

NBI-Resources, Services and Developments for ModSim1 Systems Biology Modeling - Dynamic and Quantitative Modeling of Biological Systems

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Fkz 031L0104A

Short description of the project

Methods and integrated software tools supporting the construction, simulation, and comprehensive analysis of mathematical models of biological systems are an important subfield of bioinformatics which is not supported directly by the de.NBI HUBs. Now as part of the **NBI-SysBio** node, we close this gap by adding new resources (in particular, the software tools **COPASI** and **CellNetAnalyzer**) and services (extended user support and training) for modeling in **systems biology**.

Whereas **NBI-ModSim2** (Klamt group) supports constraint-based and qualitative modeling of cellular networks, **NBI-ModSim1** offers tools and services for dynamic and quantitative modeling of biological systems.

de.NBI service: COPASI

COPASI (Hoops et al., 2006, Mendes et al., 2009), developed in the group of Ursula Kummer at Heidelberg University, together with the group of Pedro Mendes (Connecticut, USA), is a systems biology software that integrates standard and novel algorithms for the modeling, simulation and analysis of process-based non-spatial models, mostly at the cellular level. COPASI supports both ODE-based as well as stochastic (discrete particle based) formalisms. In addition, COPASI features include steady state calculation, sensitivity analyses, optimization, parameter fitting, parameter scanning and computing nonlinear dynamical systems properties such as Lyapunov exponents, among others. COPASI can be run via a user-friendly GUI or via backend version, e.g. on compute clusters.

General information on the project

The project pays for one full time post doc (Bergmann, FT). Other staff involved include Ursula Kummer and Sven Sahle.

Publications

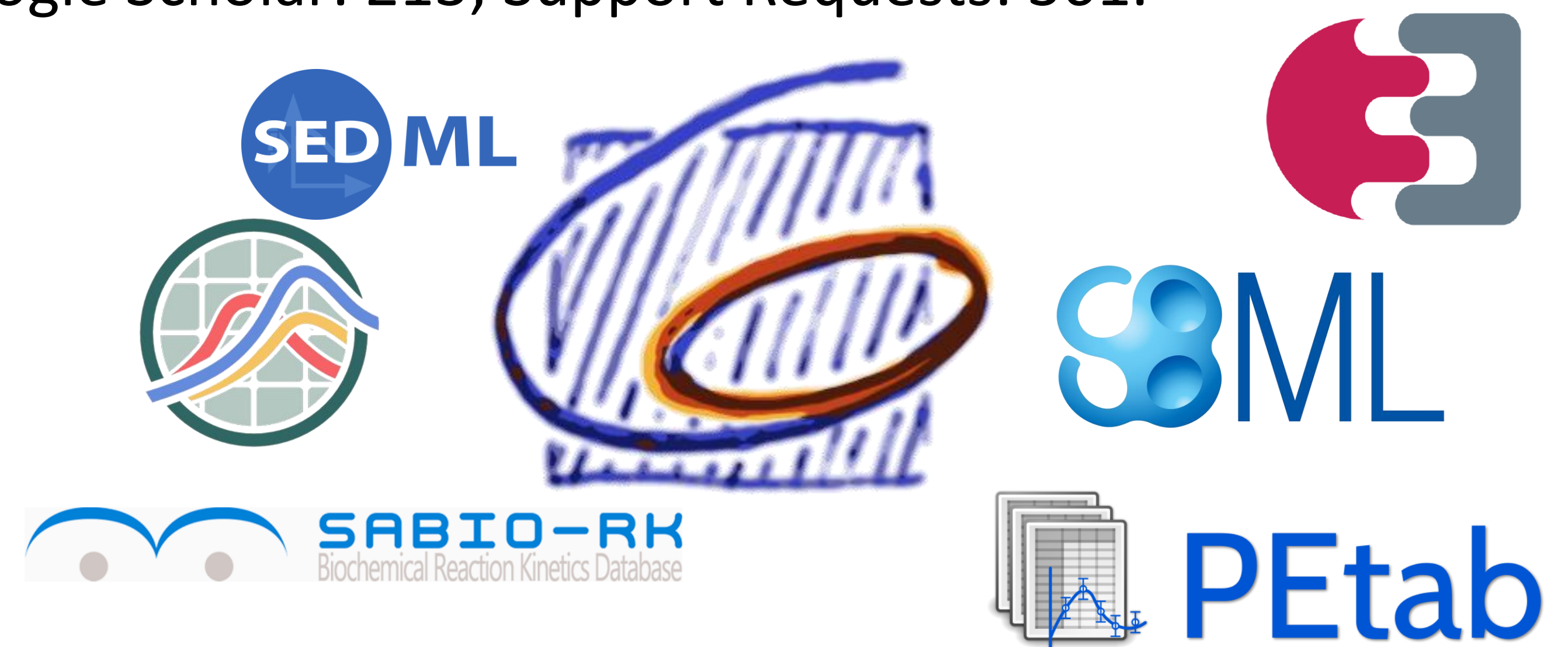
- Bergmann FT, Hoops S, Klahn B, Kummer U, Mendes P, Pahle J, Sahle S. Applying COPASI in biotechnology. *Journal of Biotechnology* (de.NBI special issue in *J. Biotech.*) 215-220, 2017.
- Hoops S, Sahle S, Gauges R, Lee C, Pahle J, Simus N, Singhal M, Xu L, Mendes P, Kummer U. COPASI-a complex pathway simulator. *Bioinformatics*, 22(24):3067–3074, 2006.
- Mendes, P., Hoops, S., Sahle, S., Gauges, R., Dada, J.O. and Kummer, U. (2009). *Computational Modeling of Biochemical Networks Using COPASI*. Methods in Molecular Biology, Humana Press. 500: 17-59.

Progress report

In the period of 2018/2019 (since the last SAB meeting), we continued to improve compatibility of COPASI with community Standards SBML and SED-ML, and improved support of the COMBINE archive format. To make it easier to interface with other tools from the de.NBI network (like Sabio-RK), we implemented a URL scheme in COPASI that allows opening models directly from web applications. We are supporting the University of Stuttgart in creating a new standard format for describing enzyme kinetics. With the University of Bonn and the Helmholtz Zentrum München we are working on support for PTab, that will allow us to exchange parameter estimation setups freely between software tools.

KPIs for the period 1.1.2019 / 31.12.2019:

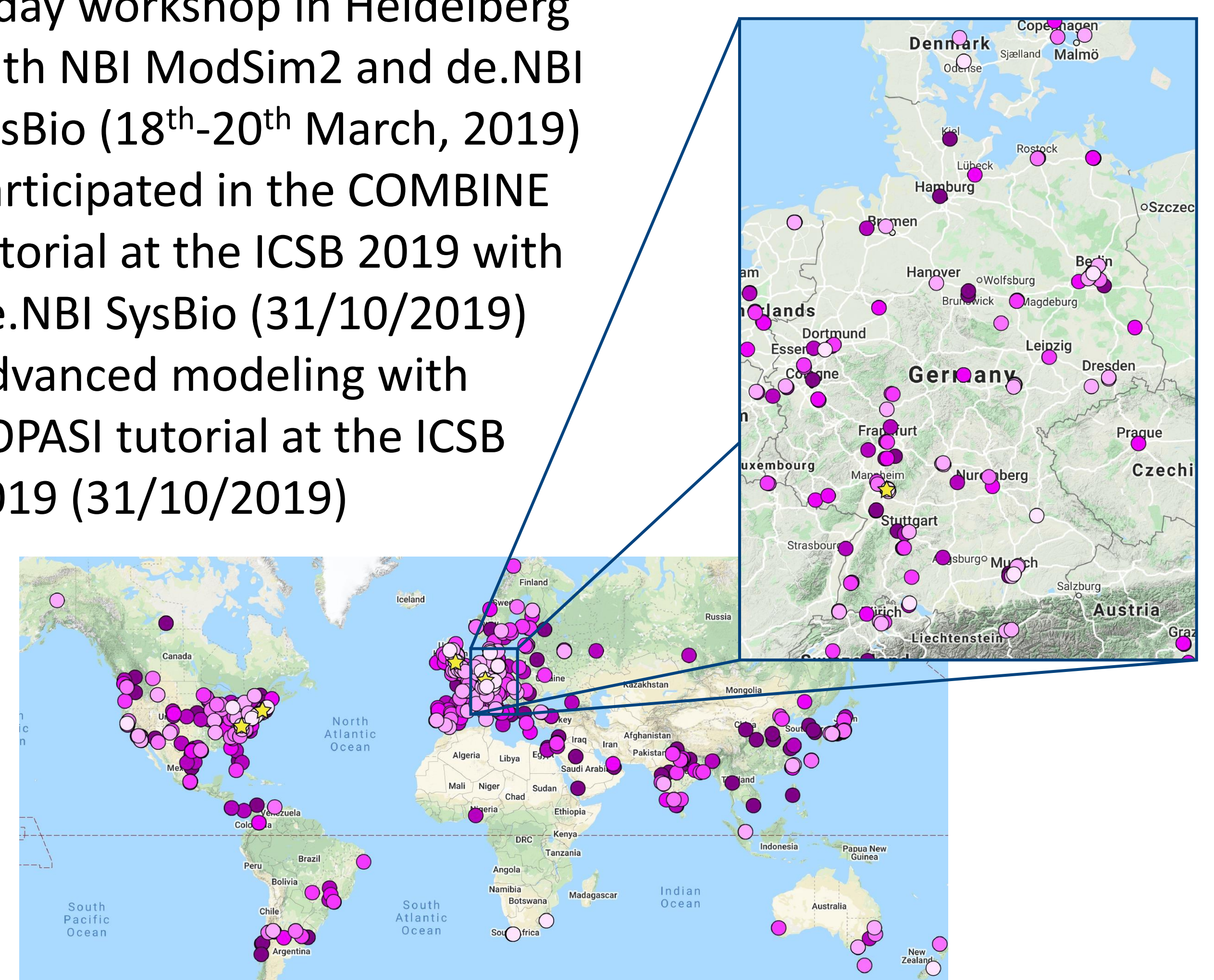
Downloads: 16030; Citations: Web of Science: 120, Google Scholar: 213; Support Requests: 361.



de.NBI Training and education

Training courses given since the last SAB meetings:

- 3 day workshop in Heidelberg with NBI ModSim2 and de.NBI SysBio (18th-20th March, 2019)
- Participated in the COMBINE tutorial at the ICSB 2019 with de.NBI SysBio (31/10/2019)
- Advanced modeling with COPASI tutorial at the ICSB 2019 (31/10/2019)



Manually curated map, of locations of researchers that published papers using COPASI. In 2019 110 additional papers were recorded, (acknowledging funding from BMBF:3, DFG:5) bringing the total to 815 (acknowledging funding from BMBF:41, DFG:30). For the full interactive list see: <http://copasi.org/Research/>