

A proposal to store qualitative simulation data in an SBML file

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Proposal description

Our proposal would be to use SBML files with additional `<qualitativeLaws>` `</qualitativeLaws>` tags which are stored within `<reaction>` `</reaction>` tags in replace of the `<kineticLaw>` `</kineticLaw>` tags.

Thus, we use the `<listOfReactants>` `</listOfReactants>` tags as Duncan Berenguier and Nicolas Le Novre use their `<listOfInputs>` `</listOfInputs>` tags and we use the `<listOfProducts>` `</listOfProducts>` tags as they use their `<listOfOutputs>` `</listOfOutputs>` tags.

1 Why did we choose those tags?

We have done that way because :

- We thought it was the most respectful option to the SBML *philosophy*. Actually, qualitative evolution rules can be seen as abstractions of quantitative evolution rules.
- It was a practical approach to encode hybrid (ODE/qualitative) models in SBML. Indeed all the reactions are stored in `<reaction>` tags; the `<kineticLaw>` tag is used for quantitative modeling and the `<qualitativeLaws>` tag is used for qualitative modeling.

2 What issue did we encounter?

The main issue we encounter was the computation of SBML model which has the same *Output* species in several different reactions. We found 2 ways to overcome this difficulty:

1. Only allow SBML files with unique *Output* species in `<qualitativeLaws>` `</qualitativeLaws>` tags.

2. Defining rules to construct unique evolution rule from several indications stored in several reaction descriptions. In that case the information such as *is involved in stimulation* or *is involved in inhibition* seems to be required.

3 Some practical experience

This format using `<qualitativeLaws>` `</qualitativeLaws>` tags in an annotated section with a specific namespace to remain compatible with SBML standard has been used for the storage of qualitative models and made it possible to read and write annotated SBML files.