Modeling with membranes in RGNC from micro to macro

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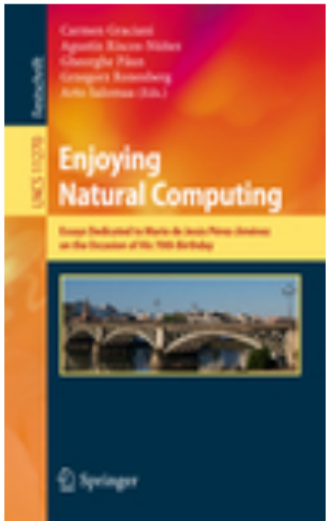
Basic references



Enjoying Natural Computing

Graciani et al. (Eds.) 2018

Bulletin of the IMCS

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.

- **something such as an object, plan, or set of rules that is used to show what something else is like or how it works:**

  a scale/working model *Retailers expect to have a working model and retail pricing information by summer.*

  economic/financial/mathematical model *No economic model can forecast growth in jobs in industries that are just being created.*

  statistical/strategic model *The charts shows a predicted oil price that is calculated using a statistical model.*

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.

Membrane computing

New modeling framework

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

Simulation algorithms

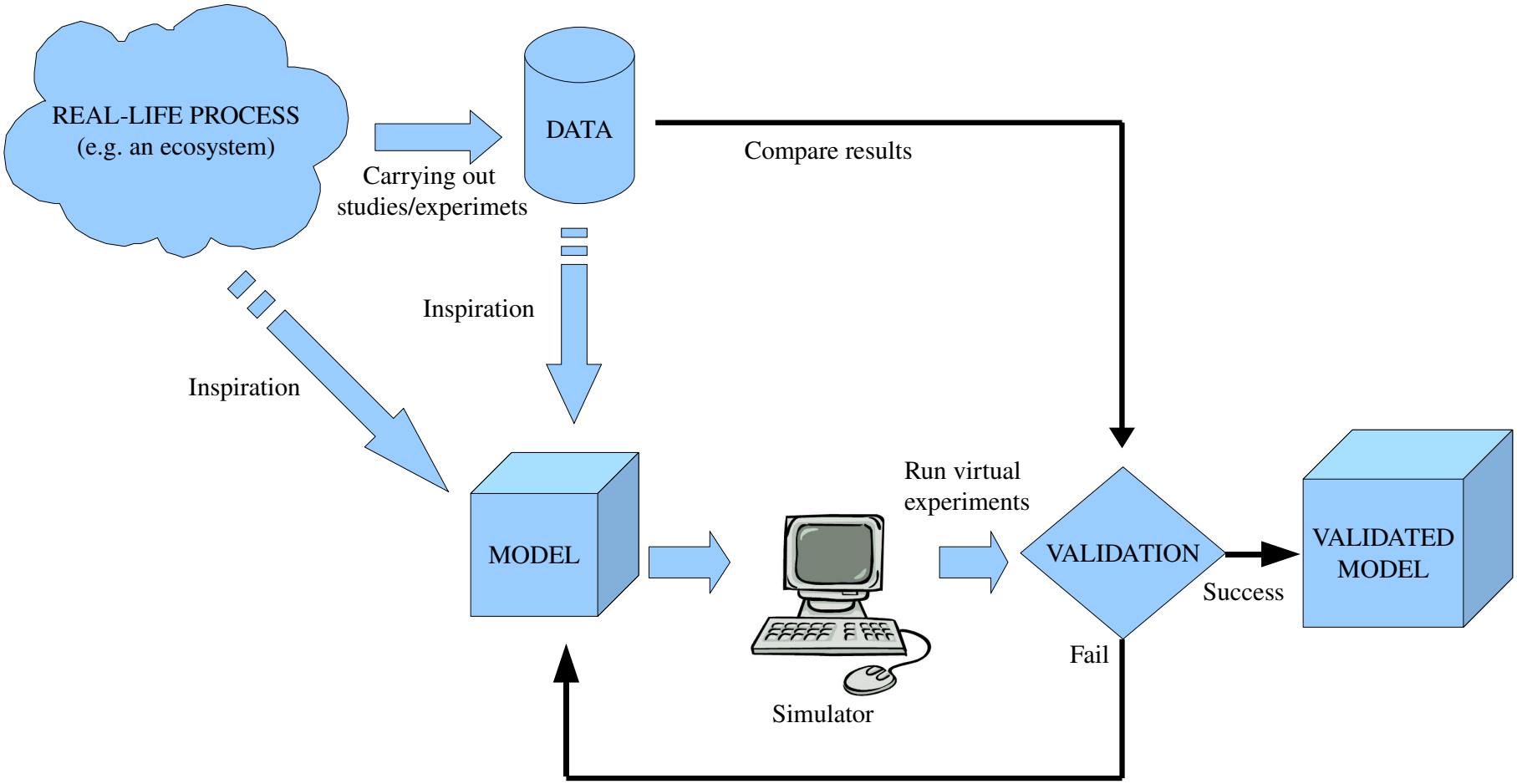
- Reproduce the behaviour of the models
- Validation
- Virtual experimentation

Software

- Implements the algorithms
- GUI for the end-user

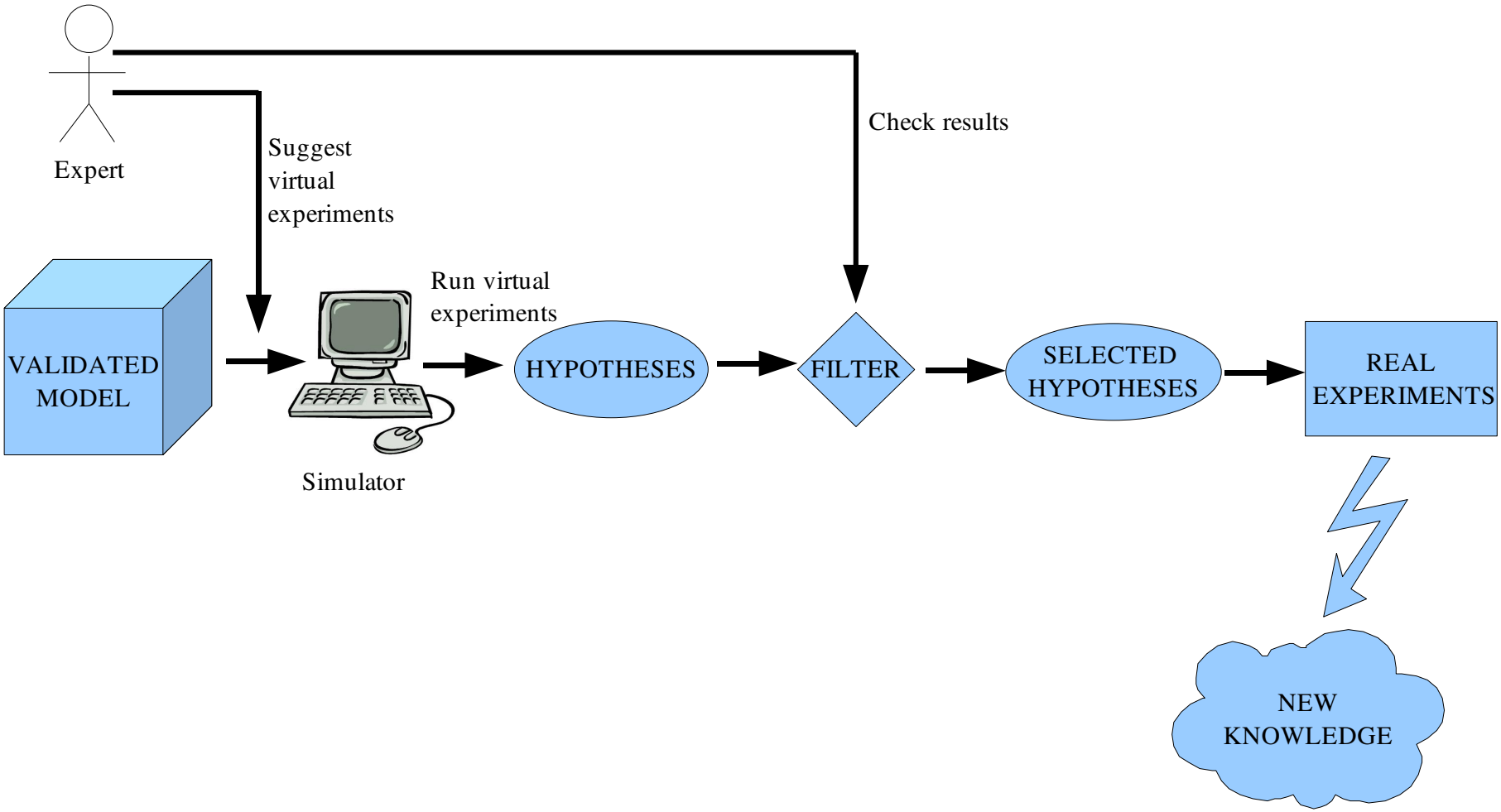
Where do models come from?

Validation process



Born to Run

Virtual Experiments



First micro-modeling works

- Epidermal growth factor receptor (EGFR) signalling pathways

  Modelling EGFR signalling network using continuous membrane systems.

  M.J. Pérez-Jiménez, F.J. Romero-Campero, In: *CMSB 2005*, pp. 118–129.

- Apoptosis mediated by FAS protein

  Simulating FAS-induced apoptosis by using P systems.

  S. Cheruku et al. *Prog. Nat. Sci.* 17, 424–431 (2007)

- Gene regulation systems: Lac Operon in E. coli

  Modelling gene expression control using P systems: The Lac Operon, a case study.

  F.J. Romero-Campero and M.J. Pérez-Jiménez, *Biosystems*, 91, 438-457 (2008)

- Quorum sensing in Vibrio fischeri

  A model of the Quorum Sensing System in Vibrio fischeri using P systems.

  F.J. Romero, M.J. Pérez-Jiménez *Artificial Life*, 14, 1 (2008), 95–109.

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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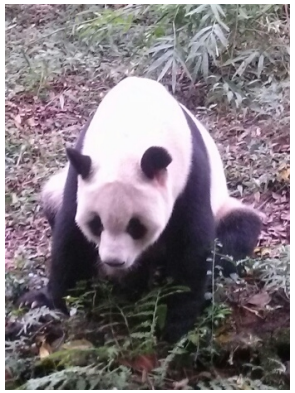


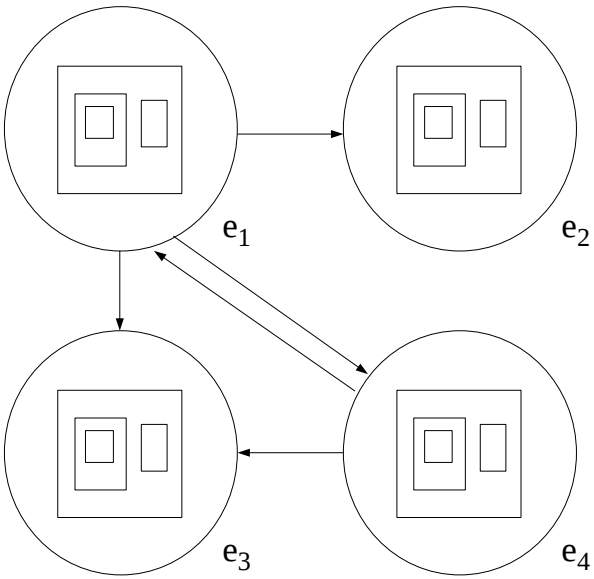
Photo by A. Riscos

- **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).

Need to define a new variant of P Systems

- Cooperation
- Randomness
- Communication between environments
- Membrane polarization

A P system based modeling framework



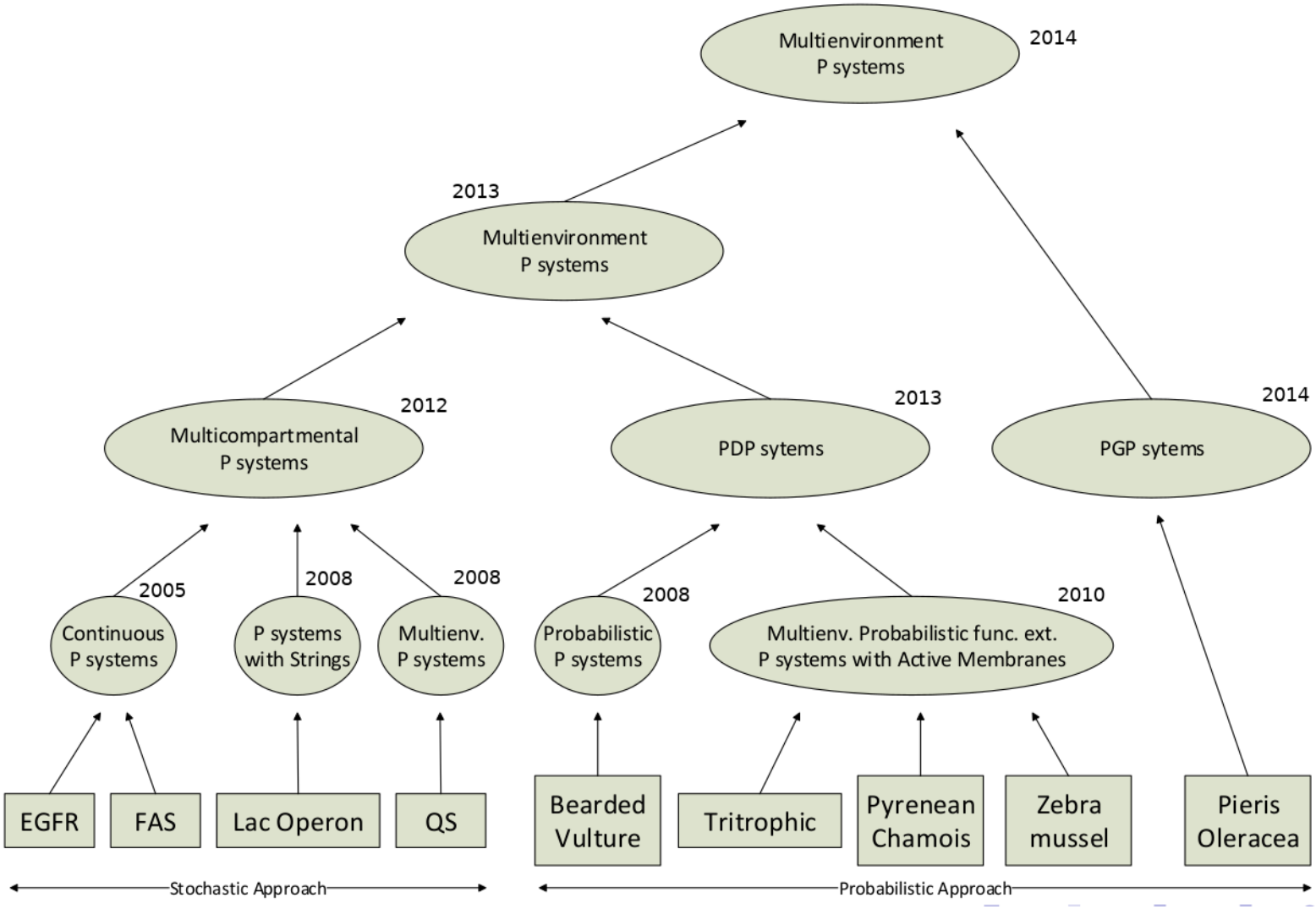
Skeleton rules

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

Environment rules

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

A P system based modeling framework



Example

Protein complex formation / dissociation

$$r_7 : [\ \text{LuxR} + \text{OHHL}\ ]_b \xrightarrow{c_7} [\ \text{LuxR.OHHL}\ ]_b$$

$$r_8 : [\ \text{LuxR.OHHL}\ ]_b \xrightarrow{c_8} [\ \text{LuxR} + \text{OHHL}\ ]_b$$

Feeding + Natural mortality

- Animals which feed and survive / don't survive.

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

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

Simulators for P systems

Simulation vs Implementation

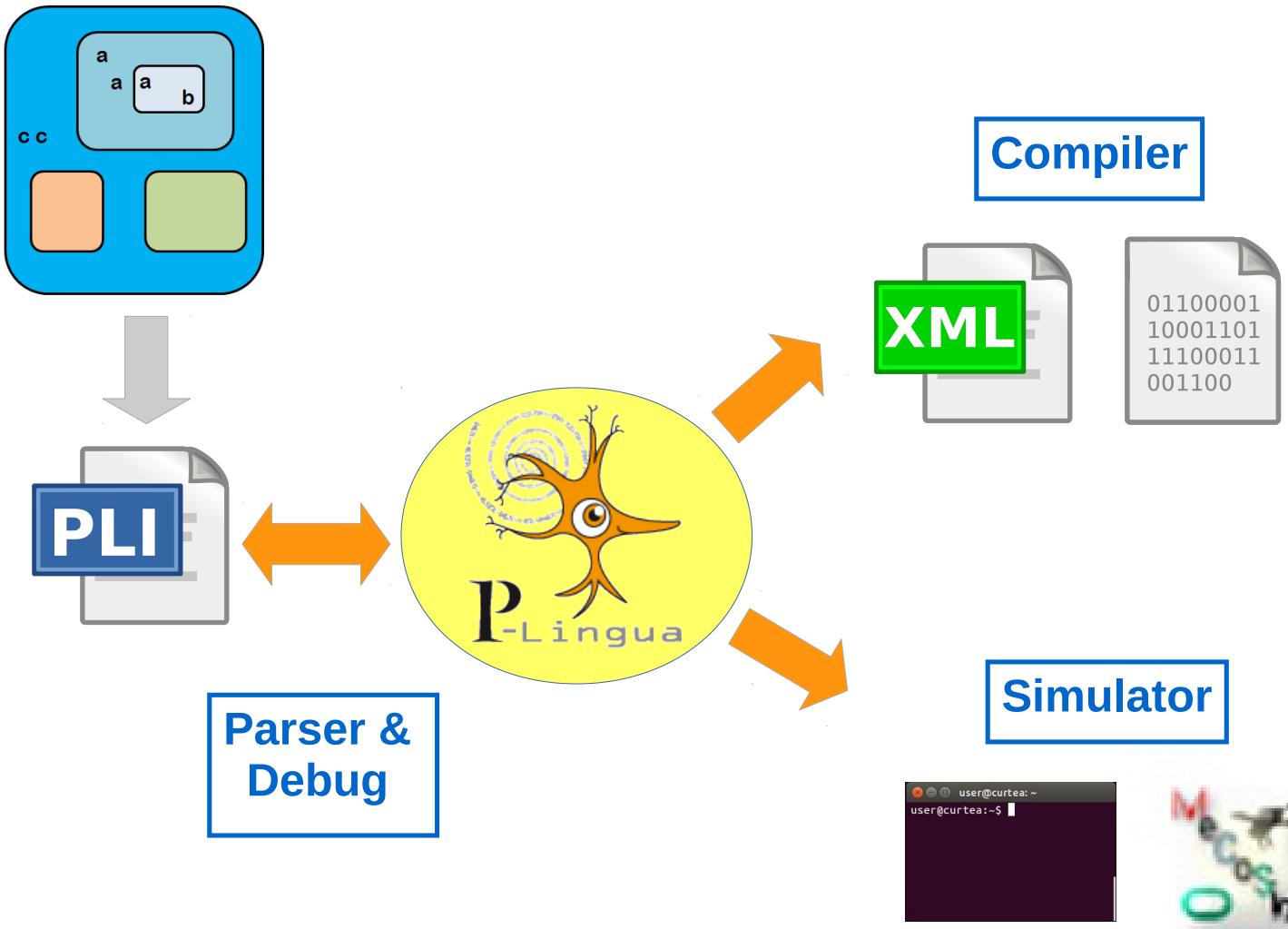
- P systems have not been implemented yet
- It is necessary software/hardware to simulate P system computations

Applications of simulators

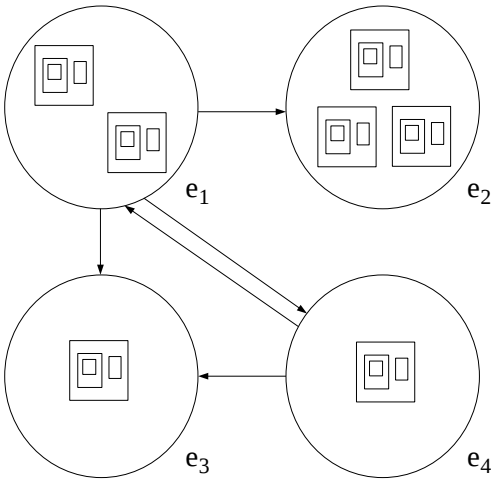
- Pedagogical tools
- Support researching in Membrane Computing
- Simulation, validation and virtual experimentation over models of real-life phenomena

pLinguaCore functionalities

Free software (GNU GPL license) `http://www.p-lingua.org`



Multicompartmental P systems



Skeleton rules

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

Environment rules

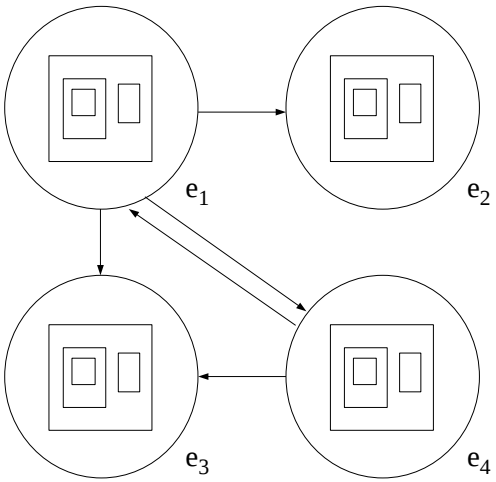
$$(a)_{e_j} \xrightarrow{fr} (b)_{e_k}$$

$$([\,]_h)_{e_j} \xrightarrow{fr} ([\,]_h)_{e_k}$$

Algorithms for stochastic approach

- Deterministic Waiting Times Algorithm
- Multicompartmental Gillespie Algorithm
- ...

Population Dynamics P systems



Skeleton rules

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Environment rules

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

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

Understanding MeCoSim philosophy

Application, Model, Scenario

Application

- Customized GUI for given model and scenario (`.XLS` file)
- Ready for virtual experimentation (end-user)

Model

- P system definition (`.PLI` file)
- might use parameters

Scenario

- Initial configuration
- Parameter values (if any)

Simulation Algorithm

- for each model, at least one simulation algorithm in *pLinguaCore*
- "`Simulation -> Options -> Simulation Algorithm`"
- can be connected to an external simulator

Understanding MeCoSim philosophy

Simulations, Cycles, Steps

Simulations

- number of repetitions (if probabilistic behaviour)

Cycles

- halting condition (number of cycles)

Steps

- a cycle is the time unit of interest when studying a biological phenomenon (30 min, 1 week, 25 years, etc.)
- for each cycle, several P system steps might be required

Future (joint) work

Please join in!

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

Thanks for your attention!