MGSmodelsDB
the database for storing Mathematical Models of Molecular Genetic Systems

F.V. Kazantsev[1], I.R. Akberdin[1], M.T. Ree[1], N.A. Ree[1], K.D. Bezmaternykh[1], V.A. Likhoshvai[1,2]*

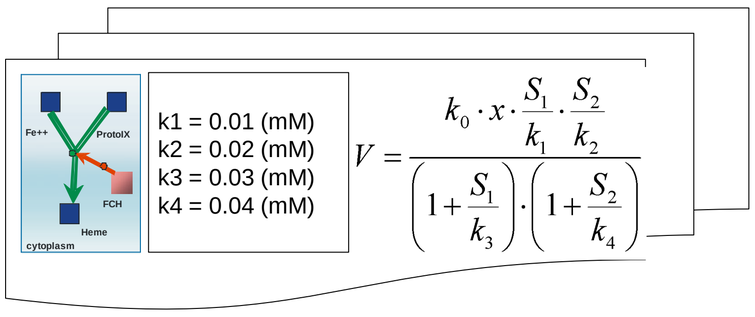
[1] *Institute of Cytology and Genetics SB RAS, Novosibirsk, Russia*

[2] *Novosibirsk State University, Novosibirsk, Russia*

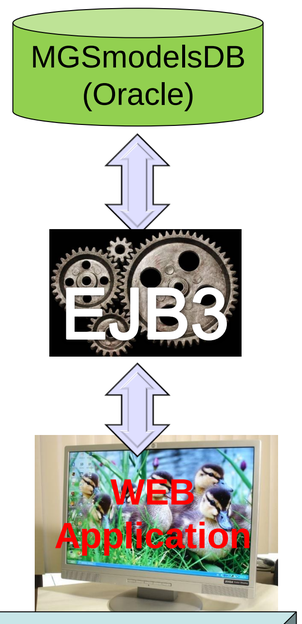
* *Corresponding author e-mail: kazfdr@bionet.nsc.ru*

Motivation:
Investigation of molecular-genetic systems mechanisms, patterns of relationship and structure is the system biology fundamental problem demanding the integration of modern experimental and theoretical approaches, in particularly mathematical modeling methods. The natural hierarchy of gene networks structure allows us to reveal an elementary subsystems (promoters, enzymes etc.) and describes them separately. Thus we can use them for making models of random gene networks structure. To implement the approach we have developed the mathematical models database of elementary cell subsystems that we call MGSmodelsDB**.**

MGSmodelsDB



The MGSmodelsDB tool was made for storing mathematical models of gene networks elementary subsystems, that are adopted to the experimental data.
Main goal of this tool is the mathematical models reuse in a complex model reconstruction.



This tool has the three tired architecture: The client Web Application for user request and data representation (JSF + Facelets); The Database where models are storing in hybrid manner, XML and relation (Oracle); And the Enterprise Java Beans that produced communication between them.

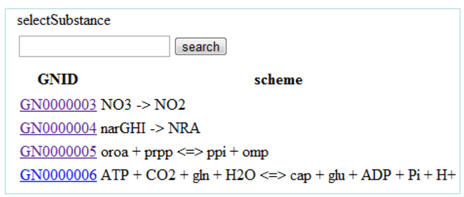
Elementary subsystem

Elementary subsystem of Gene Network is the molecular process (or set of processes), that could be modeled and analyzed in isolation from others. The typically agents of Elementary subsystems are "Enzymatic reactions" and processes of gene expression.

Each Elementary subsystem represented by triple (S,P,V), where "S" is the input variable vector, "P" is the output variable vector, "V" is the inner subsystems functioning law.

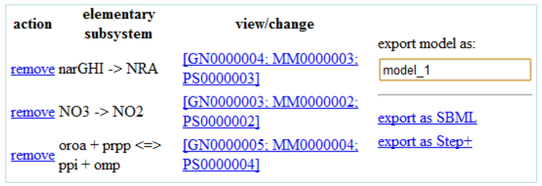
A Sample Session

Request the all models that contain reactant with selected name first


selectSubstance
search

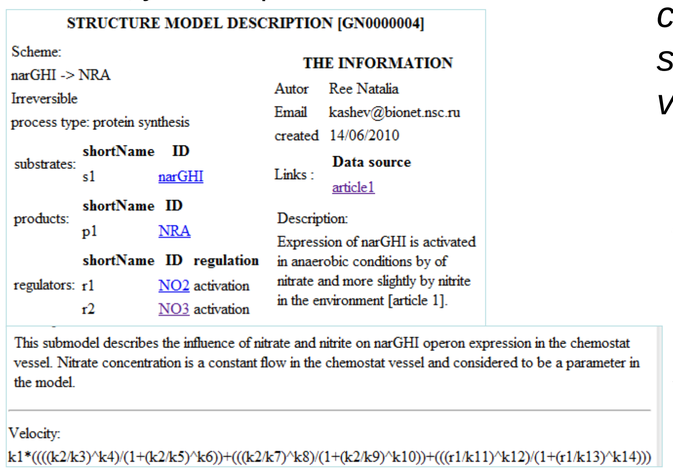
GNID	scheme
GN0000003	NO3 -> NO2
GN0000004	narGHI -> NRA
GN0000005	oroa + prpp <=> ppi + omp
GN0000006	ATP + CO2 + gln + H2O <=> cap + glu + ADP + Pi + H+

On this step you have one or more selected models in "basket" that you are interested in. There you can modify yore selection: remove elementary subsystem, change mathematical model on another existing one, or change the parameters set for selected model. After that you can do the last step



action	elementary subsystem	view/change	export model as:
remove	narGHI -> NRA	[GN0000004: MM0000003: PS0000003]	model_1
remove	NO3 -> NO2	[GN0000003: MM0000002: PS0000002]	export as SBML
remove	oroa + prpp <=> ppi + omp	[GN0000005: MM0000004: PS0000004]	export as Step+

After that you can see the selected model description, and if it's object of you interest, you can put that into the basket


STRUCTURE MODEL DESCRIPTION [GN0000004]

Scheme:
narGHI -> NRA
Irreversible
process type: protein synthesis

	shortName	ID	regulation
substrates:	s1	narGHI	
products:	p1	NRA	
regulators:	r1	NO2	activation
	r2	NO3	activation

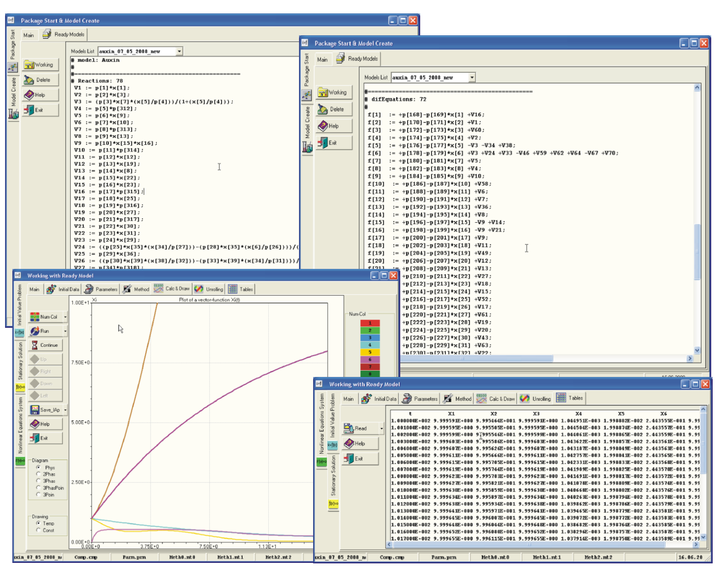
THE INFORMATION
Autor Ree Natalia
Email kashev@bionet.nsc.ru
created 14/06/2010
Links : Data source: article1
Description:
Expression of narGHI is activated in anaerobic conditions by of nitrate and more slightly by nitrite in the environment [article 1].

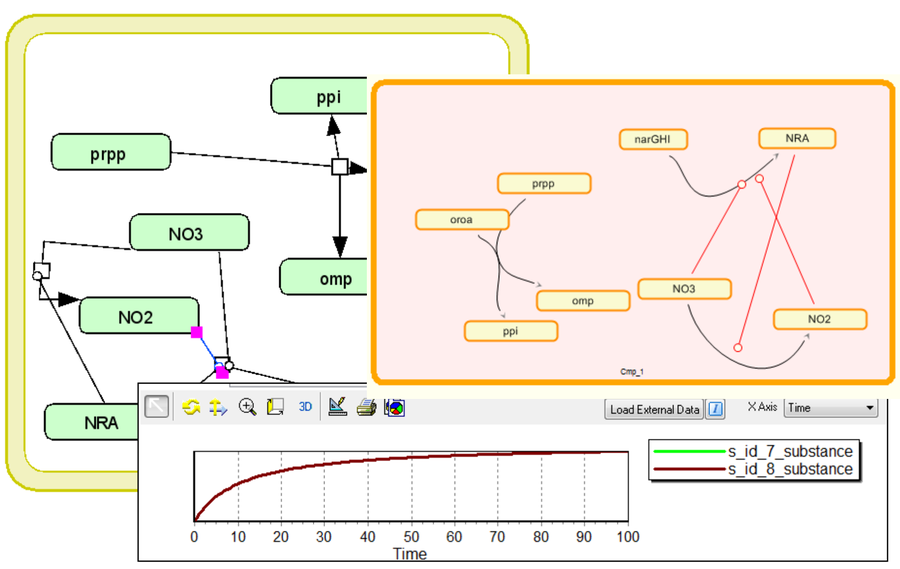
This submodel describes the influence of nitrate and nitrite on narGHI operon expression in the chemostat vessel. Nitrate concentration is a constant flow in the chemostat vessel and considered to be a parameter in the model.

Velocity:
k1*((((k2/k3)^k4)/(1+(k2/k5)^k6))+(((k2/k7)^k8)/(1+(k2/k9)^k10))+(((r1/k11)^k12)/(1+(r1/k13)^k14)))

Or you can export that in SBML format and enjoy the power of "SB*" community.

You can export the model into the STEP+ systems format and do some analysis and simulation





Integration rules

Due to the Elementary subsystems biochemical nature they could be integrated into the one complex model automatically. In this tool we do such integration by the elementary processes velocity summarize rule.

$$S_1 : \frac{dX_1}{dt} = V_1(Y_1, K_1) \quad S_2 : \frac{dX_2}{dt} = V_2(Y_2, K_2) \quad \dots \quad S_n : \frac{dX_n}{dt} = V_n(Y_n, K_n)$$

$$M : \begin{cases} \dfrac{dX}{dt} = V(Y,K), \quad V(Y,K) = \sum_{i=1}^{n} V_i(Y_i, K_i), \\ X = \cup X_i, Y = \cup Y_i, K = \cup K_i. \end{cases}$$

STEP+

Software "Step+" is oriented on the complex studying of the autonomous equations set, their stationary solutions and stability of the stationary solutions in dependence on parameters.

Also the computer system is useful for decision of the unlinear systems in a general view.

The database is accessible on the web-site:
http:// modelsgroup.bionet.nsc.ru/MGSmodelsDB

More information about the Step+ system:
http://semr.math.nsc.ru/v6/p440-456.pdf

All information relatively MGS group is available on the web-site:
http://modelsgroup.bionet.nsc.ru/

This work has been partially supported by the Grant NSh-2447.2008.4,
and by the SB RAS Interdisciplinary project Nos. 107, 119, and also by the RAS projects 21.26, 22.8, 23.29