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Nikolaus Sonnenschein

Ph.D.

Research Interests

Various aspects of computational systems and synthetic biology, in particular models of metabolism, eukaryotic and prokaryotic gene regulation, dynamics on networks, analysis of high-throughput data, kinetic modeling of biological processes, *in silico* cell factory design, and scientific software development.

Education

January 2011 *Ph.D.* in Bioinformatics, *Jacobs University Bremen*, Germany, with special distinction.

July 2007 *Diplom* in Biology (equivalent to M.Sc.), *Technical University of Darmstadt*, Germany, with distinction (overall grade: 1.0, very good).

May 2004 *Vordiplom* in Biology (equivalent to B.Sc.), Technical University of Darmstadt, Germany.

Professional Experience

since August 2013 Research Scientist, The Novo Nordisk Foundation Center for Biosustainability, DTU, Denmark.

Modeling work for cell factory engineering projects run in the iLoop Core Unit. Software development of cameo, a Python package for *in silico* cell factory design (see also Scientific Software). Supervision of three PhD students working on interpreting genetic variation in the context of metabolic models, a genome-scale metabolic reconstruction of *Methylococcus capsulatus*, and a kinetic model of *Escherichia coli* central carbon metabolism. Furthermore, supervision of one postdoc working on dedicated strain engineering projects in the iLoop project.

March 2011 – Postdoctoral Researcher, University of California, San Diego, USA.

July 2013 Development of the next-generation modeling environment for kinetic modeling of metabolic systems (MASS toolbox; see also Scientific Software). Involved in the construction of genome-scale kinetic models of the human erythrocyte and central carbon metabolism of *E. coli*. Detailed enzyme module reconstructions from bibliomic data and calibration using derivative based and derivative free optimization techniques.

- September 2007 PhD Student, Jacobs University Bremen, Germany.
 - January 2011 Combination of constraint-based modeling techniques and graph theoretical methods for the following purposes: (1) Topological classification of medium-dependent essentiality, (2) integration of gene-expression data with metabolic reconstructions of $E.\ coli$ and the human, and (3) the analysis of metabolite correlation networks. Application of point-process statistics to the transcriptional regulatory network and spatial gene organization of $E.\ coli$.
 - August 2006 **Diploma Student**, Technical University of Darmstadt, Germany.
 - July 2007 Correlation study of perturbed metabolic systems, comparing flux balance analysis and cellular automata dynamics.
 - October 2005 Research Assistant, Technical University of Darmstadt, Germany.
 - July 2006 Topological reasons for dynamical stability. Implementation of systems of linear ODEs and cellular automata dynamics on random network topologies.
 - February 2005 **Student Assistant**, Berlin-Brandenburg Academy of Sciences and Hu-June 2006 manities, Germany.
 - Help with planning the curriculum of a new biophysics study program in the biology department of the Technical University of Darmstadt.
 - July 2005 **Internship**, Max-Planck Institute for Brain Research, Frankfurt, Germany. August 2005 Cell migrations in the Rhombencephalon. In situ hybridization study of genes expressed during early mouse brain development.

Publications

Full publication list also available at scholar.google.com/citations?user=8RqKcm0AAAAJ. Articles

- [1] A. Bordbar, D. McCloskey, D. C. Zielinski, **N. Sonnenschein**, N. Jamshidi, and B. Ø. Palsson. "Personalized Whole-Cell Kinetic Models of Metabolism for Discovery in Genomics and Pharmacodynamics". In: *Cell Systems* 1.4 (Oct. 2015), pp. 283–292. ISSN: 24054712. DOI: 10.1016/j.cels.2015.10.003.
- [2] J. G. R. Cardoso, M. R. Andersen, M. J. Herrgard, and **N. Sonnenschein**. "Analysis of genetic variation and potential applications in genome-scale metabolic modeling." In: Frontiers in bioengineering and biotechnology 3 (2015), p. 13. DOI: 10.3389/fbioe.2015.00013.
- [3] A. Ebrahim, E. Almaas, E. Bauer, A. Bordbar, A. P. Burgard, R. L. Chang, A. Dräger, I. Famili, A. M. Feist, R. M. Fleming, S. S. Fong, V. Hatzimanikatis, M. J. Herrgard, A. Holder, M. Hucka, D. Hyduke, N. Jamshidi, S. Y. Lee, N. Le Novere, J. A. Lerman, N. E. Lewis, D. Ma, R. Mahadevan, C. Maranas, H. Nagarajan, A. Navid, J. Nielsen, L. K. Nielsen, J. Nogales, A. Noronha, C. Pal, B. Ø. Palsson, J. A. Papin, K. R. Patil, N. D. Price, J. L. Reed, M. Saunders, R. S. Senger, N. Sonnenschein, Y. Sun, and I. Thiele. "Do genome-scale models need exact solvers or clearer standards?" In: Molecular Systems Biology 11.10 (Oct. 2015), pp. 831–831. ISSN: 1744-4292. DOI: 10.15252/msb.20156157.
- [4] Z. A. King, A. Dräger, A. Ebrahim, **N. Sonnenschein**, N. E. Lewis, and B. Ø. Palsson. "Escher: A Web Application for Building, Sharing, and Embedding Data-Rich Visualizations of Biological Pathways." In: *PLoS computational biology* 11.8 (2015), e1004321. DOI: 10.1371/journal.pcbi.1004321.

- [5] D. Machado, K. H. Zhuang, **N. Sonnenschein**, and M. J. Herrgard. "Editorial: Current Challenges in Modeling Cellular Metabolism". In: *Frontiers in bioengineering and biotechnology* 3 (2015), p. 107. DOI: 10.3389/fcell.2015.00017.
- [6] K. R. Kildegaard, B. M. Hallström, T. H. Blicher, N. Sonnenschein, N. B. Jensen, S. Sherstyk, S. J. Harrison, J. Maury, M. J. Herrgard, A. S. Juncker, J. Forster, J. Nielsen, and I. Borodina. "Evolution reveals a glutathione-dependent mechanism of 3-hydroxypropionic acid tolerance." In: *Metabolic engineering* 26C (2014), pp. 57–66. DOI: 10.1016/j.ymben.2014.09.004.
- [7] I. Thiele, N. Swainston, R. M. T. Fleming, A. Hoppe, S. Sahoo, M. K. Aurich, H. Haraldsdottir, M. L. Mo, O. Rolfsson, M. D. Stobbe, S. G. Thorleifsson, R. Agren, C. Bölling, S. Bordel, A. K. Chavali, P. Dobson, W. B. Dunn, L. Endler, D. Hala, M. Hucka, D. Hull, D. Jameson, N. Jamshidi, J. J. Jonsson, N. Juty, S. Keating, I. Nookaew, N. Le Novère, N. Malys, A. Mazein, J. A. Papin, N. D. Price, E. Selkov, M. I. Sigurdsson, E. Simeonidis, N. Sonnenschein, K. Smallbone, A. Sorokin, J. H. G. M. van Beek, D. Weichart, I. Goryanin, J. Nielsen, H. V. Westerhoff, D. B. Kell, P. Mendes, and B. Ø. Palsson. "A community-driven global reconstruction of human metabolism." In: *Nature biotechnology* 31.5 (2013), pp. 419–425. DOI: 10.1038/nbt.2488.
- [8] M. E. Beber, C. Fretter, S. Jain, N. Sonnenschein, M. Müller-Hannemann, and M.-T. Hütt. "Artefacts in statistical analyses of network motifs: general framework and application to metabolic networks." In: Journal of the Royal Society, Interface / the Royal Society 9.77 (2012), pp. 3426–3435. DOI: 10.1098/rsif.2012.0490.
- [9] N. Sonnenschein, J. F. Golib Dzib, A. Lesne, S. Eilebrecht, S. Boulkroun, M.-C. Zennaro, A. Benecke, and M.-T. Hütt. "A Network Perspective on Metabolic Inconsistency." In: BMC systems biology 6.1 (2012), p. 41. DOI: 10.1186/1752-0509-6-41.
- [10] N. Sonnenschein, C. Marr, and M.-T. Hütt. "A topological characterization of medium-dependent essential metabolic reactions." In: *Metabolites* 2.3 (2012), pp. 632–647. DOI: 10.3390/metabo2030632.
- [11] N. Sonnenschein, M. Geertz, G. Muskhelishvili, and M.-T. Hütt. "Analog regulation of metabolic demand". In: *BMC Systems Biology* 5.1 (2011), p. 40. ISSN: 1752-0509. DOI: 10.1186/1752-0509-5-40.
- [12] **N. Sonnenschein**, M.-T. Hütt, H. Stoyan, and D. Stoyan. "Ranges of control in the transcriptional regulation of *Escherichia coli*." In: *BMC systems biology* 3 (2009), p. 119. DOI: 10.1186/1752-0509-3-119.

Book chapters

[13] B. Bergdahl, N. Sonnenschein, D. Machado, M. Herrgård, and J. Forster. "Genome-Scale Models - Fundamental Bioengineering". In: Fundamental Bioengineering. Wiley-VCH Verlag GmbH & Co. KGaA, 2015, pp. 143–182. ISBN: 9783527697441. DOI: 10.1002/9783527697441.ch06.

In Preparation

[14] J. G. R. Cardoso, K. Jensen, E. Özdemir, M. J. Herrgård, and **N. Sonnenschein**. Cameo: A Python Library for Computer Aided Metabolic Engineering and Optmiziation of Cell Factories. in preparation.

[15] N. Sonnenschein, A. Sastry, D. Zielinski, S. P. James de Bree, A. Thomas, A. Bordbar, N. Jamshidi, and B. Ø. Palsson. The MASS Toolbox: Accessible dynamic modeling. revised manuscript will be submitted soon.

Oral Conferences Contributions

7th Copenhagen Novo Nordisk Foundation, Hillerørd, Denmark, May 2015, Chairman of Bioscience "Modeling" session. Speakers: Bernhard Palsson (University of California, Conference San Diego), Nathan Price (Institute for Systems Biology), and Hector

Garcia Martin (Joint BioEnergy Institute)

COBRA Charlottesville, Virginia, USA, May 2014, Invited talk: Putting constraint-based modeling at the fingertips of bench biologists, N. Sonnenschein and M. Herrgård

Winter q-bio Waikiki, Hawaii, USA, February 2013, Contributed talk: *Dynamic modeling* Meeting for the masses: the MASS toolbox, N. Sonnenschein, D.C. Zielinski, A. Bordbar, N. Jamshidi, B.Ø. Palsson,

A complex Organized by *Volkswagen Stiftung*, Berlin, Germany, April 2009, Consystems view on tributed talk: *A Network Perspective on Metabolic Inconsistency*, N. Sonproduction and nenschein, J.F. Golib Dzib, S. Boulkroun, A. Lesne, M.-C. Zennaro, A. distribution Benecke, and M.-T. Hütt

Grants and Fellowships

Ongoing

2016 – 2020 H2020: New bioinformatics approaches in service of biotechnology (BIOTEC-2-2015), co-written application, role of scientific deputy in the consortium.

Past

2007 – 2011 PhD fellowship awarded by Jacobs University Bremen, Germany.

May 2009 Travel stipend, German Academic Exchange Service (DAAD), awarded to attend Systems Biology Short Course & Human Reconstruction Jamboree, Center of Systems Biology, Reykjavik, June 2009.

Teaching Experience

2012 – 2013, *BENG 123, Systems Biology and Bioengineering*, University of California, annually San Diego, undergraduate level, instructor

2010, occasionally $Bioinformatics \ and \ Computational \ Biology \ I,$ Jacobs University Bremen, graduate level, substitute lecturer

2007 – 2010, Advanced Bioinformatics Laboratory Course III: Genomics and Elementary annually Systems Biology, Jacobs University Bremen, graduate level, substitute lecturer

Scientific Software

MASS toolbox The Mass-Action Stoichiometric Simulation (MASS) toolbox is a modeling opencobra. software package that focuses on the construction and analysis of kinetic github.io/MASS- and constraint-based models of biochemical reactions systems. It has been toolbox developed in the group of Bernhard Palsson at the University of California, San Diego. It is licensed under BSD open source license. A publication will be re-submitted soon (see Publications).

Cameo cameo.bio

A python package for computer aided metabolic engineering and optimization of cell factories. Cameo is a high-level python library developed to aid the strain design process in metabolic engineering projects. The library provides a modular framework of simulation methods, strain design methods, and access to models, that targets developers that want custom analysis workflows. Furthermore, it exposes a high-level API to users that simply want to compute promising strain designs. It is licensed under Apache License (v2.0) open source license. A publication is in preparation (see Publications).

github.io/optlang

optlang Optlang provides a common interface to a series of optimization software biosustain. and relies on the popular symbolic mathematics package sympy for problem formulation (constraints, objectives, variables, etc.). Optlang is also used in cameo to solve optimization problems encountered in genome-scale metabolic modeling. It is licensed under Apache License (v2.0) open source license.

driven.bio

Driven Driven provides state-of-the-art methods to analyze omics data using constraint-based models. It is a project by one of my PhD students and is currently under active development. It is licensed under Apache License (v2.0) open source license.

Editorial and Peer Review Duties

Peer review Reviewer for BMC Evolutionary Biology, BMC Systems Biology, Physical Review E, Biotechnology and Bioengineering, Bioinformatics, and Scientific Reports. Verified peer review record available at publicom/author/643329.

Editor for EPJ Nonlinear Biomedical Physics (since 2013) and guest editor for Frontiers in Bioengineering research topic Current challenges in modeling cellular metabolism.

Technical skills

languages

Programming Mathematica, Python, R, C, Matlab, C++,

Javascript

Version control GIT, SVN, Github, Bitbucket

Databases MySQL, SQLite, HDF5,

pytables

Systems Apple OS X, Linux, BSD, and other UNIX variants, Microsoft Windows

Bioinformatics BLAST, Biopython, Chemoinformatics Open Babel, ChemAxon

KEGG API, Pathway

Marvin (Java API and command-line tools),
SMILES, InChI, SMARTS,

ChEBI API

Modeling tools cobrapy, cameo, driven, Optimization CPLEX, Gurobi, GLPK,

COBRA Toolbox, Copasi, GAMS, NEOS optimiza-

 ${\it Cell Designer, SBW} \qquad \qquad {\it tion server, inspyred}$

Languages

German Native speaker English Fluent

Greek Fluent Danish Basic