

MaBoSS Tutorial

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19th European Conference on Computational Biology

September 1, 2020

<https://github.com/migp11/ECCB2020-T05>

README.md



ECCB2020-T05

Computational modelling of cellular processes: regulatory vs metabolic systems

This repo contains all the material for the tutorial 05 of ECCB

Use with binder



This will open a window which will launch the Jupyter notebook.

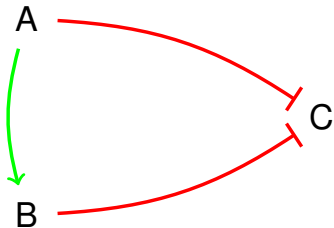
Use with docker

To run this notebook using the built docker image, run :

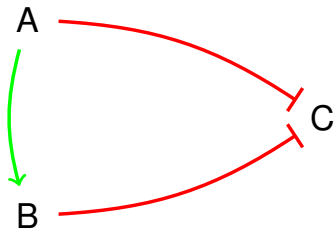
```
docker run -p 8888:8888 -d sysbiocurie/eccb2020-t05
```

Then open a window at <http://localhost:8888/tree/ECCB2020-T05>

Introduction

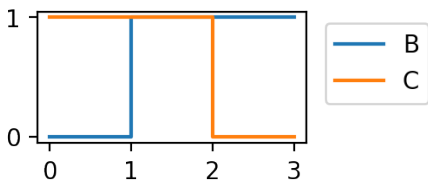


Introduction

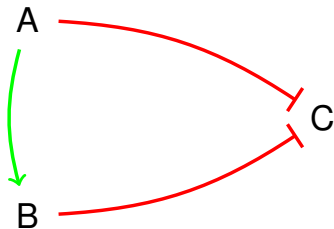


Boolean

- › A: input
- › B: A
- › C: !A & !B

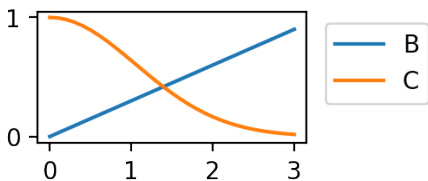


Introduction



ODEs

- › $\frac{dA}{dt} = 0$
- › $\frac{dB}{dt} = k_1 \cdot A$
- › $\frac{dC}{dt} = -k_2 \cdot A \cdot B \cdot C$



Methodology article | [Open Access](#) | Published: 29 August 2012

Continuous time boolean modeling for biological signaling: application of Gillespie algorithm

[Gautier Stoll](#) , [Eric Viara](#), [Emmanuel Barillot](#) & [Laurence Calzone](#)

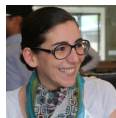
[BMC Systems Biology](#) 6, Article number: 116 (2012) | [Download Citation](#) 
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Gautier Stoll



Eric Viara



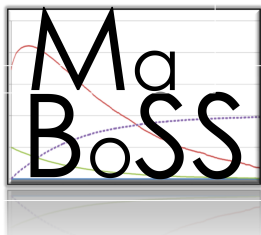
Laurence Calzone



Emmanuel Barillot

Introduction

Markovian Boolean Stochastic Simulator



<https://maboss.curie.fr/>

- › Boolean
- › Model asymptotic and transient behavior
- › Physical time
- › Handle different time scale processes (transcription, phosphorylation, etc.)

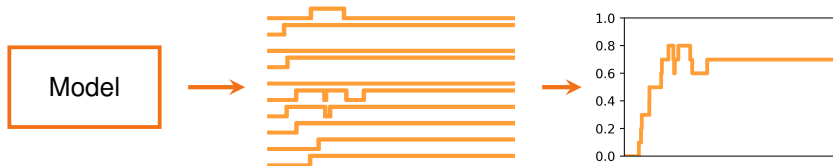
⇒ Fills the gap between ODE and Boolean modeling

Introduction

Continuous time Markov process applied on a Boolean network state space

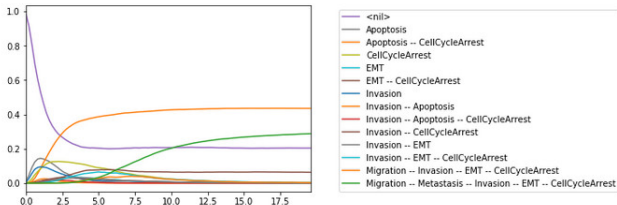
Transition rate :

$$p(S \rightarrow S') = \begin{cases} R_{up}(S), & \text{if } S_i = 0 \\ R_{down}(S), & \text{if } S_i = 1 \end{cases}$$

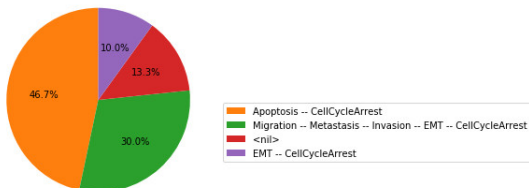


Introduction

› State distribution trajectories



› Final states distribution



Introduction

BND file : Network definition

```
1 node A {
2     logic = 1;
3     rate_up = @logic ? 1 : 0;
4     rate_down = 0;
5 }
6
7 node B {
8     logic = A & !C;
9     rate_up = @logic ? $act_B : 0;
10    rate_down = 0;
11 }
12
13 node C {
14     logic = A & !B;
15     rate_up = @logic ? $act_C : 0;
16     rate_down = 0;
17 }
18
```

CFG file: Model and Simulation settings

```
1 A.istate = FALSE;
2 B.istate = FALSE;
3 C.istate = FALSE;
4
5 $act_B = 1;
6 $act_C = 1;
7
8 max_time = 20.0;
9 sample_count = 1000.0;
10 use_physrandgen = 1.0;
11 thread_count = 1.0;
12
```

pyMaBoSS

- › Initially developped by Nicolas Levy
- › Maintained by Aurelien Naldi, Loic Pauleve, me
- › Available on Pypi:
\$ pip install maboss
- › Available on Conda:
\$ conda install -c colomoto pymaboss



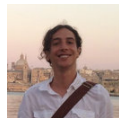
Nicolas Levy



Aurelien Naldi



Loïc Paulevé



Vincent Noël

Tutorial

- › How to create a MaBoSS model
 - › By hand
 - › From an existing boolean model
- › View results
 - › As figures
 - › As pandas dataframes
- › How to modify simulation/model parameters
 - › Initial states
 - › Model parameters
 - › Create mutants
 - › Reducing states combinatorials

We have state distributions, which can show different phenotypes, but the size of the whole population is fixed.

What if we want to use MaBoSS to create population models, whose population size is evolving ?



New Results

[Comment on this paper](#)

UPMaBoSS: a novel framework for dynamic cell population modeling

Gautier Stoll, Aurélien Naldi, Vincent Noël, Eric Viara, Emmanuel Barillot, Guido Kroemer,
 Denis Thieffry, Laurence Calzone

doi: <https://doi.org/10.1101/2020.05.31.126094>



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Eric Viara



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Emmanuel Barillot



Aurelien Naldi



Vincent Noël



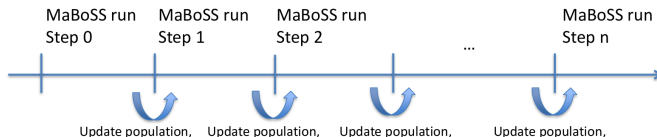
Denis Thieffry



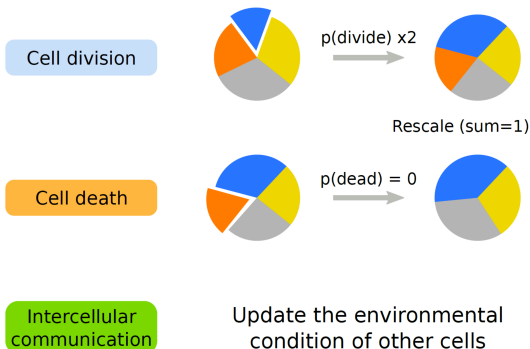
Guido Kroemer

UPMaBoSS

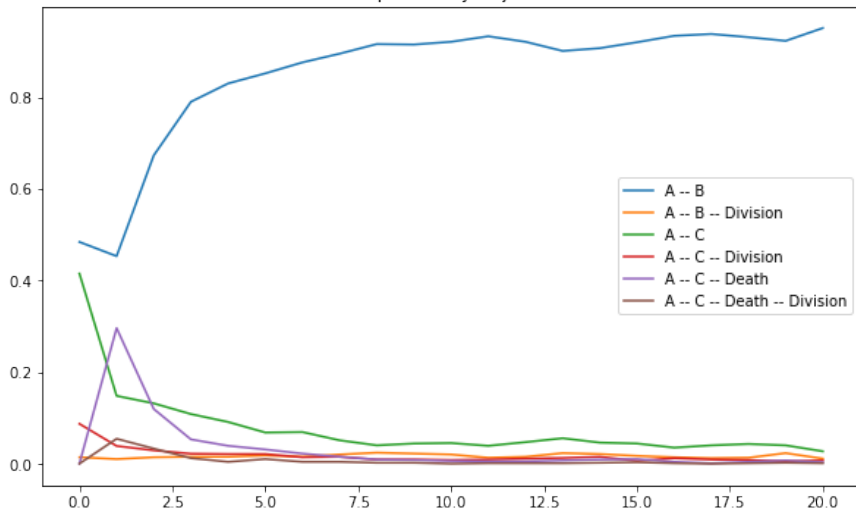
- › We start from an existing MaBoSS model
- › We add model nodes for division and death
- › We add inter-cellular communication
- › Chaining MaBoSS simulations, updating population and communication between each

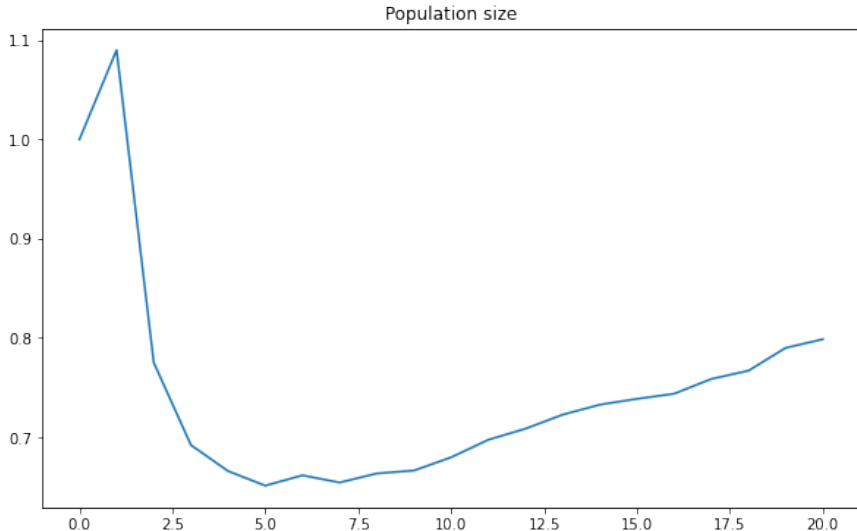


Updating population:



State probability trajectories





- › How to create an UPMaBoSS model from a MaBoSS model
- › View results
- › How to add an cell-cell communication as an external variable, which allow one phenotype to control another phenotype's death

Perspectives

MaBoSS usecases are evolving :

- › Using UPMaBoSS models to model Immunogenic Cell Death
- › Using MaBoSS in PhysiCell Agent-Based simulation using PhysiBoSS
- › A MaBoSS web interface to simplify teaching
- › Ensembles of boolean/MaBoSS models

<http://maboss.curie.fr>

<http://github.com/colomoto/pyMaBoSS>

<https://pymaboss.readthedocs.io/>

Aknowledgments



MaBoSS early team



Gautier Stoll



Eric Viara



Laurence
Calzone



Emmanuel
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MaBoSS ecosystem team



Aurelien
Naldi



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Loïc
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Levy



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Pol



Arnau
Montagud



Vincent
Noël



Gaëlle
Letort



Mihaly
Koltai



Andrei
Zinovyev



Randy
Heiland



Paul
Macklin



Jonas
Beal



Stéphanie
Chevalier



Andrea
Checcoli



Lorenzo
Pantolini



Marco
Ruscone



Gerard
Pradas