

# CellTransformer: A Tool to Generate Reaction Networks through Graph Transformation

Brendan Sheehan, Aaron Quigley

Systems Research Group, School of Computer Science and Informatics,  
University College Dublin, Belfield, Ireland

E-mail: brendan.sheehan@ucd.ie, aaron.quigley@ucd.ie

## Extended Abstract

A major problem when modelling molecular interaction networks is dealing with combinatorial complexity both in the specification of the model and subsequent simulation [2]. For a static network of  $n$  proteins there exist  $n^2$  possible interactions (of a particular kind). If we allow a finer specification of the model at the level of protein domains then the number of possible interactions increases even further. Another problem is dealing with data at various levels of resolution. For example we may have interaction data at the level of protein domains or just at the level of individual proteins. We may or may not have quantitative information concerning the reactions.

In our current work we are only concerned with the specification of reactions in the model. We are concerned with simulation only insofar as we seek to generate reactions. The modeller seeks to specify in their model reactions that are relevant to the model. It is desirable to simplify the model as far as possible by not including reactions that are irrelevant or of only minor importance to the overall behaviour of the aspect of the system we are interested in. A rule-based system such as CellTransformer can be used to generate reactions based on multi-resolution interaction data. CellTransformer is based on a specific kind of rule based system called a graph transformation system (GTS) [5] where rules are used to transform a graph into another graph according to some well-defined approach. A graphical model is suitable for describing many kinds of biological data such as protein interaction networks and cell-signalling pathways [4].

CellTransformer implements a formalism for describing bio-molecular systems specified by Blinov *et al.* [1] as far as possible through a GTS based tool called AGG [6]. There exist many tools to specify and simulate biomolecular systems. The forthcoming version of CellDesigner [3] provides an API for the development of plugins to extend its functionality. We use this API as much as possible to integrate CellTransformer with the model specification tools of CellDesigner and by extension with the SBML format for bio-molecular models. Here we discuss the challenges faced when implementing Blinov *et al.*'s formalism in AGG and its integration with CellDesigner/SBML.

## References

- [1] Michael L. Blinov, Jin Yang, James R. Faeder, and William S. Hlavacek. Graph theory for rule-based modeling of biochemical networks. 4230:89–106, 2006.
- [2] J.R. Faeder, M.L. Blinov, B. Goldstein, and W.S. Hlavacek. Combinatorial complexity and dynamical restriction of network flows in signal transduction. In *Systems Biology*,

