

NBI-ModSim/2

Resources, Services, and Developments for Systems Biology Modeling

- Constraint-Based and Qualitative Modeling of Cellular Networks with CellNetAnalyzer -

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Short description of the project

Methods and integrated software tools supporting the construction, simulation, and comprehensive analysis of mathematical models of biological systems are an important subfield of bioinformatics. As part of the NBI-SysBio node, the partner project NBI-ModSim serves this field by resources (in particular, the software tools COPASI and CellNetAnalyzer) and services (user support, training courses, and different tutorials) for modeling in systems biology.

Whereas NBI-ModSim1 (Kummer group) supports dynamic and quantitative modeling of biological systems, NBI-ModSim2 offers tools and services for constraint-based and qualitative modeling of cellular networks.

de.NBI services

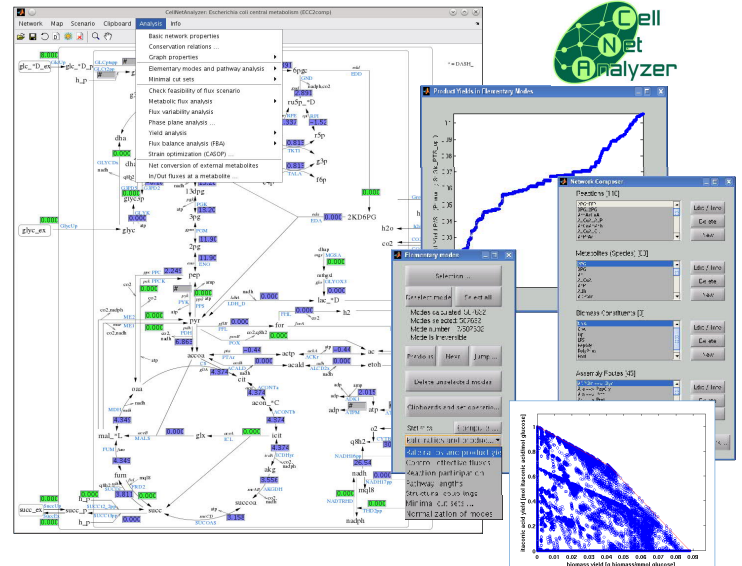
CellNetAnalyzer (CNA) is a MATLAB-toolbox providing various (partially unique) algorithms for analyzing structure and function of biological networks on the basis of topological, stoichiometric, qualitative (logical) and semi-quantitative modeling approaches. CNA facilitates the study of metabolic networks based on constraint-based modeling techniques, including methods for rational engineering of metabolic networks for biotechnological applications. Signaling / regulatory networks can be encoded and studied as interaction (influence) graphs, logical (Boolean) networks, or logic-based ODEs. CNA provides a user-friendly graphical user interface („interactive network maps“) but can also be used in command line mode via an Application Programming Interface (API).

Publications

von Kamp A, Thiele S, Hädicke O, Klamt S (2017) Use of CellNetAnalyzer in metabolic engineering and biotechnology. Journal of Biotechnology 261:221-228.

Hädicke O, von Kamp A, Aydogan T, Klamt S (2018) OptMDFpathway: Identification of metabolic pathways with maximal thermodynamic driving force and its application for analyzing the endogenous CO2 fixation potential of Escherichia coli. PLoS Computational Biology 13:e1006492.

Bekiaris PS, Klamt S (2020) Automatic construction of metabolic models with enzyme constraints. BMC Bioinformatics 21: 19.



Progress report

- communication infrastructure site installed together with NBI-ModSim1
- extended user support: new user forum for CellNetAnalyzer
- learning material (video tutorials) for CellNetAnalyzer
- training courses (software hands-on exercises) and workshops organized with NBI-ModSim1 and de.NBI-SysBio, see below)
- improved inter-operability of CellNetAnalyzer by extended support of new model standards (e.g., SBML Flux Balance Constraints) and COBRA format
- registered at ELIXIR bio.tools
- user survey 01/2019
- CellNetAnalyzer now released as open source

de.NBI Training and education

- Tutorial and hands-on exercise on CellNetAnalyzer at de.NBI-SysBio workshops (09/2017, 04/2018, 03/2019, planned for 04/2020) and at conferences (ICSB 10/2018, MPA 08/2019, FOSBE 10/2019)
- online video tutorial for CellNetAnalyzer

General information on the project

- 1 FTE (2*50%) paid from de.NBI grant
- 2 FTE additionally involved