DOI 10.18699/MM-HPC-BBB-2018-23

Creation of a modular model of metabolic processes in skeletal muscles during moderate physical load using BioUML platform

I.N. Kiselev[1, 2]*, V.I. Baranov[3], F.A. Kolpakov[1, 2]
[1] *Institute of Computational Technologies, SB RAS, Novosibirsk*
[2] *LLC «BIOSOFT.RU» Ltd., Novosibirsk*
[3] *Institute of Physiology and Basic Medicine, Novosibirsk*
** e-mail: axec@dote.ru*

Key words: mathematical model, modular modeling, skeletal muscles, metabolism, physiology, BioUML

Motivation and Aim: Global aim of this project is studying molecular mechanisms in muscles along with gene expression regulation. First step in this direction is creation of mathematical model of metabolic processes in muscle which can be further extended and linked with genetic expression in skeletal muscle under different influences.
Methods and Algorithms: Software platform BioUML (www.biouml.org) provides graphical representation and automatic generation of Java code for numerical modeling of the systems dynamics, it utilizes modular approach which implies creation of models as a set of interconnected parts (modules) each of modules is a mathematical model itself and describes particular subsystem. Modules can be modular itself, creating nested hierarchy of models. Modular representation facilitates understanding and consequent work with the model, which can be updated by adding new modules, improving existing and combining mathematical models obtained from different sources. It allows mathematical modeling of wide range of biological systems using different mathematical formalisms.
Results: We have implemented model of metabolic processes in muscles [1] as a modular model in BioUML. Model consists of 5 main modules: arteries, veins, blood flow through capillary, transport of metabolites from muscle fiber and muscle fiber. Muscle fiber module is a modular model itself. It consists of cytosol, mitochondria and block representing transport of metabolites between them. Such decomposition leads the way to further addition of new parts and/or replacing of existing blocks with more complicated and improved versions. For example modular version of this model from the same authors [2] can be obtained by duplicating muscle fiber block and initializing of two fibers with different parameters (representing red and white muscle fibers). Similarly we can construct models with other types of muscles in arms, legs, back, etc. Other ways to improve the model is adding new blocks describing: – heart, lungs, liver, etc.; – different types of training; – molecular mechanism of gene expression regulation during physical load.
Conclusion: *W*e have shown decomposition into modules and creation of a modular model with BioUML platform on the example of the muscle metabolism model. Created modular model is initial point for further improvement by adding new blocks and improving of existing blocks.
Availablility: Created model is freely available as a part of BioUML platform at http://wiki.biouml.org/index.php/Muscle_metabolism.
Acknowledgements: *S*upported by RFBR, research project No. 17-00-00296 KOMFI.

References

1. Li Y., Dash R.K., Kim J., Saidel G.M., Cabrera M.E. (2009) Role of NADH/NAD+ transport activity and glycogen store on skeletal muscle metabolism during exercise: in silico studies. Am J Physiol Cell Physiol. 296:25-46.
2. Li Y., Lai N., Kirwan J.P., Saidel G.M. (2012) Computational Model of Cellular Metabolic Dynamics in Skeletal Muscle Fibers during Moderate Intensity Exercise. Cell Mol Bioeng. 5(1):92-112.