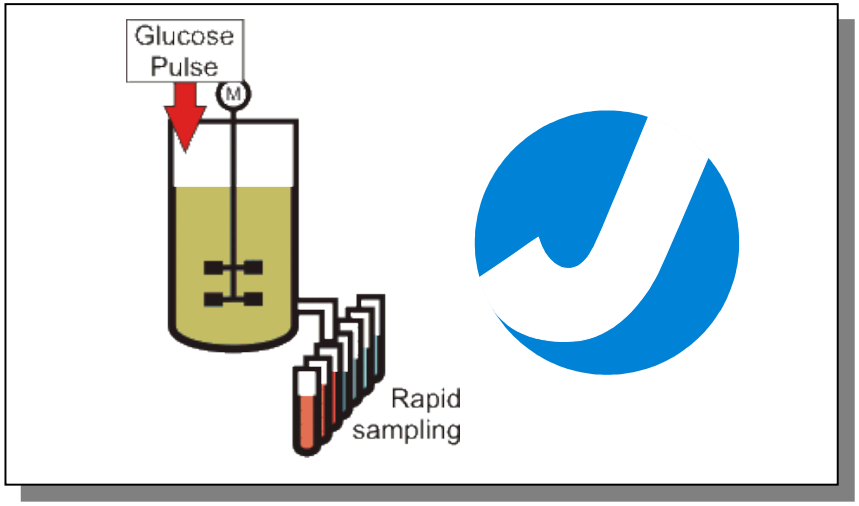
Poster-Session

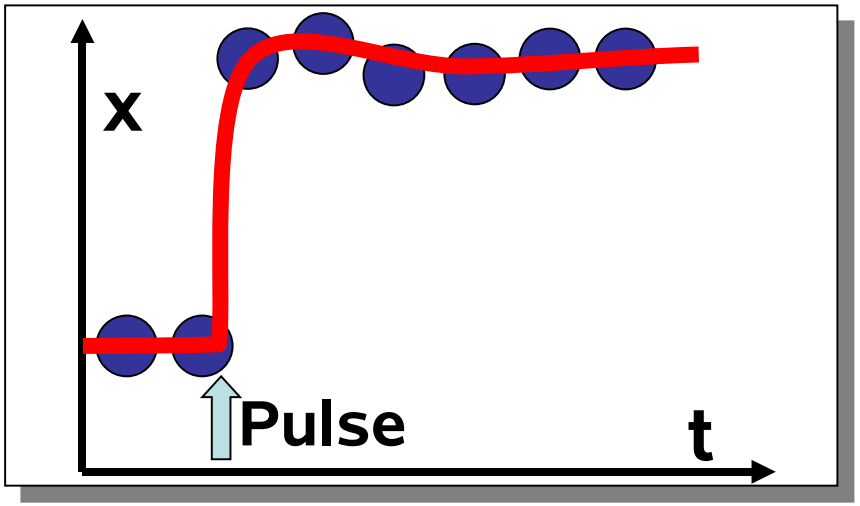
- **Roland Reichardt**
  - Simulation of Mechanical Alloying
- **Thomas Haschke**
  - Numerical Simulation of the Evaporation of Solute Droplets on Polymer Polymer Substrates
- **Marc Kalkuhl**
  - Generation of synthetic SAR-rawdata - Problems and Methods
- **Frieder Hadlich**
  - Simplification of Biochemical Network Models
- **Attiya Elsheikh**
  - Automatic Differentiation of Modelica Models
- **Michael Weitzel**
  - The Topology of Metabolic Isotope Labeling Networks

Introduction

Experiment



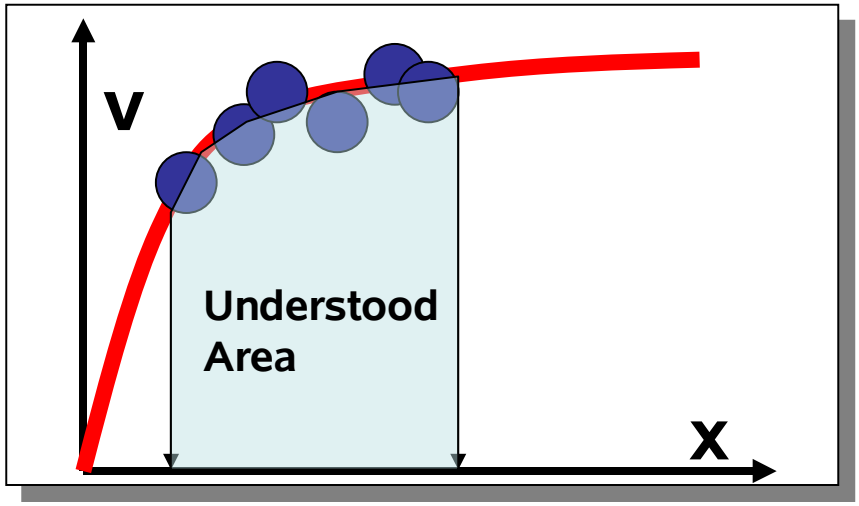
Concentration Course



Modelling

$$\dot{x} = N \cdot v(x, \alpha)$$

In vivo Kinetic ?

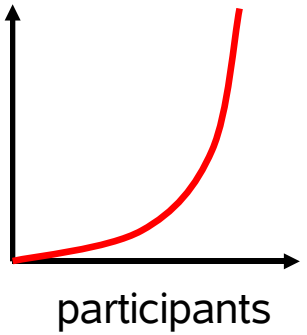


Kinetic types

MECHANISTIC KINETICS

- exact formulation of enzymatic effect mechanism
- many parameters for reactions with few participants
- f. i. Michaelis-Menten, Hill, …

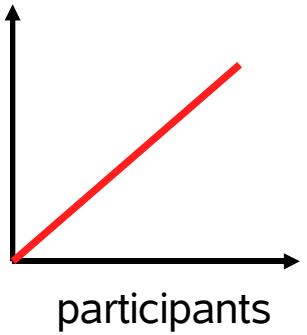
$$r_{\mathrm{GAPDH}} = \frac{r^{\max}_{\mathrm{GADPH}} \left(C_{\mathrm{gap}} C_{\mathrm{nad}} - \frac{C_{\mathrm{pgp}} C_{\mathrm{nadh}}}{K_{\mathrm{GAPDH,eq}}} \right)}{\left(K_{\mathrm{GAPDH,gap}} \left(1 + \frac{C_{\mathrm{pgp}}}{K_{\mathrm{GAPDH,pgp}}} \right) + C_{\mathrm{gap}} \right) \left(K_{\mathrm{GAPDH,nad}} \left(1 + \frac{C_{\mathrm{nadh}}}{K_{\mathrm{GAPDH,nadh}}} \right) + C_{\mathrm{nad}} \right)}$$



➔ 4 participants, 6 parameter

APPROXIMATIVE KINETICS

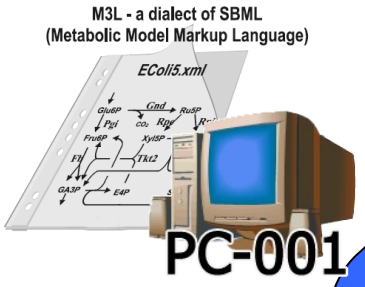
- less informational formulation of enzymatic effect mechanism in observed concentration space
- less parameters
- f. i. LinLog, Generic, PowerLaw



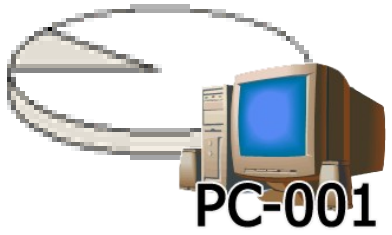
Automatic Model Simplification

Iteration Process:

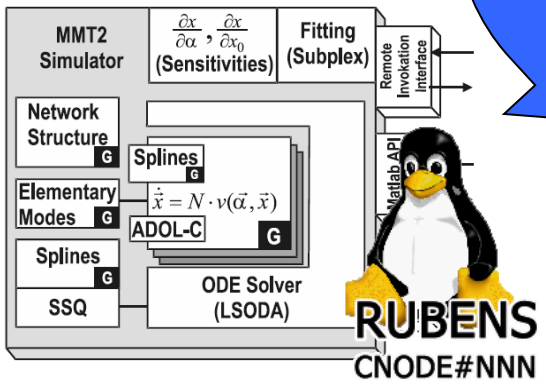
Model Generation



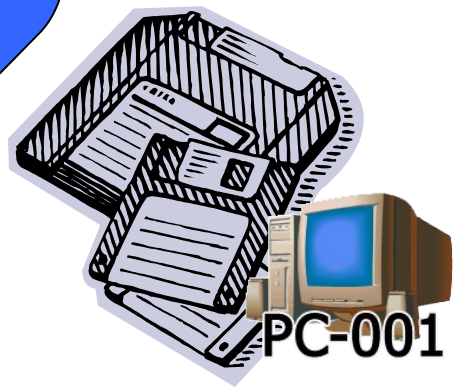
Result Analysis



1 PC:
min. 189h



MMT2 - Parameterfitting

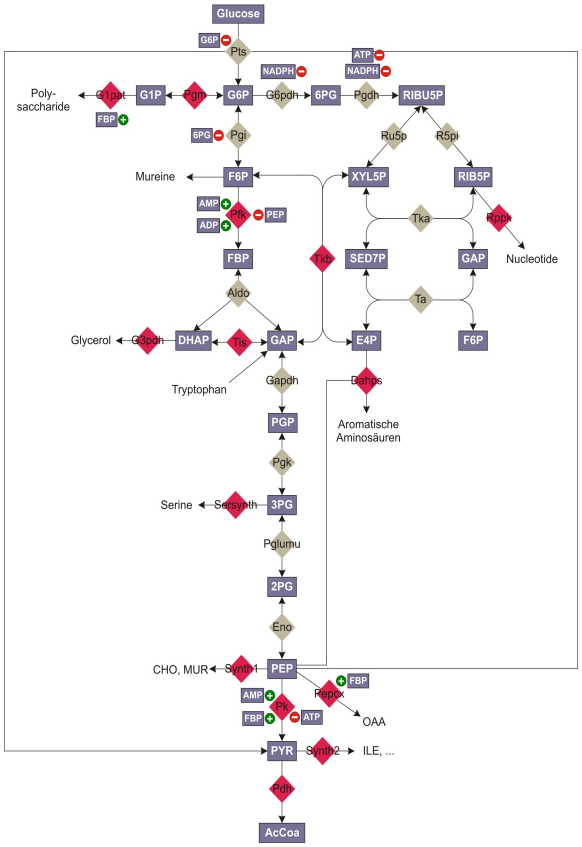


Result Storage

Results

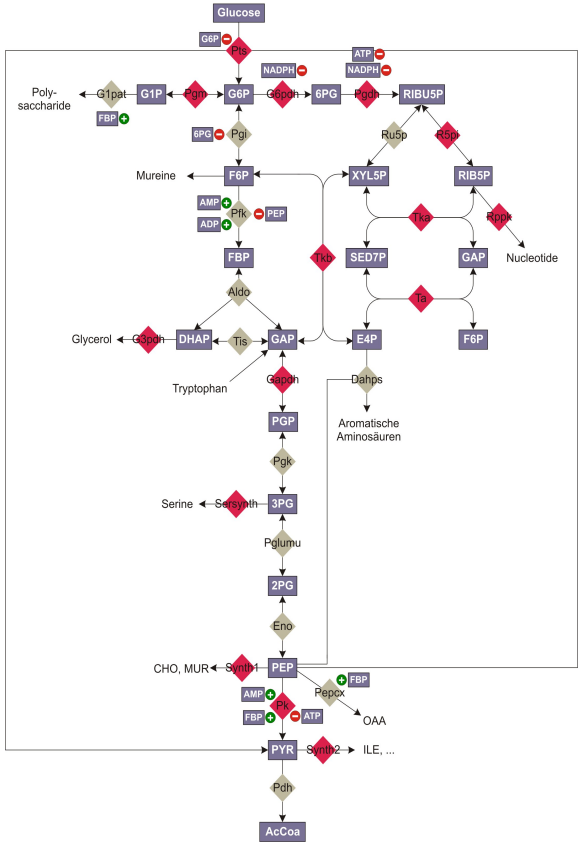
Results of *E.Coli* Model:

PowerLaw



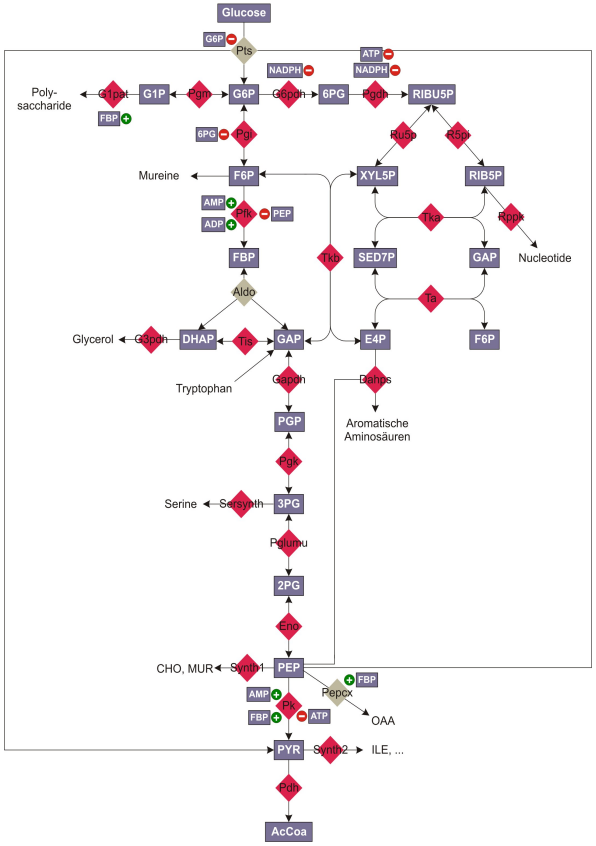
14 Substitutions (87)

Generic



15 Substitutions (93)

LinLog



24 Substitutions (81)