

Workshop: COMBINE Tutorial - Modelling and Simulation Tools in Systems Biology

Participants 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 quantitative models
- Parameter estimation, optimization and model fitting
- Simulation, analysis and visualization of biochemical models
- Database supported modelling: integrated data management and model databases
- Community standards and formats for systems and synthetic biology models

Target audience

Expected number of participants: 60-90

Experimentalists and modellers with some very basic experience in modelling and simulation of biological networks and everybody who would like to learn more about the tools and standards. Attendees are expected to bring their own computer for hands-on training.

Tutors (tentatively confirmed):

Akira Funahashi & Noriko F Hiroi: [Keio University](#) (Yokohama, Japan)

Martin Golebiewski, Ron Henkel & Andreas Weidemann: [HITS, Heidelberg](#) (Germany)

Stefan Hoops: [Biocomplexity Institute](#) - Virginia Tech (Blacksburg, VA, USA)

Ursula Kummer, Frank Bergmann, Jürgen Pahle & Sven Sahle: [Heidelberg University](#) (Germany)

Leslie M. Loew & Michael Blinov: [University of Connecticut Health Center](#) (Farmington, CT, USA)

Pedro Mendes: [University of Connecticut Health Center](#) (Farmington, CT, USA)

Chris Myers: [University of Utah](#) (Salt Lake City, UT, USA)

Date and Venue:

Saturday, August 12th, 2017 (09:00 – 18:00)

Covered tools, platforms and databases

- CellDesigner: <http://www.celldesigner.org>
- COPASI: <http://www.copasi.org/>
- iBioSim: <http://www.async.ece.utah.edu/ibiosim>
- JWS Online: <http://jjj.biochem.sun.ac.za/>
- SABIO-RK: <http://sabio.h-its.org/>
- SBOLDesigner: <http://www.async.ece.utah.edu/SBOLDesigner>
- SEEK/FAIRDOMhub: <http://fair-dom.org/seek>
- Virtual Cell (VCell): <http://vcell.org>

Introduced standard formats

Some commonly used community standards for model and modelling data exchange, as well as for model visualization will be introduced (SBGN, SBML and SED-ML) 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>

Tutorial Organization

Martin Golebiewski

Email: martin.golebiewski@h-its.org

HITS gGmbH

Schloss-Wolfsbrunnenweg 35

D-69118 Heidelberg (Germany)

Phone: +49-6221-533-281

Agenda (tentative)

- 09:00 – 9:30 **COMBINE and its Standards (BioPax, SBGN, SBML, SED-ML, CellML, SBOL, NeuroML)**
Martin Golebiewski (HITS, Germany) & Chris Myers (University of Utah, UT, USA)
- 9:30 – 10:00 **SABIO-RK – Reaction Kinetics Database**
Andreas Weidemann & Martin Golebiewski (HITS, Germany)
- 10:00 – 10:30 **CellDesigner – Modeling Tool for Biochemical Networks**
Akira Funahashi & Noriko Hiroi (Keio University, Yokohama, Japan)
- 10:30 – 11:00 **VirtualCell (VCell)**
Leslie M. Loew & Michael Blinov (Univ. of Connecticut Health Center, CT, USA)
- 11:00 - 11:30 *Coffee Break*
- 11:30 - 12:00 **COPASI – Biochemical System Simulator**
Frank Bergmann, Jürgen Pahle, Sven Sahle, Ursula Kummer (Heidelberg University, Germany), Stefan Hoops (Virginia Tech, Blacksburg, VA, USA), Pedro Mendes (University of Connecticut Health Center, CT, USA)
- 12:00 - 12:30 **Integrated Data and Model Management: FAIRDOM and SEEK**
Ron Henkel, Andreas Weidemann & Martin Golebiewski (HITS, Germany)
- 12:30 – 13:00 **Synthetic Biology Tools: iBioSim, SBOLDesigner and SynBioHub**
Chris J. Myers (University of Utah, Salt Lake City, UT, USA)
- 13:00 - 14:00 *Lunch Break*
- 14:00 - 15:30 **Demo and Hands-on Sessions 1 (parallel)**
- 15:30 - 16:00 *Coffee Break*
- 16:00 - 17:30 **Demo and Hands-on Sessions 2 (parallel)**
- 17:30 - 18:00 **Conclusions & Wrap-Up Session**