



COMBINE Tutorial

Modelling and Simulation Tools in Systems Biology

Participants of this one-day tutorial will learn how to set up computer models of biological systems (e.g. metabolic or signalling networks) using experimental kinetic data and how to simulate them in different systems biology platforms. Hands-on sessions, lectures and software demonstrations will be included, providing attendees with the necessary skills to access experimental kinetics data from available resources, to assemble computer models with these data, and finally to simulate the generated models using simulation tools. Also handling and exchange of biological models based on existing community standards will be demonstrated along with the basic principles of the underlying standard formats.

The topics will include:

- Model setup using different software tools and systems biology platforms
- Using experimental data for setting up kinetic models
- Parameter estimation, optimization and model fitting
- Simulation, analysis and visualization of biochemical models
- Database supported modelling: Data management and model databases
- Community standards and formats for systems biology models

Target audience

Experimentalists and modellers with some basic experience in modelling and simulation of biological systems.

Covered tools, platforms and databases

- **BioModels Database:** <http://www.ebi.ac.uk/biomodels/>
- **CellDesigner:** <http://www.celldesigner.org>
- **COPASI:** <http://www.copasi.org/>
- **CombineArchive Toolkit:** <https://sems.uni-rostock.de/projects/combinearchive/>
- **LigDig:** <http://mcm.h-its.org/ligdig/>
- **Pathway Commons:** <http://www.pathwaycommons.org/about/>
- **SABIO-RK:** <http://sabiork.h-its.org>
- **SEEK:** <http://fair-dom.org/seek>
- **SYCAMORE:** <http://sycamore.eml.org/>
- **webPIPSA:** <http://pipsa.h-its.org/>

Introduced standard formats

Some commonly used community standards for model and data exchange, as well as for model visualization will be introduced (**BioPax**, **SBGN**, **SBML**, **SED-ML**, **CellML**, **SBOL**) in practical examples using the covered tools. More information about the standards can be found on the **COMBINE (Computational Modeling in Biology Network)** website:
<http://co.mbine.org>

Tutors

The list of tutors currently is preliminary and subject to change.

Vijayalakshmi Chelliah, BioModels Team, European Bioinformatics Institute (EMBL-EBI, Cambridge, UK)

Emek Demir, Memorial Sloan Kettering Cancer Center (New York City, NY, USA)

Akira Funahashi and **Noriko Hiroi**, Keio University (Yokohama, Japan)

Martin Golebiewski and **Antonia Stank**, Heidelberg Institute for Theoretical Studies (HITS, Germany)

Pedro Mendes, University of Connecticut Health Center (Farmington, CT, USA) and University of Manchester (UK)

Sven Sahle and **Jürgen Pahle**, University of Heidelberg (Germany)

Dagmar Waltemath, University of Rostock (Germany)

Date and Venue

Wednesday, November 25th, 2015 (9:00 - 18:00)

Yong Loo Lin School of Medicine, National University of Singapore (NUS)

Block MD1 (rooms MD1-08-01E and MD1-08-03E)

Map and directions: <https://www.sph.nus.edu.sg/contact>

Tutorial Organization

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Agenda

9:00 - 10:30 Standards and Tools for Systems Biology Modelling (Plenary 1)

9:00 - 9:10 Introduction

Martin Golebiewski (HITS, Heidelberg, Germany)

9:10 - 9:30 COMBINE and its Standards (BioPax, SBGN, SBML, SED-ML, CellML, SBOL)

Dagmar Waltemath (University of Rostock, Germany) & Martin Golebiewski (HITS, Heidelberg, Germany)

9:30 - 9:50 BioPAX and Pathway Commons

Emek Demir (Memorial Sloan Kettering Cancer Center, New York City, NY, USA)

9:50 - 10:10 BioModels Database

Vijayalakshmi Chelliah (EMBL-EBI, Cambridge, UK)

10:10 - 10:30 Integrated Data and Model Management and the CombineArchive Toolkit

Dagmar Waltemath (University of Rostock, Germany)

10:30 - 10:50 Coffee Break

10:50 - 12:30 Tools and Databases for Systems Biology Modelling (Plenary 2)

10:50 - 11:10 SABIO-RK

Martin Golebiewski (HITS, Heidelberg, Germany)

11:10 - 11:40 CellDesigner

Akira Funahashi and Noriko Hiroi (Keio University, Yokohama, Japan)

11:40 - 12:10 COPASI

Sven Sahle and Jürgen Pahle (University of Heidelberg, Germany) & Pedro Mendes (University of Connecticut Health Center, Farmington, CT, USA and University of Manchester, UK)

12:10 - 12:30 LigDig, webPIPSA and SYCAMORE

Antonia Stank (HITS, Heidelberg, Germany)

12:30 - 14:00 Lunch

14:00 - 15:30 Parallel Demo and Hands-on Session 1

1) COPASI, SABIO-RK, LigDig, webPIPSA, SYCAMORE and CombineArchive Toolkit

Martin Golebiewski, Pedro Mendes, Jürgen Pahle, Sven Sahle, Antonia Stank and Dagmar Waltemath

2) CellDesigner, BioModels Database, BioPAX and Pathway Commons

Vijayalakshmi Chelliah, Emek Demir, Akira Funahashi and Noriko Hiroi

15:30 - 16:00 Coffee Break

16:00 - 17:30 Parallel Demo and Hands-on Session 2

1) COPASI, SABIO-RK, LigDig, webPIPSA, SYCAMORE and CombineArchive Toolkit

Martin Golebiewski, Pedro Mendes, Jürgen Pahle, Sven Sahle, Antonia Stank and Dagmar Waltemath

2) CellDesigner, BioModels Database, BioPAX and Pathway Commons

Vijayalakshmi Chelliah, Emek Demir, Akira Funahashi and Noriko Hiroi

17:30 - 18:00 Closing Plenary Session

Mutual information exchange between the parallel groups

How to apply tools and standards for concerted setup, editing, simulation and handling of models