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

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This article presents an algorithm that allows modeling of biological networks in a qualitative framework with continuous time. Mathematical modeling is used as a systems biology tool to answer biological questions, and more precisely, to validate a network that describes biological observations and to predict the effect of perturbations.

We propose a modeling approach that is intrinsically continuous in time. The algorithm presented here fills the gap between qualitative and quantitative modeling. It is based on continuous time Markov process applied on a Boolean state space. In order to describe the temporal evolution, we explicitly specify the transition rates for each node. For that purpose, we built a language that can be seen as a generalization of Boolean equations. The values of transition rates have a natural interpretation: it is the inverse of the time for the transition to occur. Mathematically, this approach can be translated in a set of ordinary differential equations on probability distributions; therefore, it can be seen as an approach in between quantitative and qualitative.

We developed a C++ software, MaBoSS, that is able to simulate such a system by applying Kinetic Monte-Carlo (or Gillespie algorithm) in the Boolean state space. This software, parallelized and optimized, computes temporal evolution of probability distributions and can also estimate stationary distributions. Applications of Boolean Kinetic Monte-Carlo have been demonstrated for two qualitative models: a toy model and a published p53/Mdm2 model. Our approach allows to describe kinetic phenomena which were difficult to handle in the original models. In particular, transient effects are represented by time dependent probability distributions, interpretable in terms of cell populations.

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