

Workshop: COMBINE & de.NBI 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

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.

Date and Venue:

VirginiaTech - Squires student center

290 College Avenue
Blacksburg, Virginia 24061

Sunday, August 6th, 2017 (09:00 – 18:00)

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

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

Covered tools, platforms, databases and standard formats

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

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 website of **COMBINE (Computational Modeling in Biology Network)**: <http://co.mbine.org>

Agenda (tentative)

- 09:00 – 9:15 Introduction: **Modelling and Simulation Tools in Systems Biology**
Martin Golebiewski (HITS, Germany)
- 09:15 – 9:45 **COMBINE and its Standards:**
BioPax, SBGN, SBML, SED-ML, CellML, SBOL, NeuroML
<http://co.mbine.org>
Martin Golebiewski (HITS, Germany)
- 9:45 – 10:20 **SABIO-RK – Reaction Kinetics Database** (presentation/demo)
<http://sabio.h-its.org/>
Andreas Weidemann & Martin Golebiewski (HITS, Germany)
- 10:20 - 10:45 *Coffee Break*
- 10:45 – 12:45 **CellDesigner – Modeling Tool for Biochemical Networks** (presentation/hands-on)
<http://www.celldesigner.org>
Akira Funahashi & Noriko Hiroi (Keio University, Yokohama, Japan)
- 12:45 - 13:45 *Lunch Break*
- 13:45 - 15:45 **COPASI – Biochemical System Simulator** (presentation/hands-on)
<http://www.copasi.org/>
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)
- 15:45 - 16:00 *Coffee Break*
- 16:00 – 16:45 **Integrated Data and Model Management: FAIRDOM&SEEK** (presentation/demo)
<http://fair-dom.org/seek>
Ron Henkel, Andreas Weidemann & Martin Golebiewski (HITS, Germany)
- 16:45 – 17:55 **VCell - VirtualCell** (presentation/demo)
<http://vcell.org>
Leslie M. Loew (Univ. of Connecticut Health Center, CT, USA)
- 17:55 – 18:00 **Conclusions & Wrap-Up**

Tutorial Organization

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