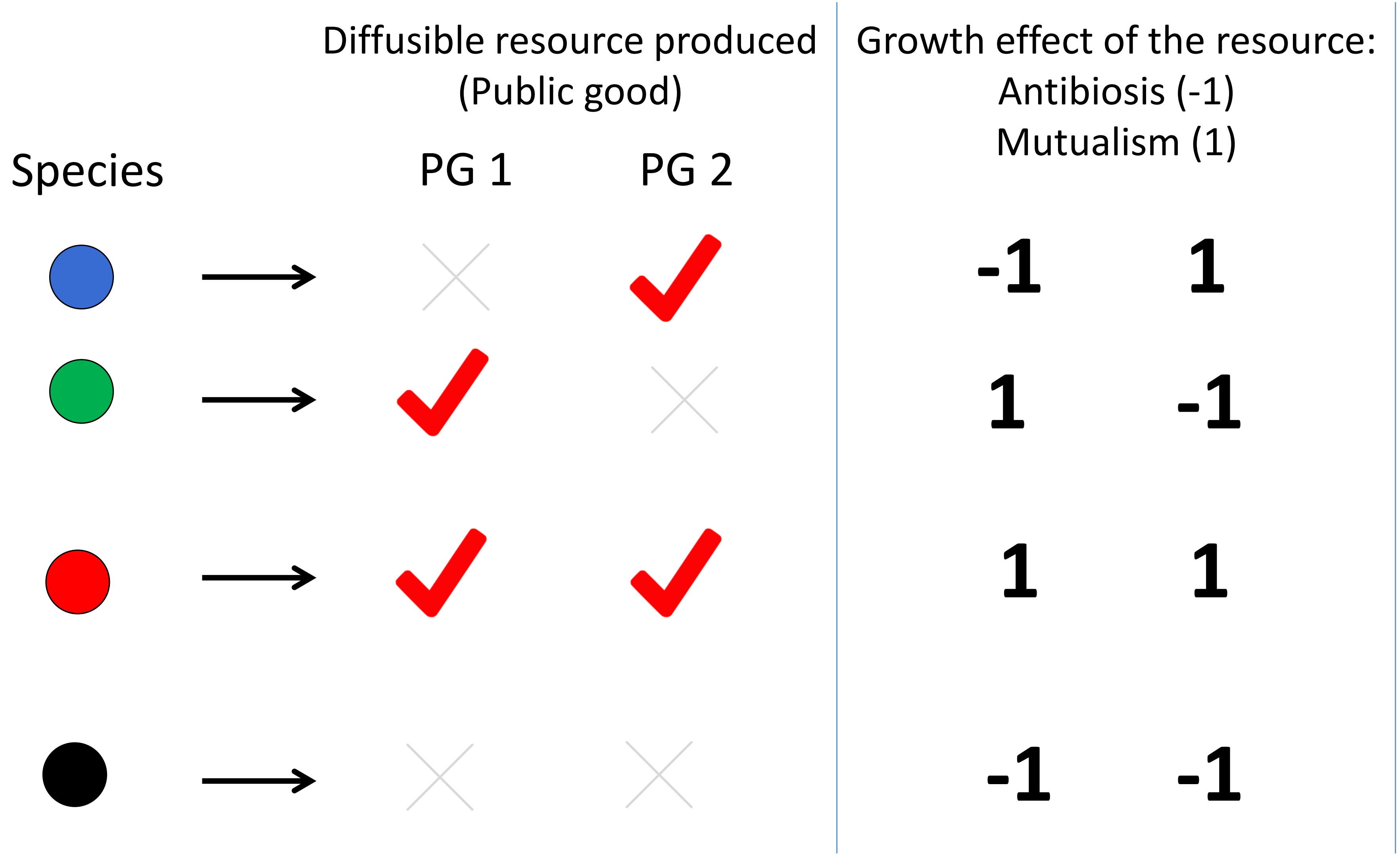


IBM & Gradient model



IBM & Gradient model

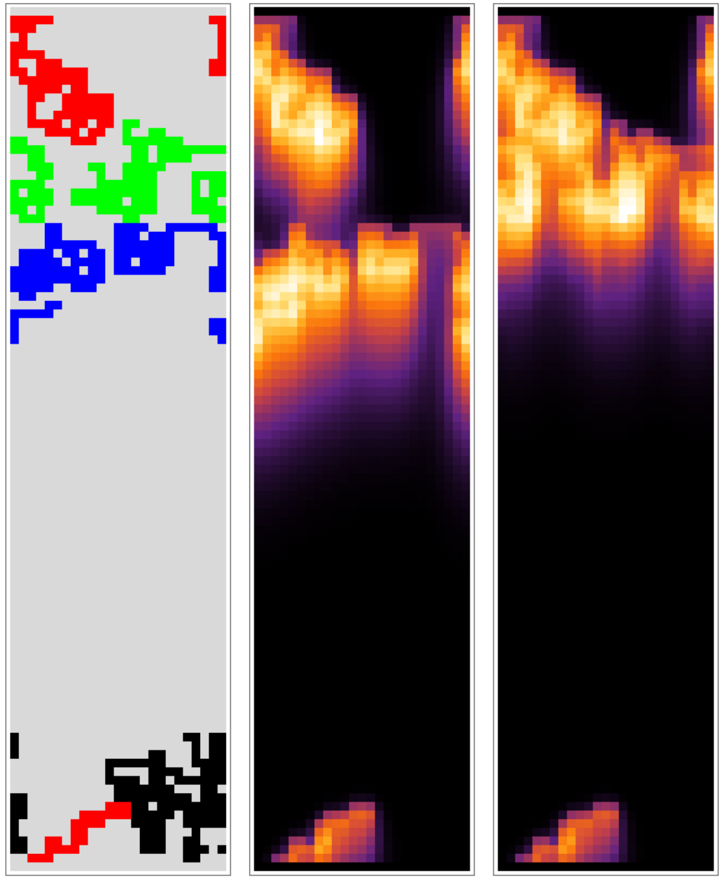
& Specialists – Generalist – Free-rider/Sensitive

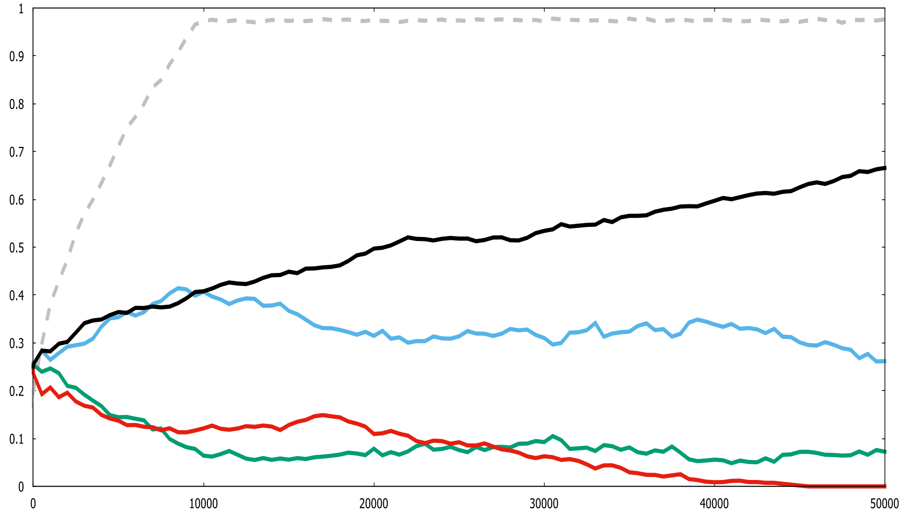


IBM & Gradient model

& Specialists – Generalist – Free-rider/Sensitive

Gradient-oriented diffusion rate surplus = 0.25



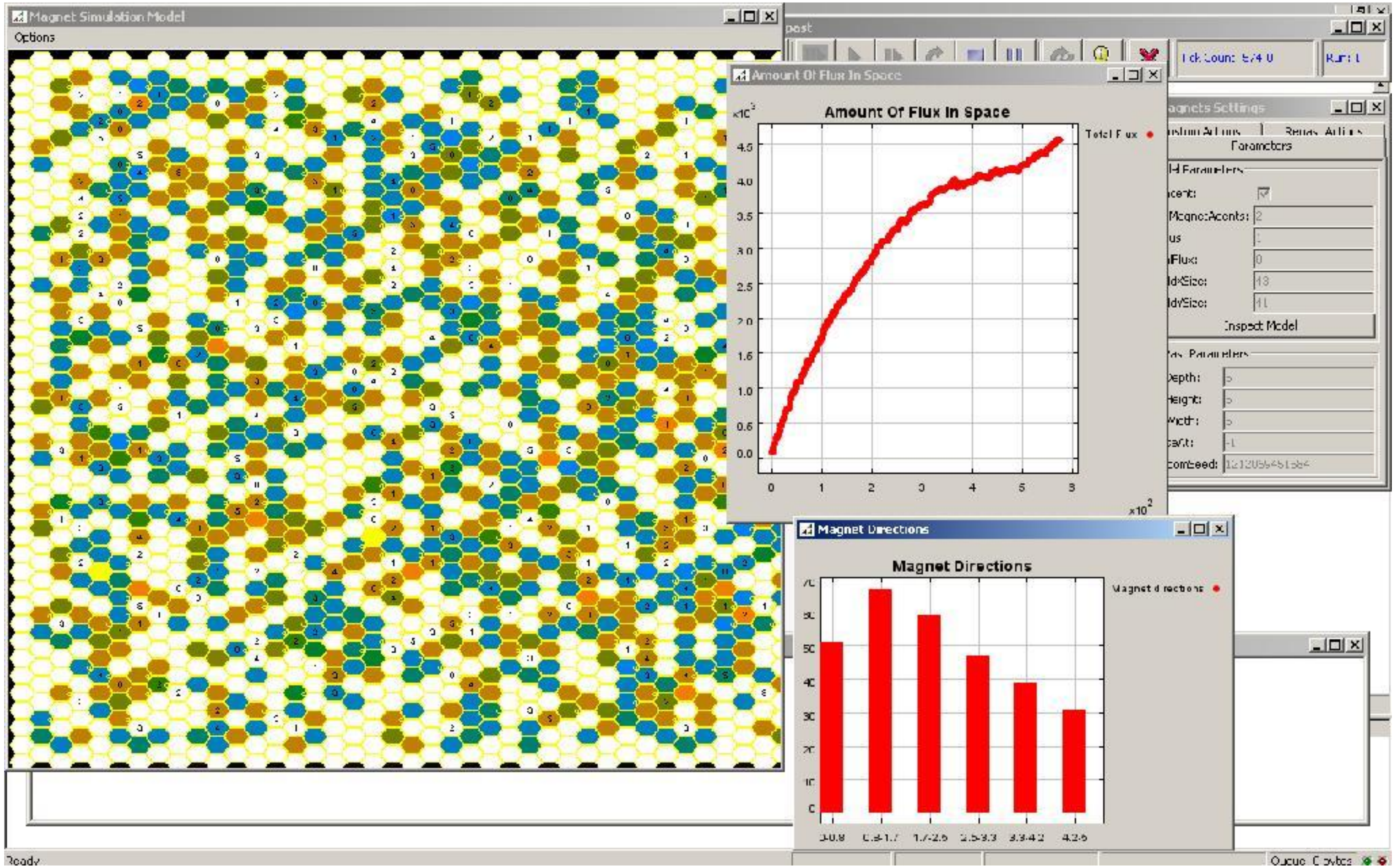


ABM platforms

- Specialized softwares: AnyLogic, NetLogo, Repast (Repast-HPC), Sesam, Swarm, etc.
  + Lower entry barrier, graphical GUI, specialized libraries, online simulations
  - Slower simulation speed, limited scalability, limited capacity
- General-purpose programming languages: C, C++, Java, Julia, Pascal, MATLAB, Mathematica, Python
  + Almost unlimited scalability (HPCs), debugging
  - Higher entry barrier, skills and time is necessary for coding, GUI is less easy to learn
- Combined solutions
  - Model in AnyLogic/NetLogo, output analysis in R
  - Model using specialized libraries of general-purpose languages (e.g., JAS-mine/ JAVA)

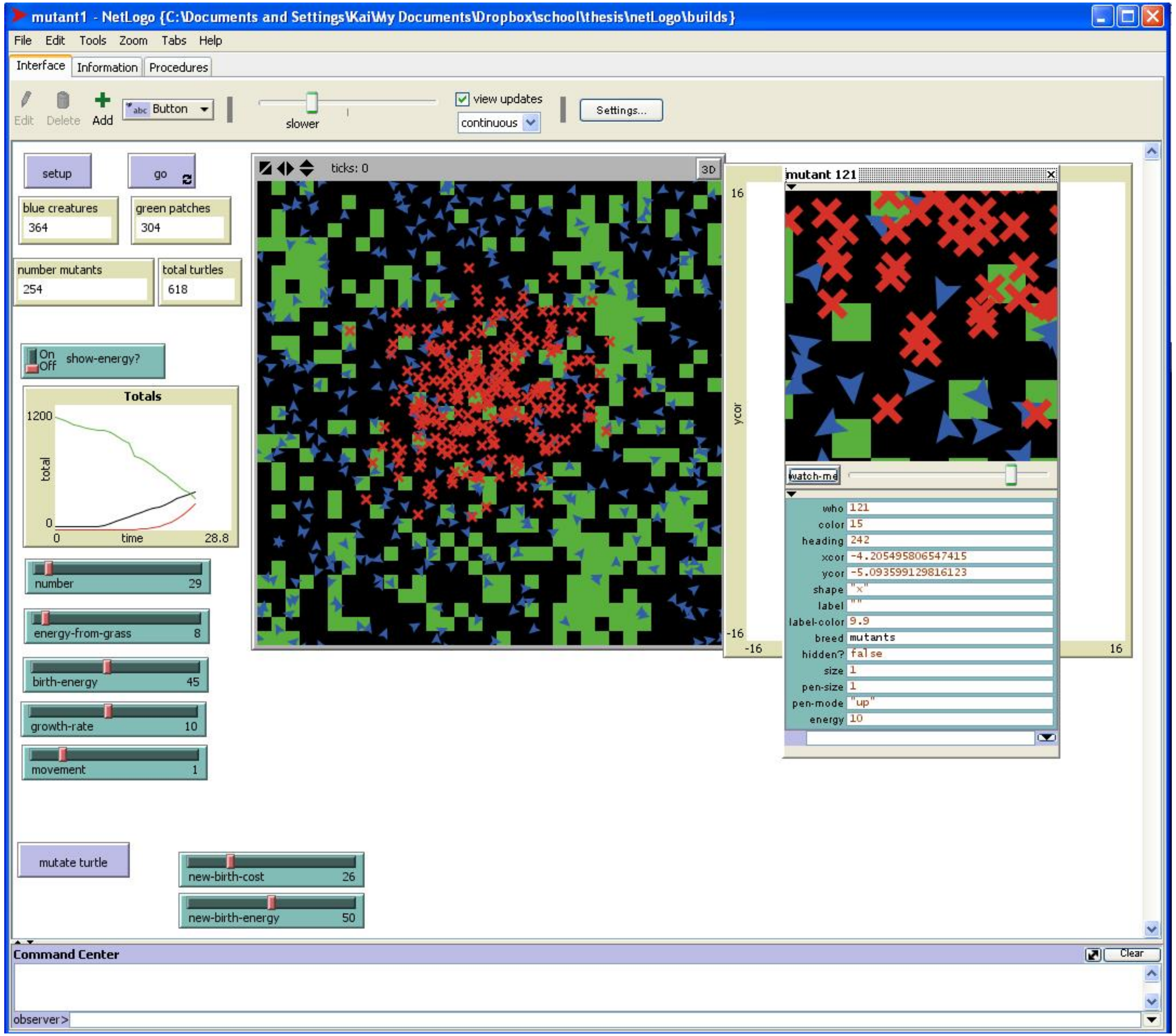
- ABM software comparison
  - https://en.wikipedia.org/wiki/Comparison_of_agent-based_modeling_software

Repast (Java)



Magnet Simulation Model
Options
Amount Of Flux In Space
Amount Of Flux In Space
Total Flux
Magnet Directions
Magnet Directions
Magnet directions
Parameters
Inspect Model
Ready

NetLogo



mutant1 - NetLogo {C:\Documents and Settings\Kai\My Documents\Dropbox\school\thesis\netLogo\builds}
File Edit Tools Zoom Tabs Help
Interface Information Procedures
Edit Delete Add Button
slower
view updates
continuous
Settings...
setup
go
blue creatures 364
green patches 304
number mutants 254
total turtles 618
On Off show-energy?
Totals
1200
total
0
0 time 28.8
number 29
energy-from-grass 8
birth-energy 45
growth-rate 10
movement 1
mutate turtle
new-birth-cost 26
new-birth-energy 50
ticks: 0
3D
16
ycor
-16
-16
16
mutant 121
watch-me
who 121
color 15
heading 242
xcor -4.205495806547415
ycor -5.093599129816123
shape "x"
label ""
label-color 9.9
breed mutants
hidden? false
size 1
pen-size 1
pen-mode "up"
energy 10
Command Center
Clear
observer>

ABM challenges

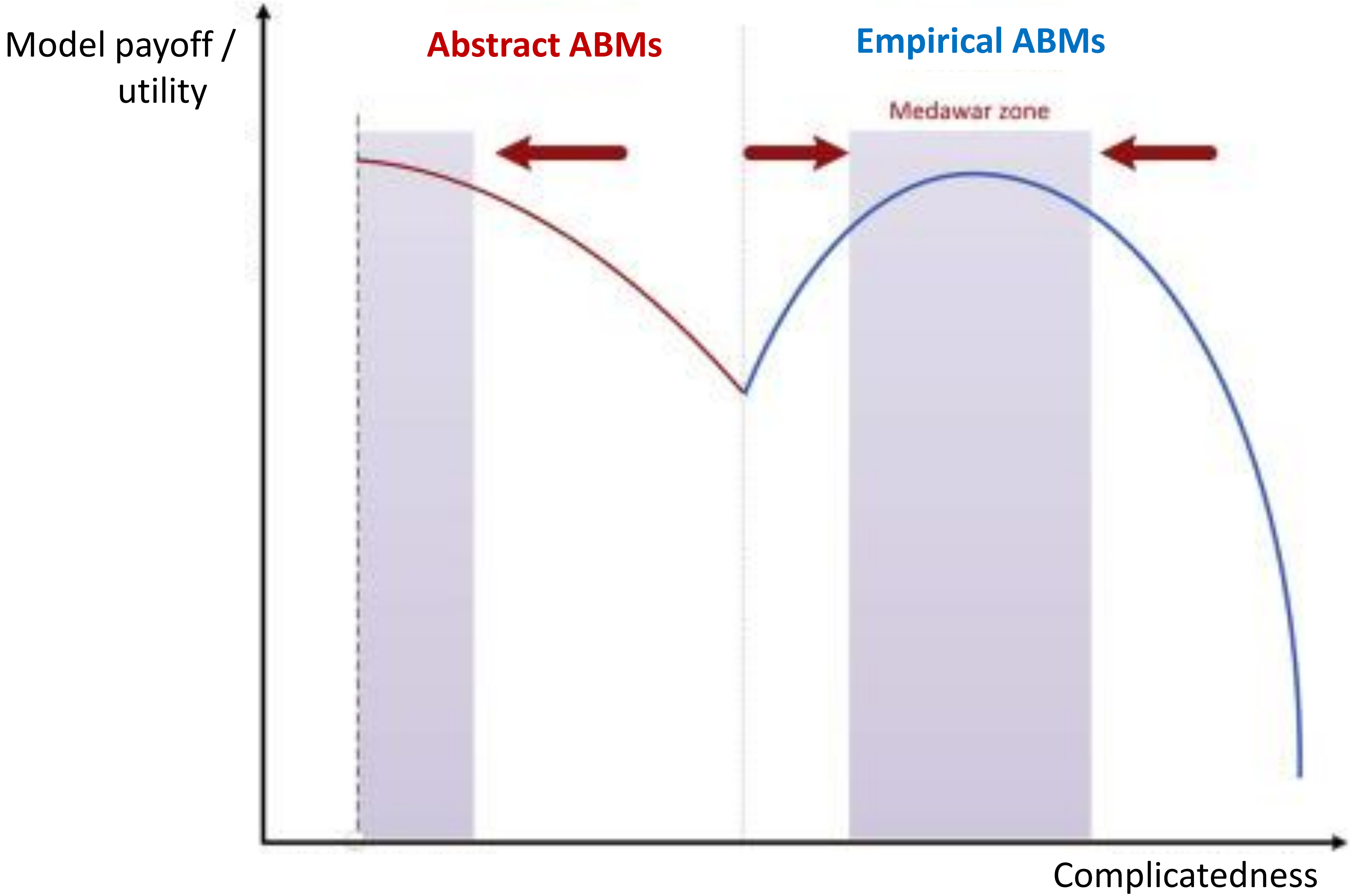
1. Optimize model complexity, choose the right modelling framework.

2. Compare ABMs and their results, predictions (problem of transparent and universal documentation).

3. Verify and validate ABMs.

ABM challenges

1. Optimize model complexity:



(Sun et al. 2016)

ABM challenges

2. Compare ABMs:

transparent and universal documentation.

O	1. **Purpose and patterns**
	2. **Entities, state variables and scales**
	3. **Process overview and scheduling** *Submodel A* *Submodel B* …
D	4. **Design concepts**
D	5. **Initialization**
	6. **Input data**
	7. **Submodels** *Submodel A (Details)* *Submodel B (Details)* …

Basic principles
Emergence
Adaptation
Objectives
Learning
Prediction
Sensing
Interaction
Stochasticity
Collectives
Observation

- Model code sharing
  - Specialised platforms
    comses.net
    cloud.anylogic.com
    runmycode.org
  - GitHub

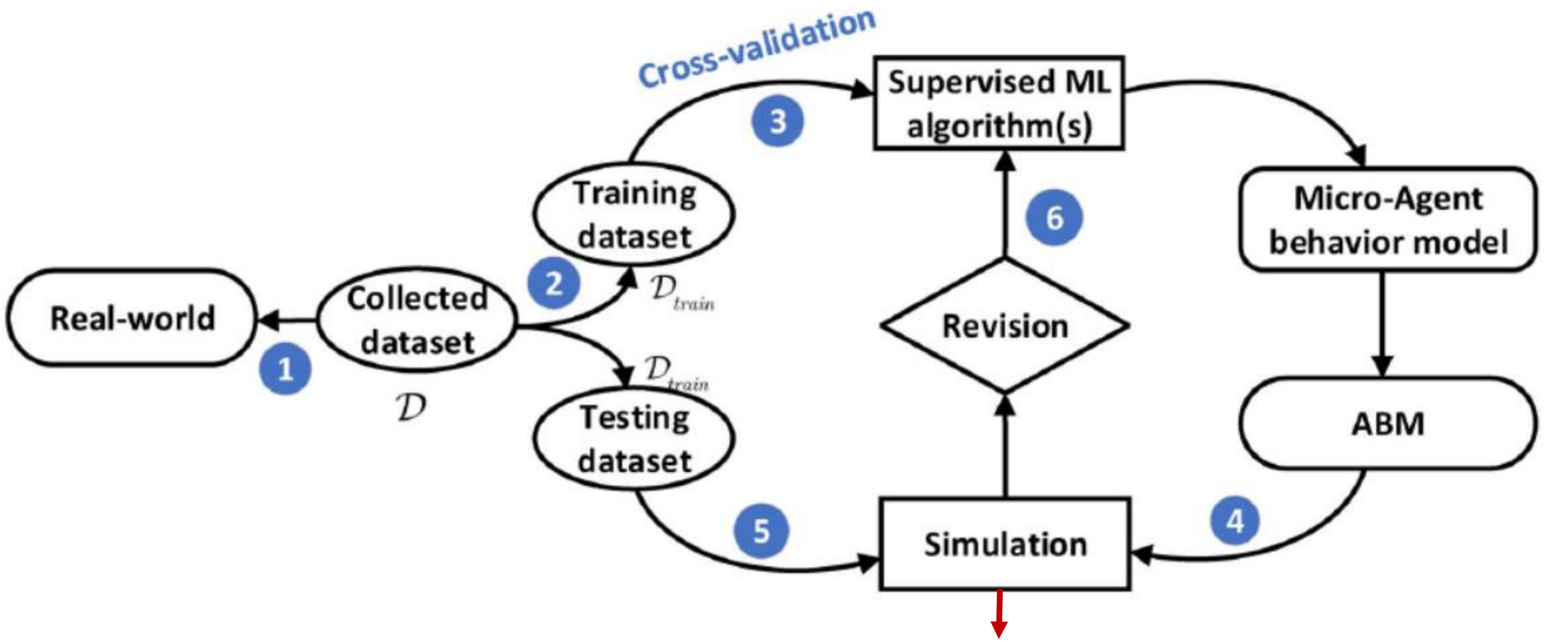
(Grimm et al. 2020)

ABM challenges

3. Verify and validate ABMs.

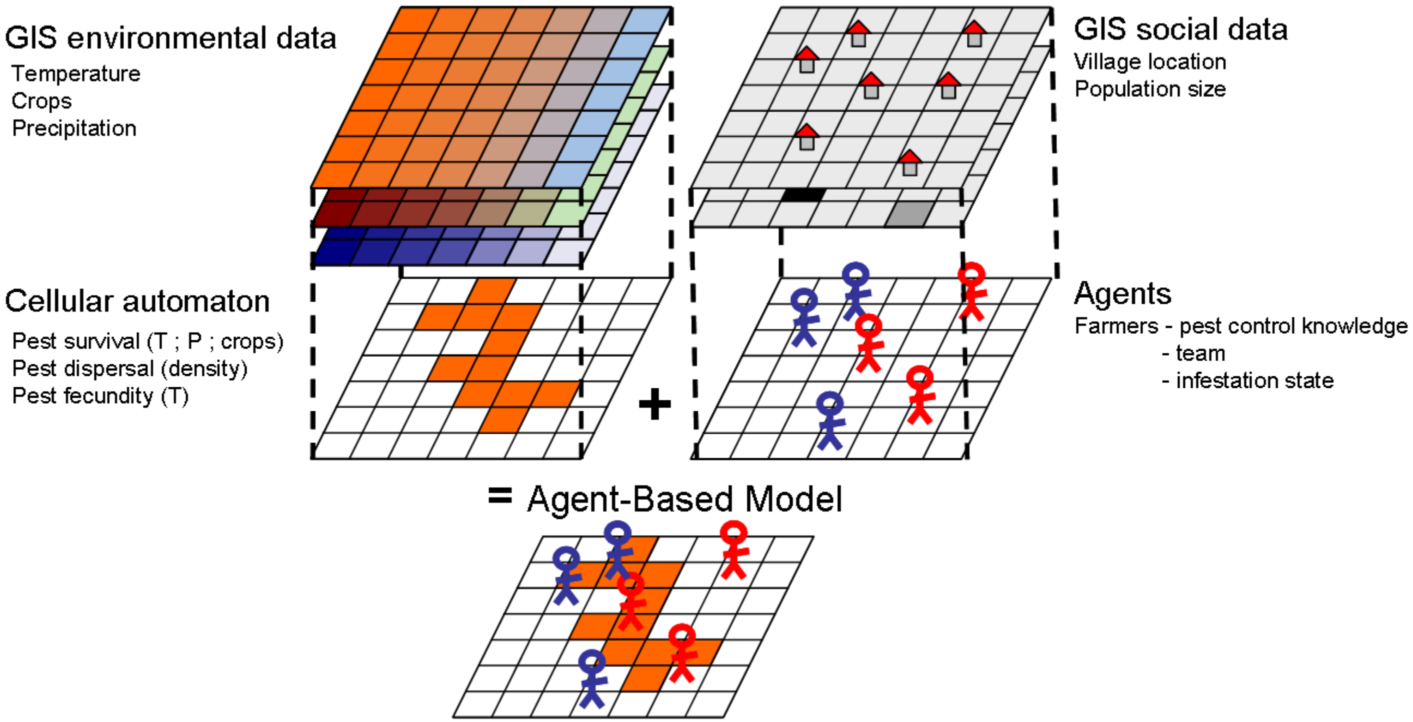
Baseline behavior. Validate model with known parameters, retrieve published outcomes.

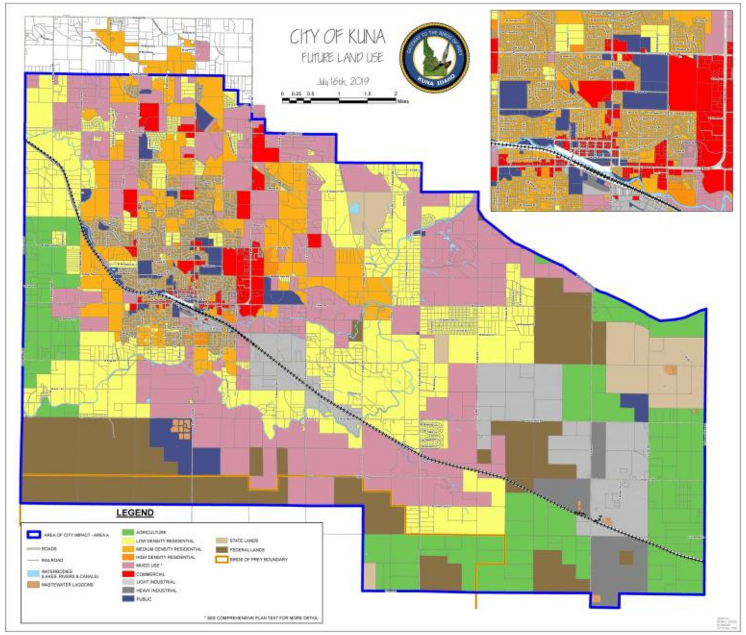
Data-driven modelling. Train functions, parameters, behavioral components with data.



(Zhang et al. 2021)

Complex ABM with multiple GIS Data layers

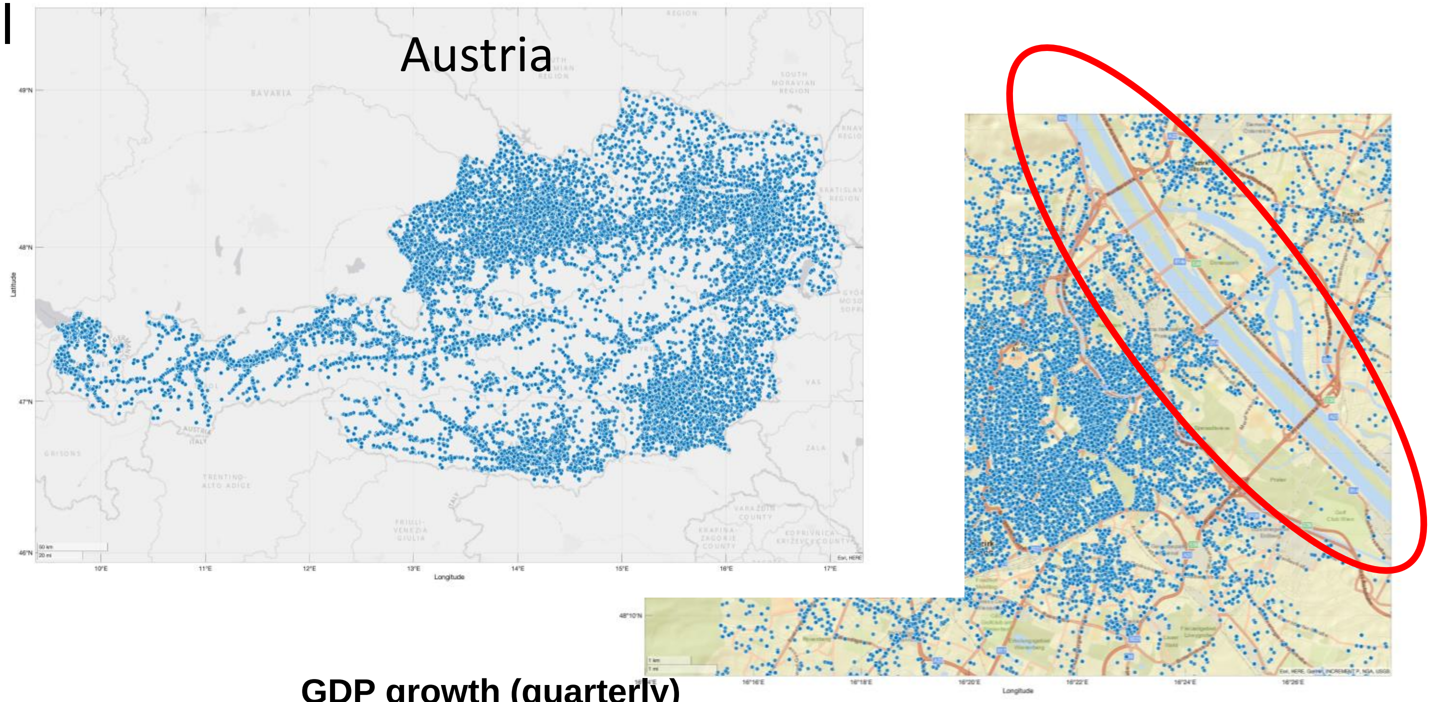


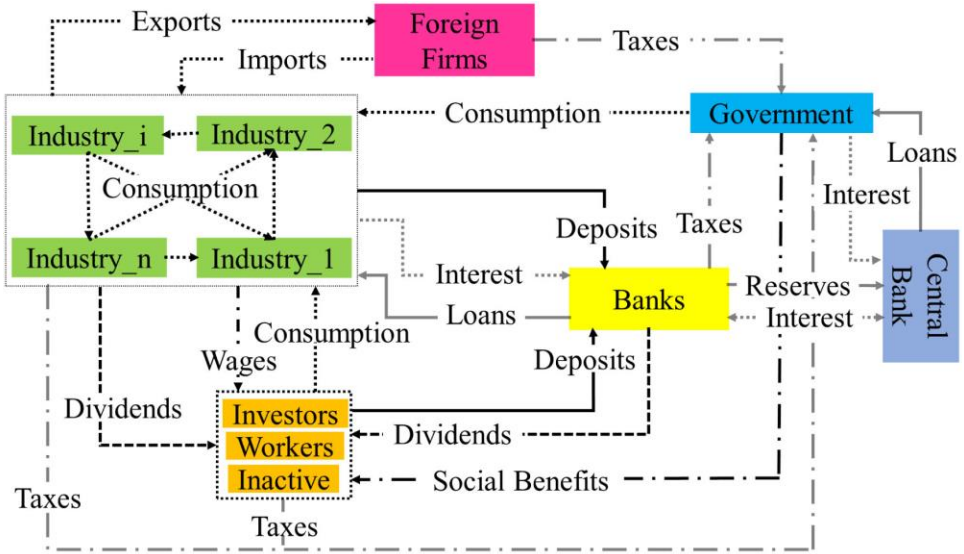


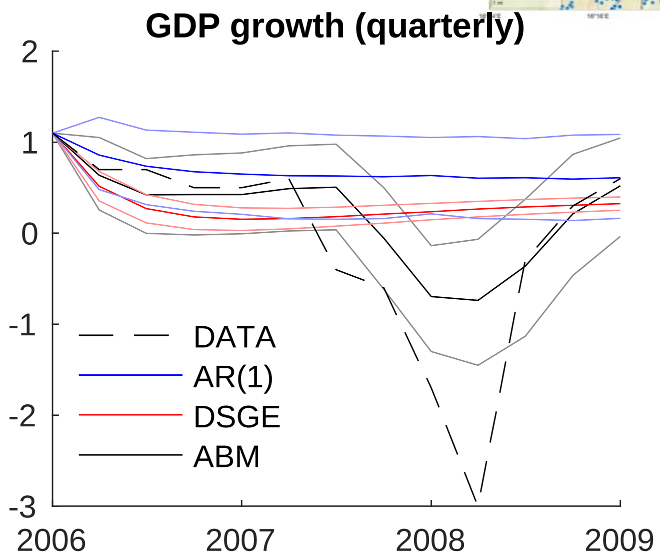
(Rebaudoa et al. 2011)

Macroeconomic agent-based model for the macro-economy

- Agent-based model with explicit sector detail and millions of interacting agents;
- intersectoral input-output and financial linkages;
- calibrated micro- and macroeconomic pms;
- microfoundations for heterogeneous agents, financial frictions, and bounded rationality



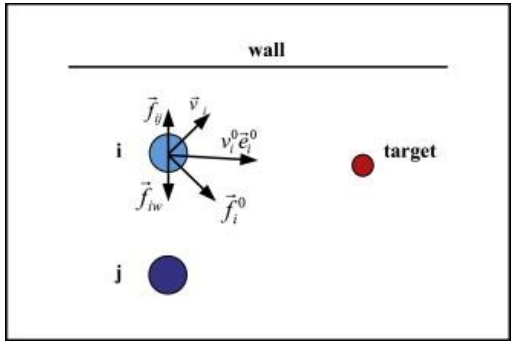


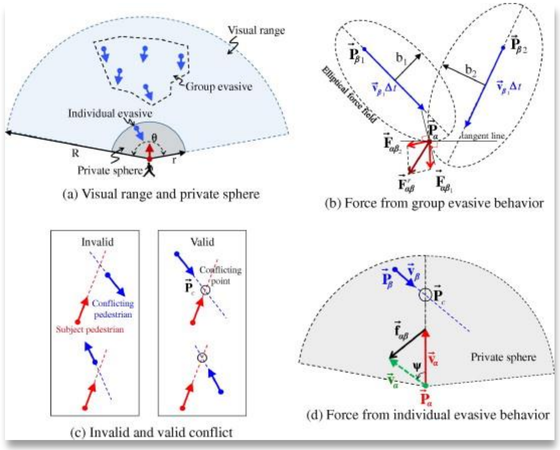


ABM GDP forecasts from the last quarter of 2006 for the euro area

(Poledna et al. 2020)

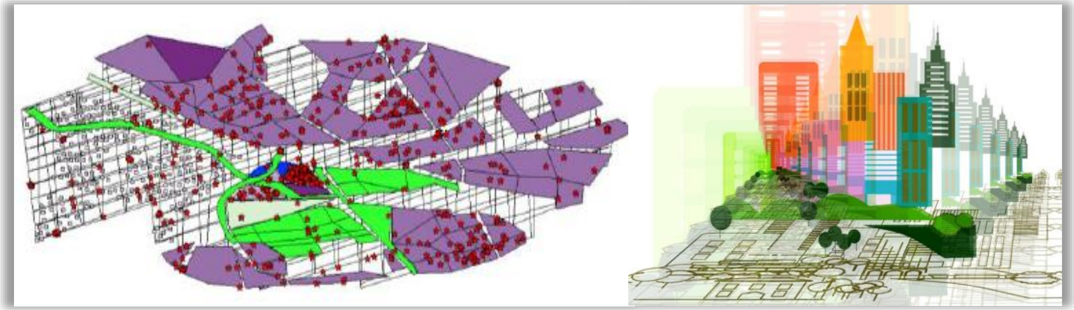
Social-force model: pedestrian behavior

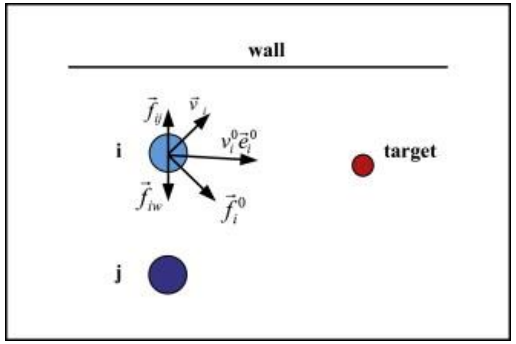


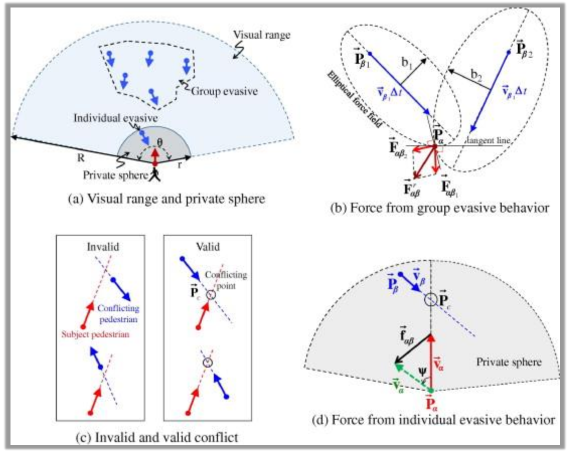


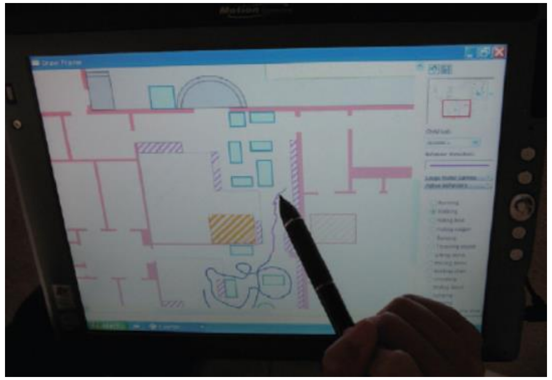
(Helbing and Molnár 1995; Johansson & Krietz 2011; Dam et al. 2014; Zeng et al. 2014; Gorrini et al. 2016; smartctlab.web.illinois.edu; unalab.eu)

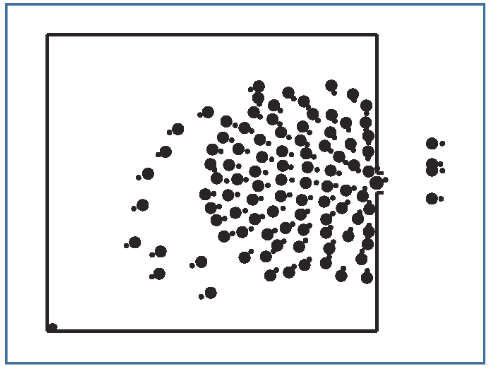
Social-force model: pedestrian behavior

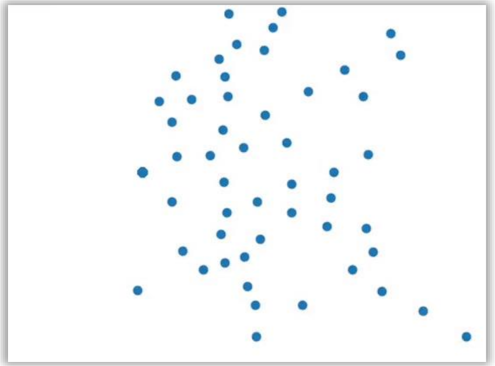






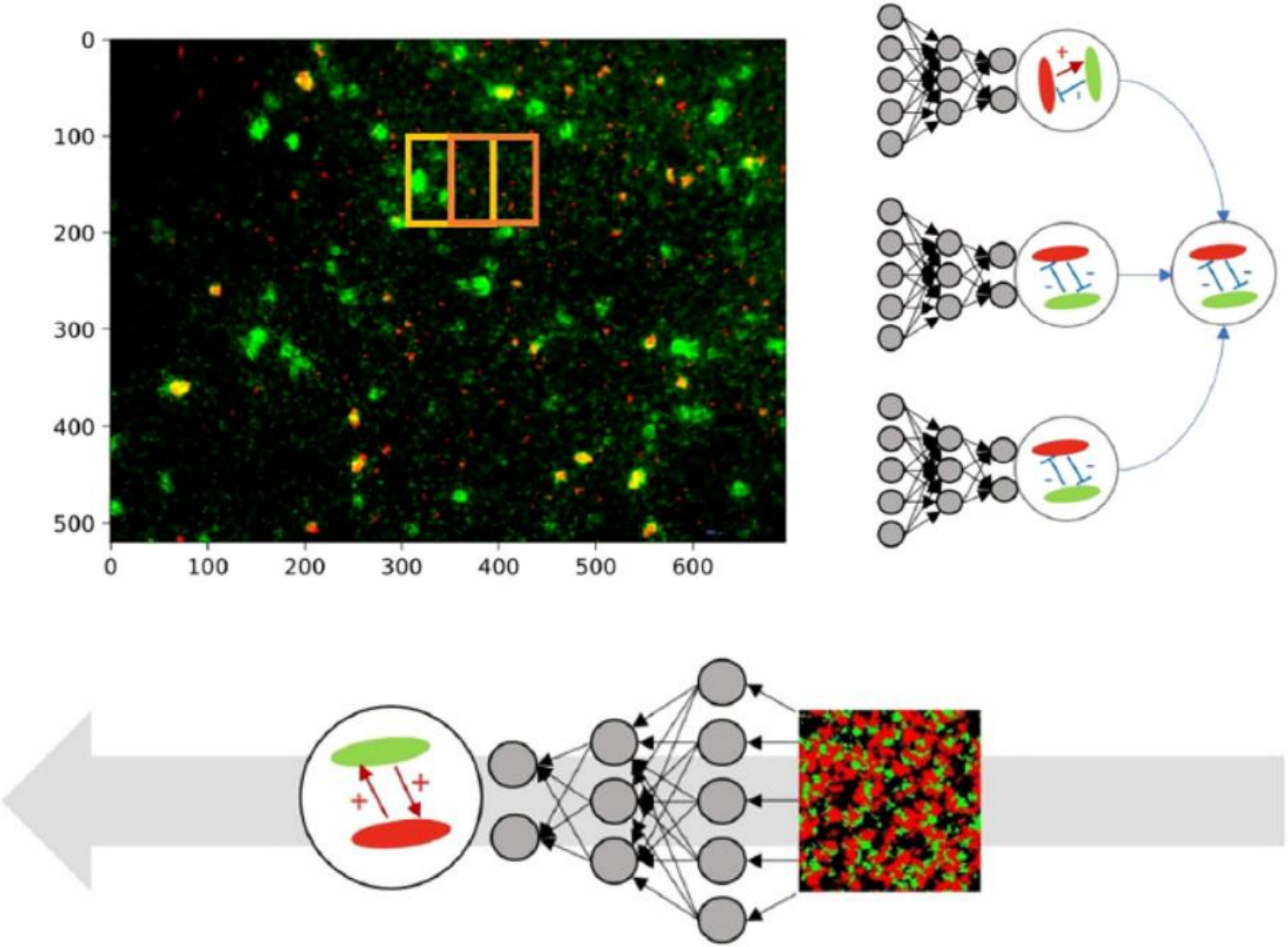






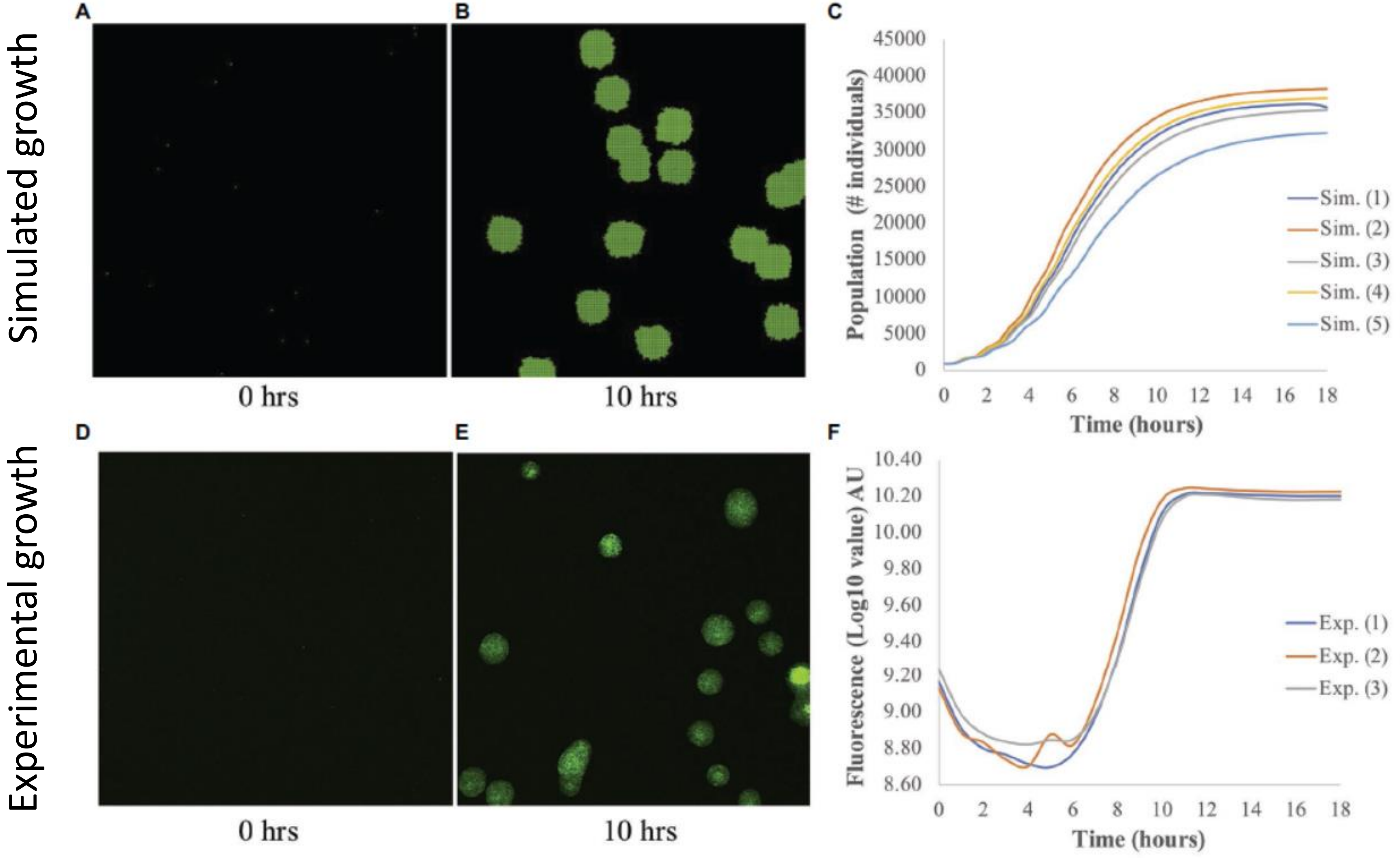
(Helbing and Molnár 1995; Johansson & Krietz 2011; Dam et al. 2014; Zeng et al. 2014; Gorrini et al. 2016; van Dam et al. smartctlab.web.illinois.edu; unalab.eu)

ABM & Machine learning: understanding interaction networks



(Lee et al. 2020)

ABM & Machine learning: parametrizing bacterial colony growth



Parameters	Description	Values [increment] (units)
Efficiency	Thermodynamic reactions efficiency	0.37 (–)*
umax_pa	Maximum growth rate of *Pantoea* individuals	0.1–10 [0.1] (h^{-1})
min/steptime	Time-scalable conversion from ticks to minutes	0.1–2 [0.5] (min)
diffusion-coefficient	Rate of redistribution of nutrients on each patch at each steptime	0–1 [0.01] (–)*
energy_maintenance_pa	Minimum carbon needed by *Pantoea* to survive in time	0.0015 ($gC_{glucose} \cdot gC_{pantoea}^{-1} \cdot h^{-1}$)
rep_pa	Minimum time needed by *Pantoea* to get ready for reproduction	20 (min)
max-time-viability_pa	Maximum time that *Pantoea* can survive without its minimum energy requirements	83 (min)
pmax	Maximum number of bacteria allowed in the same patch	1–10 [1] ($\# \cdot patch^{-1}$)
Ammonium	Initial concentration of ammonium in patches	18.7 (mM)
Glucose	Initial concentration of glucose in patches	0–100 [0.1] (mM)
Total-length-world	Value of world width and world height	605 (µm)
Depth	Depth of the first "layer" of medium where the bacteria grow	10–50 [1] (µm)
Microorganism	Initial number of *Pantoea* individuals	10–1,000 [1] (#)

(Chen et al. 2021)

Summary

- ABM is a extremely flexible modelling framework
- ABMs can be almost as complex as real life systems
- Very simple rules can recover patterns observed in the real world
- More than the sum of parts
- Modular structure, easy to develop further
- Unpredictable dynamics and resultant patterns: emergent behavior in a complex system

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Thank you!