Towards an automatic conversion from SBML core to SBML qual

Athénaïs Vaginay^(1, 2), Malika Smail-Tabbone⁽¹⁾, Taha Boukhobza⁽²⁾ ¹⁾LORIA (Université de Lorraine, CNRS, Inria); ⁽²⁾CRAN (Université de Lorraine, CNRS) Contact: <athenais.vaginay@inria.fr>



Abstract: The SBML format is the *de facto* standard to encode biological model in different formalisms. It was first developed to encode quantitative models like Differentials Equations (DEs), but the current release allows the definition of packages extending the core format. One of these packages, named qual, encodes qualitative models like Boolean Networks (BNs). To the best of our knowledge, there is no automatic pipeline to convert a quantitative model encoded in SBML core into a qualitative model encoded with the qual package. Here, we explore such a pipeline on a relatively simple system: the cell division of fission yeast, which has been studied both with a set DEs [1] and with a BN [2]. Our approach consists in extracting the model topology from the set of DEs and in solving them numerically in order to retrieve the time course data of species' concentrations on which we apply a discretization. Then we extract from these data a scarce state transition table. We are currently investigating ways to synthesize a BN fitting both topology knowledge and state transitions.



Next objectives:

- Use the knowledge about topology derived from the kinetic model to synthetize boolean functions Define pipeline validation criteria such as attractor identification and

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matching Assess the pipeline on other models

- Fully automatize the pipeline \rightarrow to be submitted to SBFC convertor

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References:

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[1] Novak et al. 'Mathematical model of the cell division cycle of fission yeast', Chaos, Mar. 2001.

[2] Davidich and Bornholdt, 'Boolean network model predicts cell cycle

[3] Leifeld *et al.* 'Identification of Boolean Network Models From Time Series Data Incorporating Prior Knowledge', Front. Physiol., Jun. 2018.