Anne Arnold
Zoran Nikoloski
Systems Biology and Mathematical Modeling Group
Max-Planck Institute of Molecular Plant Physiology, 14476 Potsdam, Germany
e-mail: `arnold@mpimp-golm.mpg.de`
e-mail: `nikoloski@mpimp-golm.mpg.de`

Comparative model analyis of the Calvin-Benson cycle

Carbon fixation, especially the Calvin-Benson cycle (CBC), is the initial pathway for energy storage in carbohydrate products in C_3-plants. Understanding the interplay between regulation and efficiency of CBC and its end-products (*e.g.*, sucrose, starch and amino acids) requires the development of mathematical models which can explain the observed dynamics of metabolic transformations. Here, we address this question by comparing and ranking the existing models of the CBC to determine the set of best-performing models.

The importance of the CBC and the related pathways for the increase of plant biomass has already resulted in 15 models with various level of detail. The existing models can be categorized biologically based on: (1) chosen boundaries, *i.e.*, models of CBC including or excluding end-product synthesis, (2) details of reaction modeling, *i.e.*, leaf, cell, or compartment-level, and (3) hierarchy of kinetics [4], translating the model structure into mathematical equations amenable to extensive analysis of spatiotemporal properties. Our focus is placed on mass action, Michaelis-Menten-like, equilibrium approximations, and special functions in conjunction with the regulation terms.

The ranking of the SBML-implemented compendium of models is carried out with respect to the following criteria: (1) stability analysis [3], (2) sensitivity analysis, (3) ability to capture key features extracted from the data [1], and (4) analysis of yield. The obtained scores are then combined through a comprehensive model ranking scheme, based on which the set of best-performing models is selected with regard to metabolomics data and detection of candidates for genetic engineering.

References

[1] S. Arrivault, *et al.*, *Use of reverse-phase liquid chromatography, linked to tandem mass spectrometry, to profile the Calvin cycle and other metabolic intermediates in arabidopsis rosettes at different carbon dioxide concentrations* Plant J **59** 826–839 (2009).

[2] W.W. Chen, M. Niepel, P.K. Sorger, *Classic and contemporary approaches to modeling biochemical reactions* Genes & Development **24** 1861–1875 (2010).

[3] S. Grimbs, J. Selbig, S. Bulik, H.G. Holzhutter, R. Steuer, *The stability and robustness of metabolic states: identifying stabilizing sites in metabolic networks* Mol Syst Biol **3** 146 (2007).

[4] S. Grimbs, et al., *Spatiotemporal dynamics of the Calvin cycle: Multistationarity and symmetry breaking instabilities* BioSystems (2011), *in press*.