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NetBioDyn, a smart Agent-Based software to intuitively model and simulate complex biological systems

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Objectives

To facilitate the process of **investigating, teaching and learning** complex biological systems

- **Creating realistic models and simulations** of complex biological systems to **investigate their dynamics** and **grasp complexity**
- **Reducing the gap** between the actual **programming skills** of (future) biologists and most modelling software needs
- Stimulating students **creativity** by promoting **abduction** (observe, build and test hypothesis)

Proposal

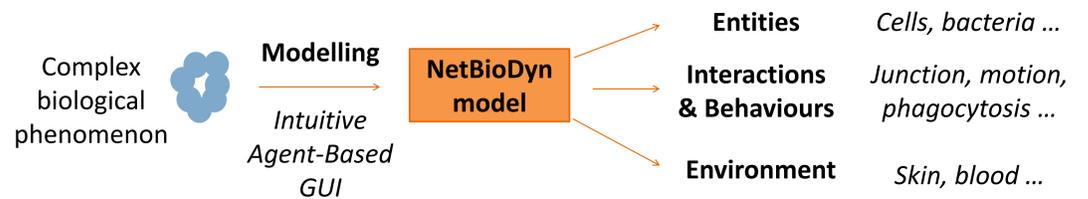
To design an **intuitive Agent-Based software** aimed at biologists (students, teachers, researchers) to easily build and simulate complex biological mechanisms observed in **multicellular** and **molecular** systems

Modelling and teaching complex biological systems

Scientific approach

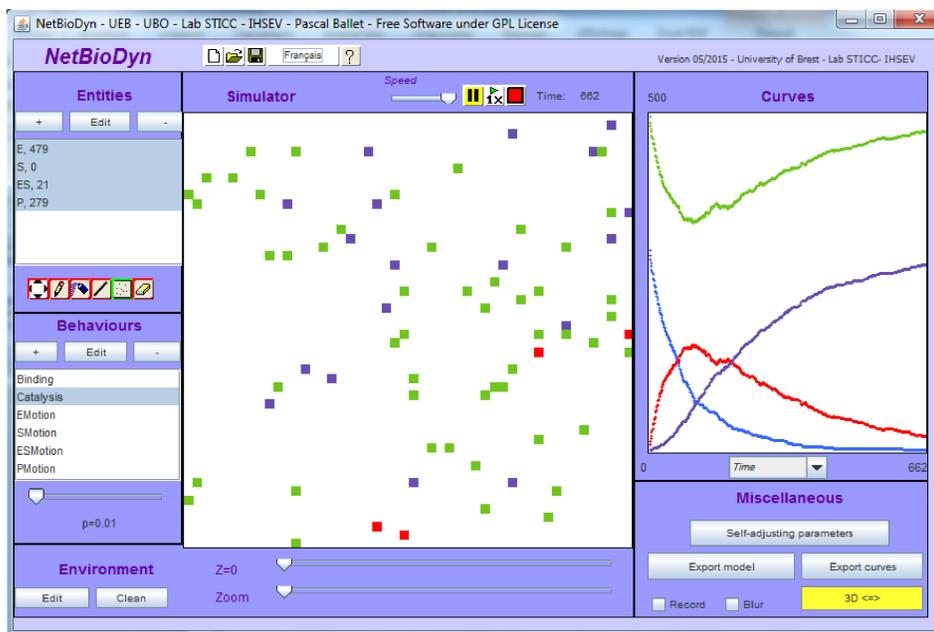
Using an **Agent-Based (discrete) approach** (vs. continuous)

- Focus on individuals (cells, molecules), their behaviour and their interactions, instead of population
 - Definition of **local interactions** leading to **global emerging behaviours**
 - **Variability** in cell population, cell differentiation
 - **Easier** to understand, do not require advanced mathematical skills
 - Model's **parameters are closer** to the field of biology
- Design of an **intuitive graphical user interface (GUI)** guided by the Multi-Agent paradigm



NetBioDyn, an intuitive and open-source software

<http://virtulab.univ-brest.fr/>



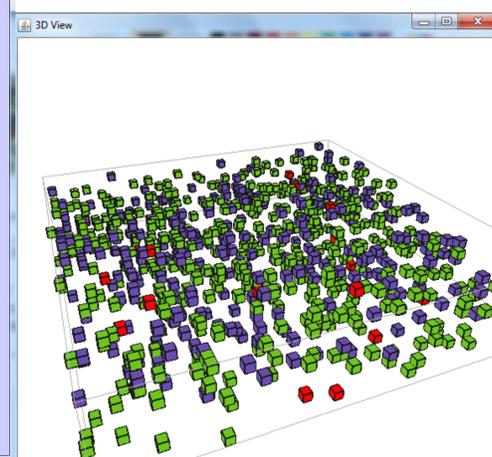
Enzyme kinetics
 $E + S \rightarrow ES \rightarrow P$

The environment is a 2D or 3D grid where entities interact according to their behaviours

- An entity occupies a whole grid cell
- Von Neumann neighbourhood: 4 neighbours in 2D and 6 in 3D
- Behaviours involving current entities are probabilistically performed at each time step

Specific graphical user interface

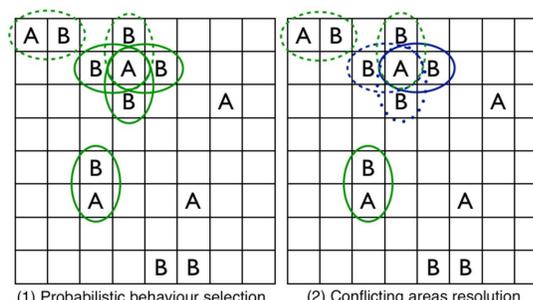
- Guided by the Multi-Agent paradigm (entities, behaviours and environment)
- No need of any prerequisite or knowledge in computer programming
- Providing at any time a simplified and complete view of the system's state (suitable *external representation*)



3D View

Self-adjusting mechanisms to calibrate the parameters of the model (*test phase*)

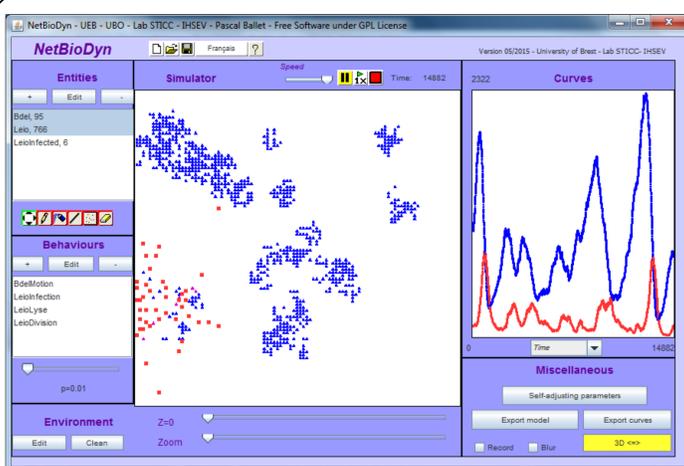
- Aiming at automatically find the proper values for all the parameters involved in a simulation
- Based on real results provided by users, obtained for example *in vitro*.



(1) Probabilistic behaviour selection

(2) Conflicting areas resolution

Name	behaviour	
Description	Short text of explanation	
Probability	Decimal number in [0, 1]	
Reactives	Positions	Products
A	+	A'
B	$\odot \uparrow$ $\leftarrow A \rightarrow$ $\downarrow \otimes$	B'
C	$\leftarrow A$ \downarrow	C'



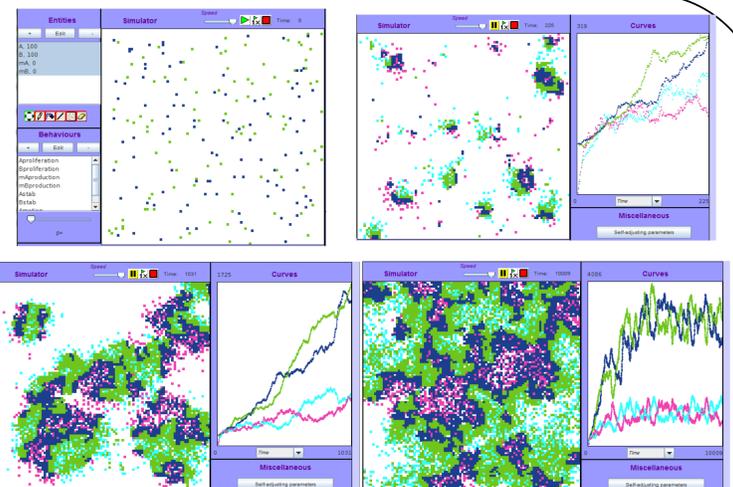
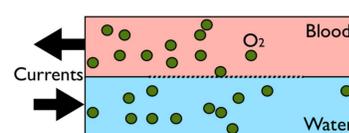
A predator-prey relationship involving two marine bacteria (*Bdellovibrio* and *Photobacterium leiognathi*)

- **Emergence** of interdependences and cycles between the two populations observed in real predator-prey systems

Examples of applications

Water-blood O₂ exchanges in Zebra Fishes

- **Investigating** the efficiency of the Zebra Fish counter-current respiratory system by **changing easily** the flow direction



A simple autopoietic system

- 4 entities: A, B and mA and mB (produced by A and B)
- A and B entities use each other's products (mA and mB) to multiply
- The system **converges** towards a balanced state

More examples of applications, tutorials and the software sources are available at <http://virtulab.univ-brest.fr/>