NATIONAL DEVELOPMENT PLAN 2020

EUROPEAN UNION
European Regional Development Fund

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European Regional Development Fund Specific Objective 1.1.1 "Improve research and innovation capacity and the ability of Latvian research institutions to attract external funding, by investing in human capital and infrastructure" 1.1.1.1. measure "Support for applied research".

Crypthecodinium cohnii and Zymomonas mobilis syntrophy for production of omega 3 fatty acid from byproducts of biofuel and sugar industry, Project No.1.1.1.1/18/A/022

Sustainable Microbial Valorisation of Waste Lipids into Biosurfactants (Waste2Surf) Project No.1.1.1.1/19/A/047

Genome scale metabolic modelling linked bioreactor control system (GenCon) Project No.1.1.1.1/20/A/137

# BioModelling Spring Riga 2022 (remotely via Zoom)
# March 22-24, 2022

**Registration:** https://lu-lv.zoom.us/meeting/register/tJMscemorDorGNFpwnfVFNk-mKXjUSomLTXK

**Files for tutorials:** https://failiem.lv/u/g44x7jmrn

Organised by:
**Computational and Systems Biology Group (https://www.biosystems.lv/)**
**House of Nature**
**University of Latvia**
**Jelgavas iela 1**
**LV 1004, Riga, Latvia**

**Speakers:**

**Dr.sc.ing. Egils Stalidzans**, Computational Systems Biology Group, University of Latvia, director of Institute of Microbiology and Biotechnology.
Research interests: kinetic and stoichiometric modeling of metabolism, modeling of paharmacokinetics, user of COPASI and COBRA.

**Dr. Ehsan Motamedian**, Computational Systems Biology Group, University of Latvia, Institute of Microbiology and Biotechnology.
Research interests: Reconstruction of metabolic networks, Systems metabolic engineering of microbial cell factories, Omics data integration and analysis, Biomedical applications of metabolic modelling, Adaptive evolution and reprogramming

**Dr. Jürgen Pahle** (COPASI developer), ,Center for Quantitative Analysis of Molecular and Cellular Biosystems (BioQuant), Heidelberg University, Germany
Research interests: data analysis, stochastic modelling and simulation, information theory.

**Johanna Daas**, Pahle Lab, Center for Quantitative Analysis of Molecular and Cellular Biosystems (BioQuant), Heidelberg University, Germany
Research interests: workflows for computational systems biology.

**Reinis Muiznieks**, Computational Systems Biology Group, University of Latvia, Institute of Microbiology and Biotechnology. Student at the University of Latvia and Riga Technical University study program "Biotechnology and Bioengineering".
Research interests: kinetic and stoichiometric modeling of metabolism, user of COPASI and COBRA.

The participants are expected to have own computers and installed COPASI (http://copasi.org/) and COBRA (https://opencobra.github.io/cobratoolbox/stable/installation.html) software if they want to follow tutorials.

**Day 1 (Tuesday, March 22, 2022)**

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| ***13:00-13:05*** | ***Welcome and introduction to BioModelling Spring*** |
| **13:05-14:30** | Constraining kinetic models on COPASI, Egils Stalidzans<br>- total enzyme concentration constraint,<br>- homeostatic constraint,<br>- reduction of the solution space by constraints. |
| **14:30-15:00** | Break |
| **15:00-16:30** | What is Flux balance analysis?, Ehsan Motamedian<br>- Convex space and polyhedral cone;<br>- Introduction of constraints and objectives. |

**Day 2 (Wednesday, March 23, 2022)**

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| **9:00-10:30** | Implementation of thermodynamic constraints in stoichiometric models using matTFA, Renis Muiznieks<br>- basics of stoichiometric model related thermodynamics;<br>- implementation of thermodynamic constraints in a model;<br>- comparison of solution space of unconstrained and constrained model. |
| **10:30-11:00** | Break |
| **11:00-12:30** | CoRC – the COPASI R Connector, Juergen Pahle, Johanna Daas<br>- importing, creating and editing models;<br>- analysis and simulation tasks;<br>- scripting workflows. |
| **12:30-13:30** | Lunch break |
| **13:30-15:00** | Introduction to simplex algorithm, Ehsan Motamedian<br>- Standard form of linear programming (LP);<br>- The Simplex Method in Tableau Format: manual solution of an example. |
| **15:00-15:30** | Break |
| **15:30-17:00** | Solving LP problems using MATLAB, Ehsan Motamedian<br>- Definition of reduced cost and shadow price<br>- Types of feasible solutions found by LP<br>- Changing upper and lower bounds and objective function |

**Day 3 (Thursday, March 24, 2022)**

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| **9:00-10:30** | Insight into functionality of COBRA toolbox, Ehsan Motamedian<br>- Core *E. coli* model as an example: Application of various functions. |
| **10:30-11:00** | Break |
| **11:00-12:30** | LAMOS: a linear algorithm for finding multiple optimal solutions, Ehsan Motamedian<br>- Comparing LAMOS and FVA: elimination of internal cycles;<br>- Using LAMOS for finding metabolic engineering strategies. |