the **combine**
computational modeling in biology network

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, Oregon Health & Science University (Portland, OR, 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 and **Martin Scharm**, 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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BIOENGINEERING INSTITUTE
THE UNIVERSITY OF AUCKLAND
NEW ZEALAND
Te Whare Wānanga o Tāmaki Makaurau

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)**
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   **Data and Model Management for Systems Biology**
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 – Reaction Kinetics Database**
Martin Golebiewski (HITS, Heidelberg, Germany)

11:10 - 11:40   **CellDesigner – Modeling Tool for Biochemical Networks**
Akira Funahashi and Noriko Hiroi *(Keio University, Yokohama, Japan)*

11:40 - 12:10   **COPASI – Biochemical System Simulator**
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 - 16:00 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, Martin Scharm, Antonia Stank and Dagmar Waltemath

2) **CellDesigner, BioModels Database, BioPAX and Pathway Commons**
Vijayalakshmi Chelliah, Emek Demir, Akira Funahashi and Noriko Hiroi

16:00 - 16:30 Coffee Break

16:30 - 18:00 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, Martin Scharm, Antonia Stank and Dagmar Waltemath

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