P Systems as a computational modeling framework

A. Riscos-Núñez

Research Group on Natural Computing
Department of Computer Science and Artificial Intelligence
Universidad de Sevilla

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Modeling

Cambridge dictionary

model *noun* [C] **(REPRESENTATION)**

A2 **something that represents another thing, either as a physical object that is usually smaller than the real object, or as a simple description that can be used in calculations:**

a plastic model aircraft

By looking at this model you can get a better idea of how the bridge will look.

to construct a statistical/theoretical/mathematical model

No computer model ***of*** *the economy can predict when the next recession will be.*

Modeling

What to Model

- **Relevant** ingredients / features
- Focus on the **Dynamics**

Why?

- Understand / Analyze
- Predict / Control

Requirements

- Keep it simple
- Simulation tools (Validation)

Computational Modeling

- Computational modeling and simulation are nowadays a cornerstone of the scientific method.

Desirable properties of a *good* model[1]

- Relevant
- Readable
- Extensible
- Computationally tractable

- **P systems** fulfill the requirements

[1] Regev, A., Shapiro, E. Cellular abstractions: Cells as computations. *Nature* **419**, 6905 (2002), 343-343.

- Differential Equations (ODEs/PDEs)

- Lindenmayer Systems `http://algorithmicbotany.org`
- Cellular Automata `http://cancerres.aacrjournals.org/content/70/1/46.abstract`
- Petri Nets
- Agent-based Systems
- Process Algebra, π–calculus
- P Systems (*Membrane Computing*) `http://www.gcn.us.es`

- P Systems based modeling framework
  - Ecosystems
  - Other bio-processes (e.g. at cellular level)
- Randomness $\rightarrow$ probabilistic/stochastic strategies

Simulation algorithms

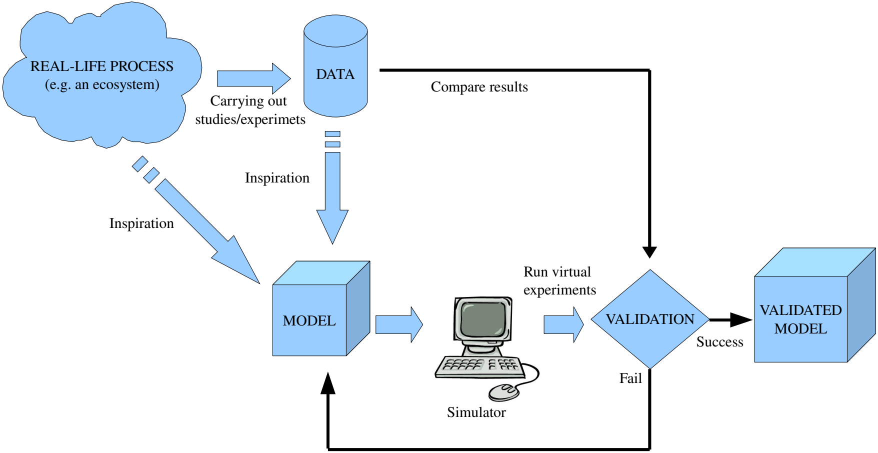
- Reproduce the behaviour of the models
- Validation
- Virtual experimentation

Software

- Implements the algorithms
- GUI for the end-user

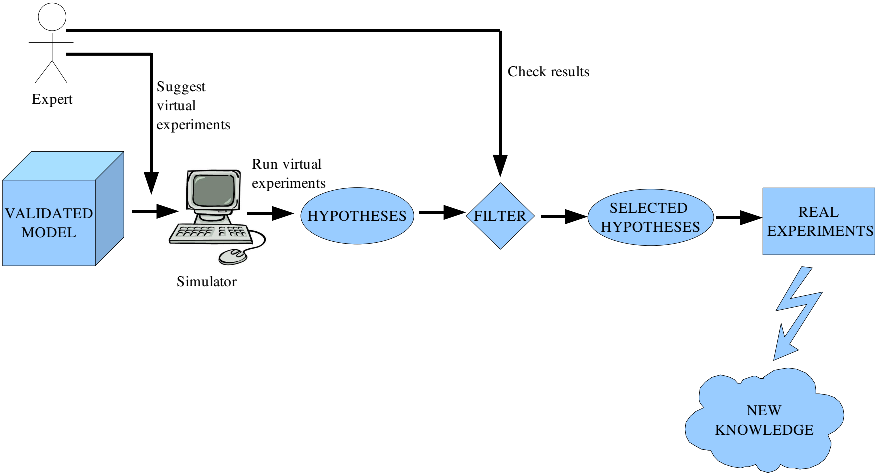
Where do models come from?

Validation process



Born to Run

Virtual Experiments



Modeling real-life ecosystems

Some studies within the RGNC

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Photo by Amy Benson, U.S. Geological Survey

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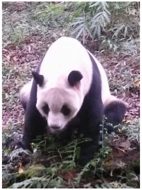


Photo by A. Riscos

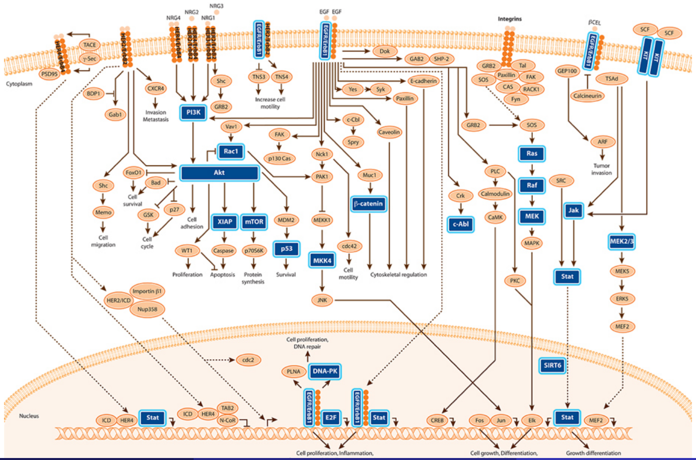
- **Modeling Ecosystems using P systems: The Bearded Vulture, a case study**. Cardona et al. *LNCS*, 5391, 137–156, (2009).
- **Modeling Population Growth of Pyrenean Chamois (Rupicapra p. pyrenaica) by Using P Systems**. M.A. Colomer et al. *LNCS*, 6501, 144–159, (2010).
- **Population Dynamics P System (PDP) Models: A Standardized Protocol for Describing and Applying Novel Bio-Inspired Computing Tools**. Colomer et al. *PLOS ONE*, 8 (4): e60698 (2013).
- **Application of a computational model for complex fluvial ecosystems: the population dynamics of zebra mussel Dreissena polymorpha as a case study**. Colomer et al. *Ecological Complexity*, 20 (2014).

Modeling at micro level (I)

In the framework of P systems

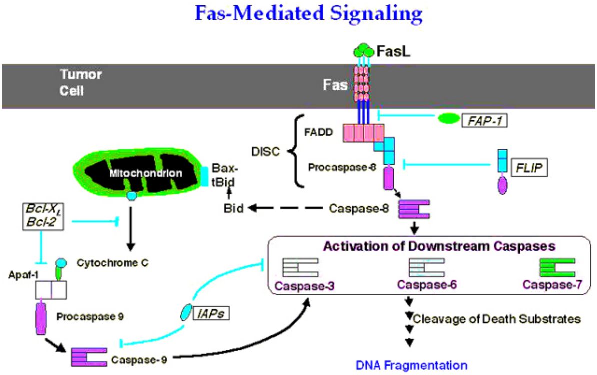
Cellular signalling pathways

- Epidermal growth factor receptor, EGFR



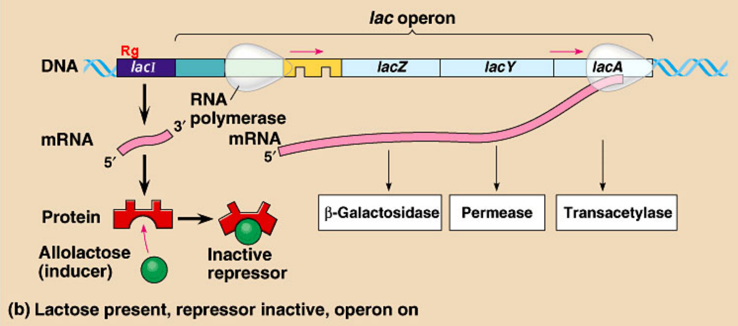
Cellular signalling pathways

- Apoptosis mediated by FAS protein



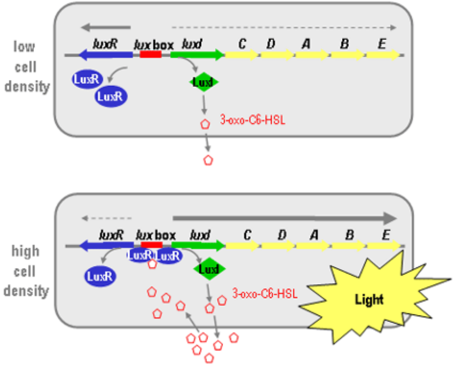
Gene regulation systems

- Lac Operon in E. coli



Quorum sensing systems in bacteria

- Cell density dependent gene regulation system



Quorum sensing in Vibrio fischeri (I)

- This phenomenon was first investigated for a marine bacteria *Vibrio fischeri*.
- *Vibrio fischeri* exhibits a **coordinated behaviour** which enables a **population of bacteria** to jointly regulate specific **genes expression** **according to the size** of the population.

Quorum sensing in Vibrio fischeri (II)

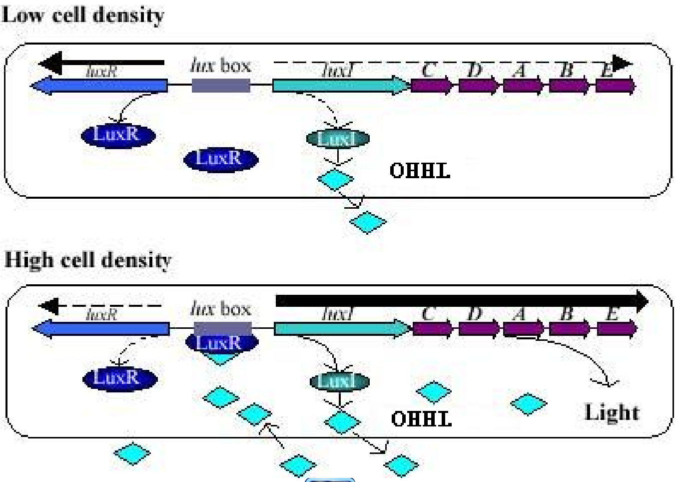
- Vibrio fischeri exists naturally either in a free-living planktonic state or as a symbiont of certain luminescent squid.
- The bacteria colonise specialised light organs in the squid.
- The source of the luminescence is the bacteria themselves.

Quorum sensing in Vibrio fischeri (III)

- Vibrio fischeri only emit light when living in colony within the luminescent organ, but not in planktonic state.
- Luminescence in the squid is involved in the attraction of prey, camouflage and communication between different individuals.

Quorum sensing in Vibrio fischeri (IV)

Molecular mechanisms (K.H. Nealson y J.W. Hasting, 1979; K.L Visic et al., 2000):



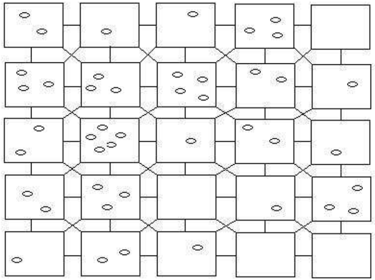
Modeling Quorum sensing system in Vibrio fischeri

We will study the behaviour of a population of N bacteria placed inside a multicompartmental P system of degree $(25, 1, N)$. [2].

$$\mathbf{ME} = (G, \Gamma, \Sigma, T, \mathcal{R}_E, \mu, \mathcal{R}, \Pi_1, \ldots, \Pi_N)$$

where:

- $G = (V = \{e_1, \ldots, e_{25}\}, S)$ is the following directed graph.



[2] F.J. Romero, M.J. Pérez-Jiménez. A model of the Quorum Sensing System in Vibrio fischeri using P systems. *Artificial Life*, **14**, 1 (2008), 95–109.

Modeling Quorum sensing system in Vibrio fischeri

- $\Gamma = \{\text{LuxR}, \text{LuxR.OHHL}, \text{LuxBox}, \text{LuxR.OHHL.LuxBox}, \text{OHHL}\}$.
- $\Sigma = \{\text{OHHL}\}$.
- $T \geq 1$.
- Rules from $\mathcal{R}_E$.

$$r_1 : (\ \text{OHHL}\ )_{e_i} \xrightarrow{c_1} (\ \ )_{e_i}$$
$$r_2 : (\ \text{OHHL}\ )_{e_i} \xrightarrow{c_2} (\ \text{OHHL}\ )_{e_j}$$
$$r_3 : (\ [\ \ ]_b\ )_{e_i} \xrightarrow{c_3} (\ [\ \ ]_b\ )_{e_j}$$

- $\mu = [\ \ ]_b$.

Modeling Quorum sensing system in Vibrio fischeri

- Rules from $\mathcal{R}$:

$$
\begin{aligned}
r_4 &: \text{OHHL} [\ ]_b \xrightarrow{c_4} [\text{OHHL}]_b \\
r_5 &: [\text{LuxBox}]_b \xrightarrow{c_5} [\text{LuxBox} + \text{OHHL}]_b \\
r_6 &: [\text{LuxBox}]_b \xrightarrow{c_6} [\text{LuxBox} + \text{LuxR}]_b \\
r_7 &: [\text{LuxR} + \text{OHHL}]_b \xrightarrow{c_7} [\text{LuxR.OHHL}]_b \\
r_8 &: [\text{LuxR.OHHL}]_b \xrightarrow{c_8} [\text{LuxR} + \text{OHHL}]_b \\
r_9 &: [\text{LuxR.OHHL} + \text{LuxBox}]_b \xrightarrow{c_9} [\text{LuxR.OHHL.LuxBox}]_b \\
r_{10} &: [\text{LuxR.OHHL.LuxBox}]_b \xrightarrow{c_{10}} [\text{LuxR.OHHL} + \text{LuxBox}]_b \\
r_{11} &: [\text{LuxR.OHHL.LuxBox}]_b \xrightarrow{c_{11}} [\text{LuxR.OHHL.LuxBox} + \text{OHHL}]_b \\
r_{12} &: [\text{LuxR.OHHL.LuxBox}]_b \xrightarrow{c_{12}} [\text{LuxR.OHHL.LuxBox} + \text{LuxR}]_b \\
r_{13} &: [\text{OHHL}]_b \xrightarrow{c_{13}} \text{OHHL} [\ ]_b \\
r_{14} &: [\text{OHHL}]_b \xrightarrow{c_{14}} [\ ]_b \\
r_{15} &: [\text{LuxR}]_b \xrightarrow{c_{15}} [\ ]_b \\
r_{16} &: [\text{LuxR.OHHL}]_b \xrightarrow{c_{16}} [\ ]_b
\end{aligned}
$$

Modeling Quorum sensing system in Vibrio fischeri

- $\Pi_k = (\Sigma, L, \mu, M_1, \mathcal{R})$, $1 \leq k \leq N$, where:
  - $\Sigma = \{\text{OHHL}\}$.
  - $L = \{b\}$.
  - $\mu = [\ ]_b$.
  - $M_1 = \{LuxBox\}$.

Stochastic Constants associated with the rules:

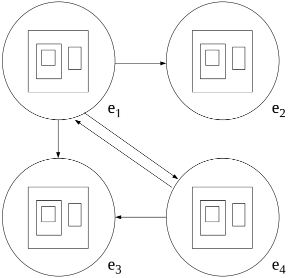
$c_1 = 5, c_2 = 8, c_3 = 2, c_4 = 1, c_5 = 2, c_6 = 2, c_7 = 9, c_8 = 1,$
$c_9 = 10, c_{10} = 2, c_{11} = 250, c_{12} = 200, c_{13} = 50, c_{14} = 30, c_{15} = 20, c_{16} = 20.$

1. Modeling framework
2. **A P system based modeling framework**
3. Example: Tritrophic Interactions
4. A software framework for Membrane Computing
   - Simulation algorithms
   - Simulation results
5. Conclusions and future work

Need to define a new variant of P Systems

- Cooperation
- Randomness
- Communication between environments
- Membrane polarization

A P system based modeling framework



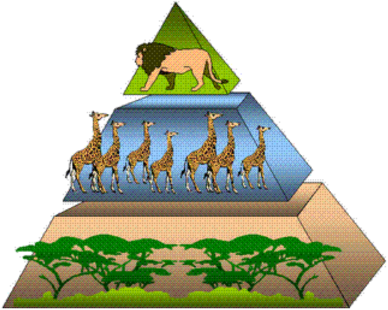
Skeleton rules

$$u\ [\ v\ ]_h^{\alpha} \xrightarrow{f_r} u'\ [\ v'\ ]_h^{\beta}$$

Environment rules

$$(a)_{e_j} \xrightarrow{f_r} (b)_{e_k}$$

Example: Tritrophic interactions



- Simplification of a real ecosystem
- Three trophic levels
  - (3) A Carnivore
  - (2) Herbivores
  - (1) Grass

Tritrophic interactions

The model consists of 5 modules

1. Reproduction + Grass production
2. Feeding / Hunting + Natural mortality
3. Lack of food: migration
4. Feeding
5. Restore Initial Config.

- represents a one-year cycle
- several computation steps per module
- 10 geographical areas

Tritrophic interactions

Reproduction + Grass production

- Grass production

$$r_{1,j} \equiv X_1[\,]_1^0 \xrightarrow{m_j} [X_1, G^{h_j}]_1^+,\ 1 \le j \le 3$$

- Females which reproduce and generate d_i offsprings.

$$r_{2,i} \equiv [X_i]_1^0 \xrightarrow{k_{i,1}\cdot 0.5} [X_i^{1+d_i}]_1^+, 2 \le i \le 7$$

- ...

Tritrophic interactions

Feeding + Natural mortality

- Animals which feed and survive.

$$r_{5,i} \equiv [X_i G^{f_i}]_1^+ \xrightarrow{1-k_{i,2}} [Y_i]_1^-, 2 \le i \le 6$$

$$r_{6,i} \equiv [X_7 X_i^{f_7}]_1^+ \xrightarrow{1-k_{7,2}} [Y_7]_1^-, 2 \le i \le 6$$

- Animals which feed and don't survive.

$$r_{7,i} \equiv [X_i G^{f_i}]_1^+ \xrightarrow{k_{i,2}} [\ ]_1^-, 2 \le i \le 6$$

$$r_{8,i} \equiv [X_7 X_i^{f_7}]_1^+ \xrightarrow{k_{7,2}} [\ ]_1^-, 2 \le i \le 6$$

Tritrophic interactions

Lack of food: migration

- Movement of objects between environments.

$$r_{12,k,s,i} \equiv (X_i)_{e_k} \xrightarrow{p_{k,s,i}} (X_i')_{e_s},\ 1 \leq k, s \leq 10, 2 \leq i \leq 7$$

- ...

Tritrophic interactions

Resources in the new area $\rightarrow$ possibility to feed and survive.

Feeding

$$r_{16} \equiv [X_i' G^{f_i}]_1^- \xrightarrow{1-k_{i,2}} [Y_i]_1^0, 2 \leq i \leq 6$$

$$r_{17} \equiv [X_7' X'^{f_7}_i]_1^- \xrightarrow{1-k_{7,2}} [Y_7]_1^0, 2 \leq i \leq 6$$

$$r_{18} \equiv [X_7' Y_i^{f_7}]_1^- \xrightarrow{1-k_{7,2}} [Y_7]_1^0, 2 \leq i \leq 6$$

Tritrophic interactions

Reinit of the cycle

$$r_{23,i} \equiv [Y_i]_1^0 \longrightarrow [X_i]_1^0, 2 \leq i \leq 7$$

$$r_{24} \equiv [R_6]_1^0 \longrightarrow [R_0]_1^0$$

$$r_{25} \equiv [X_1]_1^0 \longrightarrow X_1[\;]_1^0$$

$$r_{26,i} \equiv [X_i']_1^0 \longrightarrow [\;]_1^0, 2 \leq i \leq 7$$

$$r_{27} \equiv [G]_1^0 \longrightarrow [\;]_1^0$$

Simulators for P systems

Simulation vs Implementation

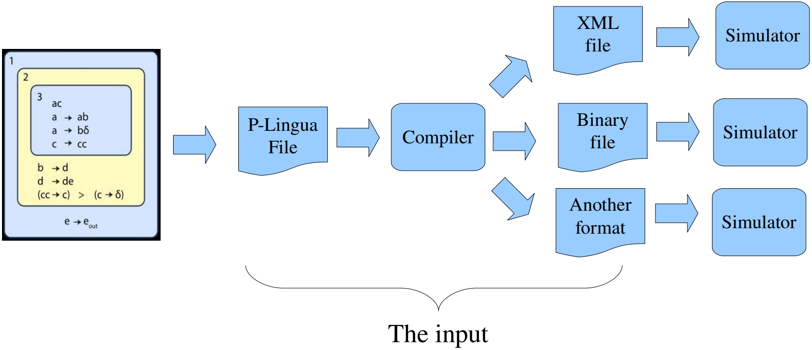
- P systems have not been implemented yet
- It is necessary software/hardware to simulate P system computations

Applications of simulators

- Pedagogical tools
- Support researching in Membrane Computing
- Simulation, validation and virtual experimentation over models of real-life phenomena

Command-line compilation tool

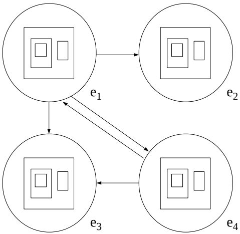
Interoperability



pLinguaCore

Java library for parsing, exporting and simulating

- Free software (GNU GPL license)
- It reads P-Lingua files
- It implements several simulation algorithms
- It exports to other file formats
- Text interface
- It can be used in other Java applications
- It can be extended
- Web page: `http://www.p-lingua.org`



Skeleton rules

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Environment rules

$$(a)_{e_j} \xrightarrow{f_r} (b)_{e_k}$$

Algorithms for probabilistic behaviour

- Binomial Block Based (**BBB**) simulation algorithm
- Direct Non-Deterministic distribution algorithm with Probabilities (**DNDP**)
- Direct distribution based on Consistent Blocks Algorithm (**DCBA**)
- . . .

Simulation algorithms

Rules are applied in a *maximal parallel way according to their probabilities*

General scheme

1. **Selection** process:
   decides which rules to apply and how many times
2. **Execution** process:
   updates the configuration according to rules RHS

BBB: Binomial Block-based

Selection

Loop over **all** blocks (🔀)

- Loop over **all*** rules (🔀)
  - choose randomly the number of applications (*Binomial distrib. on the **remaining** objects*)
  - * the last rule takes it all

DNDP: Direct Non-deterministic Distribution with Probabilities

First Selection (consistency)

Loop over **all** rules (⤨)

- If rule is consistent with previous ones (otherwise discard)
  - choose randomly the number of applications (*Binomial distrib. on the* ***total*** *available objects*)

Second Selection (maximality)

Loop over selected rules (ordered by probabilities)

- apply as many times as possible

DCBA: Direct distribution based on Consistent Blocks Algorithm

Selection: 1. Distribution; 2. Maximality; 3. Probability

1. Filter: block charges (F1); block objs. (F2); dummy objs. (F3)

Loop over rows (object,region)

- for each element: $/$ by row sum and $*$ by obj. multiplicity

Loop over columns (blocks)

- number of applications $\equiv$ minimum

2. Loop over blocks ( ): maximize applications

3. Loop over blocks: (*Multinomial distrib.*) $\Rightarrow$ rule applications

Execution stage

Execution (for BBB, DNDP, DCBA)

Loop over selected rules $\langle r, n \rangle$

- Add $n \cdot$ RHS(r)
- update charges

MeCoSim. A specific Java GUI over pLinguaCore

- **Input**
  - Initial ecosystem parameters
  - Simulation algorithm
  - Number of years (complete cycles) to simulate
  - Number of simulations per year
- **Output**
  - Evolution of the populations
  - Tables and graphs

Future (joint) work

Please join in!

- **Theoretical foundations**
- **Computational complexity**
- **Applications**
- **Simulators**
- **Implementation**

Thanks for your attention!