MaBoSS Tutorial

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19th European Conference on Computational Biology

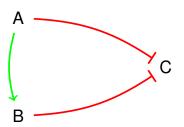
September 1, 2020





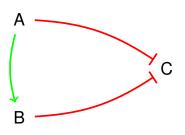






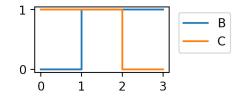


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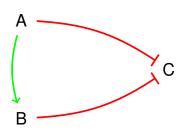


Boolean

- A: input
- > B: A
- > C: !A & !B







ODEs

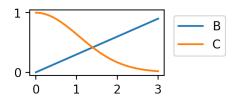
$$\frac{dA}{dt} = 0$$

$$\frac{dB}{dt} = k_1.A$$

$$\frac{dA}{dt} = 0$$

$$\frac{dB}{dt} = k_1.A$$

$$\frac{dC}{dt} = -k_2.A.B.C$$





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 \(\pm\) 6306 Accesses 32 Citations 1 Altmetric Metrics >>



Gautier Stoll



Eric Viara



Laurence Calzone



Emmanuel Barillot



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



Continuous time Markov process applied on a Boolean network state space

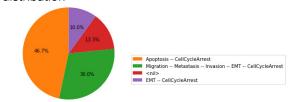
Transition rate:

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

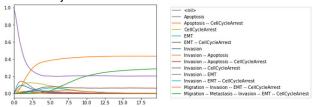


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Final states distribution



State distribution trajectories





BND file: Network definition

CFG file: Simulation settings

```
node A {
       logic = 1:
       rate up = @logic ? 1 : 0;
       rate down = 0;
6
   node B {
       logic = A \& !C;
       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;
       rate down = 0;
16
17 }
18
```

```
1  A.istate = FALSE;
2  B.istate = FALSE;
3  C.istate = FALSE;
4  
5  time_tick = 0.1;
6  max_time = 20.0;
7  sample_count = 10000.0;
8  use_physrandgen = 1.0;
9  thread_count = 1.0;
10
11  $act_B = 1;
12  $act_C = 1;
```

pyMaBoSS

- Initially developed 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

What if we want to use MaBoSS to create population models?







New Results

Comment on this paper

UPMaBoSS: a novel framework for dynamic cell population modeling

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

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



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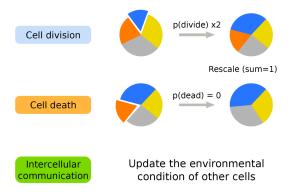


- We start from an existing MaBoSS model
- We add model nodes for division and death
- We add inter-cellular communication
- Chaining MaBoSS simulations, updating population and communication between each

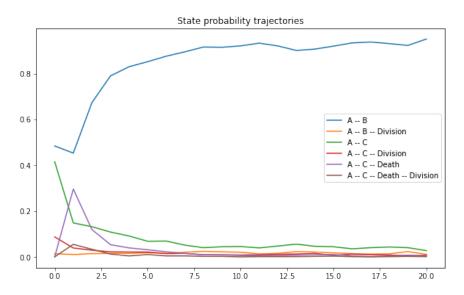




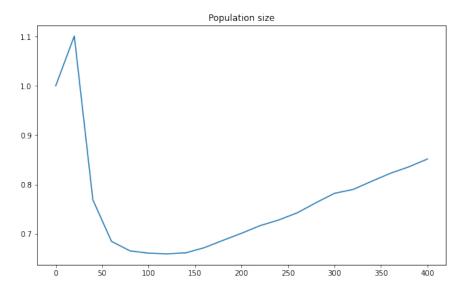
Updating population:













Aknowledgments







Aurelien

Naldi

Vincent

Noël

Jonas

Beal



MaBoSS early team



Calzone



Barillot

LaBRI













MaBoSS ecosystem team





Letort

Stéphanie

Chevalier











Checcoli













Arnau Montagud













Gerard

Pradas













Nicolas

Levy





Randy

Heiland