Andreas Hoppe

Curriculum vitae

Business address:	Institute for Biochemistry Charitéplatz 1/Virchowweg 6 10117 Berlin Phone: +49-30-450528176 Germany E-mail: hoppe@bioinformatics.org
Private address:	Schinkelstr. 8 16341 Panketal Germany
Place and Date of Birth:	Berlin, April 21th, 1970.
Citizenship:	Germany
Marital Status:	Married, four children

Education

1984-1988 Abitur at the Special School "Heinrich Hertz" of mathematics, natural sciences, and technics in Berlin.

1988-1994 Diploma in Mathematics at the Humboldt University Berlin. Study visit of Artificial Intelligence and Mathematics in Edinburgh. Internship at Akademie der Wissenschaften: "Expert system for research decisions in pharmaceutical industry." In Diploma thesis, contribution to the computational group theory software GAP at the RWTH Aachen (Joachim Neubüser) [34].

1994-1998 Dr. rer. nat. in Mathematics for a study of Normal forms in Dedekind domains in Computational Number Theory (Michael E. Pohst) at the Technical University Berlin, in cooperation with Henri Cohen, Bordeaux. Algorithm development and implementation for MAGMA (computer algebra system) [32].

Professional experience

1999–2005 Post-Doc for Protein Structure Theory (Cornelius Frömmel) at Charité Berlin, developed algorithms and software to predict molecular arrangements, used for the prediction of interactions in the drug design process.

2005–now Post-Doc in Computational Systems Biochemistry (Hermann-Georg Holzhütter) at Charité Berlin, in the VirtualLiver Network and its predecessors, HepatoSys. Modeled metabolic networks, developed algorithms for flux-balance optimization, contributed to biological thermodynamics, and the interpretation of transcription data.

Non-scientific interests

Photography, mountaineering, apnoe diving, cycling, skiing, music. Former chess player, placed 9/16/10 in national youth championships (U11/U13/U15, 1980/82/84).

Publications

Peer-reviewed article, first author

1. Abshagen K*, Hoppe A*, Thomas M, Müller I, Ebert M, Weng H, Holzhütter HG, Zanger UM, Vollmar B, Dooley S (2014). Pathobiochemical signatures of cholestatic liver disease in bile duct ligated mice. * contributed equally. Submitted to JBC.
2. Hoppe A, Ilkavets I, Dooley S, Holzhütter HG. (2012) Metabolic consequences of the cultivation of primary mouse hepatocytes and the effect of TGFβ stimulation screened from transcript data. Metabolites, 2012; 2(4): 983-1003.

3. Hoppe A. (2012) What mRNA abundances can tell us about metabolism. Metabolites, 2012; 2(3):614-631.
4. Hoppe A, Holzhütter HG. (2012) ModeScore: A method to infer changed activity of metabolic function from transcript profiles. OpenAccess Series in Informatics (OASIcs), 26:1-11.
5. Hoppe A, Richter C, Holzhütter HG. (2011) Enzyme maintenance effort as criterion for the characterization of alternative pathways and length distribution of isofunctional enzymes. BioSystems, 105(2):122–129.
6. Hoppe A, Hoffmann S, Gerasch A, Gille C, Holzhütter HG. (2011) FASIMU: flexible software for flux-balance computation series in large metabolic networks. BMC Bioinformatics, 12(1):28.
7. Gille C*, Bölling C*, Hoppe A*, Bulik S, Hoffmann S, Hübner K, Karlstädt A, Ganeshan R, König M, Rother K, Weidlich M, Behre J, Holzhütter HG. (2010) HepatoNet1: a comprehensive metabolic reconstruction of the human hepatocyte for the analysis of liver physiology. Mol Syst Biol., 6:411. * contributed equally.
8. Hoppe A, Hoffmann S, and Holzhütter HG. (2007) Including metabolite concentrations into flux-balance analysis: Thermodynamic realizability as a constraint on flux distributions in metabolic networks. BMC Syst. Biol., 1(1): 23. 53 citations as of 4.9.12.
9. Hoppe A and Frömmel C. (2003) NeedleHaystack: A program for the rapid recognition of local structures in large sets of atomic coordinates. J. Appl. Cryst. 36, 1090-1097.

Peer-reviewed article, contribution

9. Thiele I, Swainston N, Fleming RMT, **Hoppe A**, Sahoo S, Aurich MK, Haraldsdottir H, Mo ML, Rolfsson O, Stobbe MD, Thorleifsson SG, Agren R, Bölling C, Bordel S, Chavali AK, Dobson P, Dunn WB, Endler L, Hala D, Hucka M, Hull D, Jameson D, Jamshidi N, Jonsson JJ, Juty N, Keating S, Nookaew I, Le Novere N, Malys N, Mazein A, Papin JA, Price ND, Selkov Sr. E, Sigurdsson MI, Simeonidis E, Sonnenschein N, Smallbone K, Sorokin A, van Beek JHGM, Weichart D, Goryanin I, Nielsen J, Westerhoff HV, Kell DB, Mendes P, Palsson BØ. (2013) A community-driven global reconstruction of human metabolism, Nat. Biotech. 31(5):419-25.
10. Bazzani S, **Hoppe A**, Holzhütter HG. (2012) Network-based assessment of the selectivity of metabolic drug targets in Plasmodium falciparum with respect to human liver metabolism. BMC Syst Biol. 6(1):118.
11. Gille C, Hübner K, **Hoppe A**, Holzhütter HG. (2011) Metannogen: annotation of biological reaction networks. Bioinformatics 27(19):2763-4.
12. Huthmacher C, **Hoppe A**, Bulik S, Holzhutter HG. (2010) Antimalarial drug targets in Plasmodium falciparum predicted by stage-specific metabolic network analysis. BMC Syst Biol., 4(1):120.
13. Rother K, Hoffmann S, Bulik S, **Hoppe A**, Gasteiger J, Holzhütter HG. (2010) IGERS: Inferring Gibbs energy changes of biochemical reactions from reaction similarities. Biophys J., 98(11):2478-86.
14. Bauer RA, Bourne PE, Formella A, Frömmel C, Gille C, Goede A, Guerler A, **Hoppe A**, Knapp EW, Pöschel T, Wittig B, Ziegler V, Preissner R. (2008) Superimpose: a 3D structural superposition server Nucleic Acids Res., 36(W47-W54).

15. Gille C, **Hoppe A**, Holzhütter HG. (2008) Web-Links as a Means to Document Annotated Sequence and 3D-Structure Alignments in Systems Biology. Genome Inform.; 20:277-84.
16. Günther S, May P, **Hoppe A**, Froemmel C, Preissner R. (2007) Docking without docking: ISEARCH-prediction of interactions using known interfaces. Proteins. CAPRI, Special Issue. Sep 5;69(4):839-844.
17. Hoffmann S, **Hoppe A** and Holzhütter HG. (2007) Pruning genome-scale metabolic models to consistent ad functionem networks. Genome Informatics, 18(1), 308-19.
18. Hoffmann S, **Hoppe A** and Holzhütter HG. (2006) Composition of Metabolic Flux Distributions by Functionally Interpretable Minimal Flux Modes (MinModes). Genome Informatics 17(1), 195-207.

Article in book

19. Hoppe A and Frömmel C. Total surface comparison - Glimpse into the morphogenesis of Proteins. In: QSAR and Molecular Modelling in Rational Design of Bioactive Molecules. Editors: Esin Aki Sener and Ismail Yalcin. Computer-aided drug design & development society in Turkey, 2006. ISBN 975-00782-0-9.
20. Hoppe A and Frömmel C. The molecular mimicry hypothesis: Foundation and limits of rational drug design. In: Designing Drugs and Crop Protectants: processes, problems and solutions. Editors: Martyn Ford, David Livingston, John Dearden, Han Van de Waaterbeemd. Blackwell Publishings 2003. ISBN 1-4051-2516-0.

Selected conference talks

21. Thermodynamic constraints improve flux balance optimization. At: Metabolic Pathway Analysis, Oxford, 2013.
22. ModeScore — A method to infer changed activity of metabolic functions from transcript profiles. At: German Conference of Bioinformatics, Jena, 2012.
23. Integrating metabolome and expression data into optimization-based network analysis. Three approaches developed in the Holzhütter group. At: IOMPA — Integrating omics data in metabolic pathway analysis, workshop at ICSB, Edinburgh, 2010.
24. HepatoNet - Stoichiometric model of the human hepatocyte. Curation and applications. At: Brasil Deutschland Systems Biology meeting, Ouro Preto, 2008.
25. The molecular mimicry hypothesis: Foundation and limits of rational drug design. At: Euro-QSAR, Bournemouth, 2002.

Selected posters

26. Hoppe A, Richter C, Holzhütter HG. Are enzyme costs minimized in evolution? Enzyme size, efficiency and turnover as a mean for better flux predictions in FBA. At: ICSB, Edinburgh, 2010.

27. Hoppe A, Hoffmann S, Gerasch A, König M, Gille C, Holzhütter HG. FASIMU: A flexible software for flux-balance computation series in large metabolic networks. At: SBMC, Freiburg, 2010.
28. Hoppe A, Gerasch A, Hoffmann S. How visualization of flux modes helps to generate biochemical hypotheses. At: VizBi, Heidelberg, 2010.
29. Hoppe A, Hoffmann S, Holzhütter HG. Constrained optimization sheds light in the metabolic functioning of higher cells. At ICSB, Gothenborg, 2008.
30. Hoppe A and Frömmel C. Total surface comparison — Glimpse into the morphogenesis of proteins. At: Euro-QSAR, Istanbul, 2004.
31. Hoppe A and Frömmel C. Looking for the Needle in the Haystack: An Algorithm for the Rapid Recognition of Local Structures in Proteins. At: Euro-QSAR, Düsseldorf, 2000.

Theses

32. Effiziente Algorithmen zur Berechnung von Elementarteilern ganzzahliger Matrizen — Implementation in GAP. (1994) Diplomarbeit im Lehrstuhl D für Mathematik an der RWTH Aachen.
33. Normal forms over Dedekind domains, efficient implementation in the computer algebra system KANT. (1998) Accepted thesis of the department 3, Mathematics, of the Technical University of Berlin for the award of the academical degree Doctor of the natural sciences. Download pdf.

Further activities

- Reviewer of journals in systems biology and theoretical biology (e.g. Molecular Systems Biology, BMC Systems Biology, BioSystems, Bioinformatics, BMC Bioinformatics, Journal of Theoretical Biology, Molecular Genetics and Metabolism, Biotechnology and Bioengineering, Biotechnology Progress, Nucleic Acids Research).
- Author and maintainer of the freely available software package NeedleHaystack. Author and maintainer of the public license (GPL) software package FASIMU. Co-author of the visualization plug-in faBiNA.

Skills and expertise

Supervision

Co-supervision of the PhD theses of Sabrina Hoffmann, Carola Huthmacher (both succeeded), and Susanne Bazzani (in progress) as well as the Diploma thesis of Christine Richter (succeeded), see publications [11,13,18,19,10]. Supervision of Erasmus internship of Marijke Dermois, TU Eindhoven.

Grant applications

Co-ordinating partner of a collaboration project submitted to the BMBF funding initiative "Innovative Toxikologie zur Reduzierung von Tierversuchen (e:ToP)" (http://www.ptj.de/e-top).

Administration

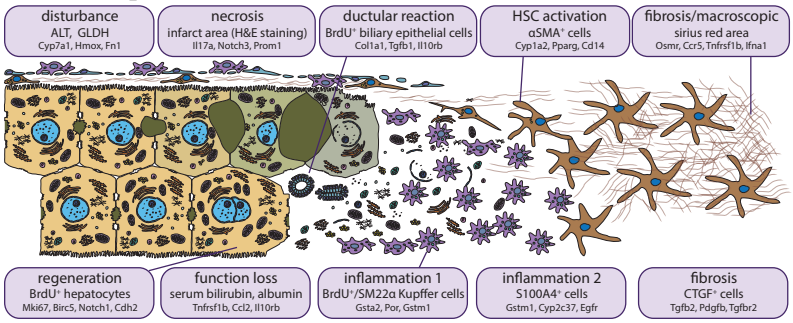
- Scientific administrator for the VirtualLiver Network consortium. Organizer and reporter for one work package (A1.1).
- Server administration for workgroups: Holzhütter group (since 2005), Frömmel group (2001-2004), Sulanke group (1993-94).
- Website administration for Holzhütter group (www.charite.de/sysbio, since 2005) and Frömmel group (www.charite.de/bioinf, 2002-05).

Programming languages

C	language of NeedleHaystack [9] and KANT/MAGMA [32]
R, octave	languages used in ModeScore [4]
AWK, bash	main languages of FASIMU [6]
java	language of faBiNA [7]
HTML, php	webpage programming including the web-accessible calculations with NeedleHaystack [9]
Pymol, rasmol	molecular geometry visualization [20,21]
LaTeX	layout and scientific visualization [5], automated process from calculations to printable documents
grace	scientific visualization [8]
GAP	group theory language [33]
Prolog, TurboPascal, Maple, Pascal	used in graduate courses and projects

Graphical design for scientific purposes

Work sample from [1]:



Languages

German	native language
English	business fluent
Russian	advanced, particularly written
Spanish	basic knowledge

Websites

www.charite.de/sysbio/hoppe	personal page
www.bioinformatics.org/fasimu	FASIMU software
www.charite.de/bioinf/haystack	NeedleHaystack software
scholar.google.com/citations?user=MdlOMGUAAAAJ	Google scholar listing

Other

Driver's license B/MSL. DLRG lifeguard (silver).

Research statement

Based on an education in mathemtics and computer science the core of my research in systems biology is the development of algorithms, first in structural molecular biology, then in metabolic modeling. In the software I developed the emphasis is not only the efficiency of the final implementation but also an efficient development process and software flexible enough to explore the properties of a system in a scientific way. In colloboration with medical doctors, biologist, and biophsicists I was also involved in the interpretation of the computation results. Thus, I developed algorithms which followed the lines of thinking of the biologist and medical scientist.

In molecular geometry I implemented a 3D search algorithm [9] with the emphasis on speed to utilize database searches of molecular interfaces in the DFG-Forschgruppe "Molekulare Bibliotheken". In modeling of metabolic networks I introduced a new approach [8] and developed the software FASIMU [6] for the exploration of metabolic networks with flux-balance optimizitions. It was also used for the testing in reconstruction projects of genome-wide metabolic networks for human cells [7,10].

Currently, I'm involved in several projects based on omics data for which I develop specifically adapted tools which utilize available domain knowledge to generate testable hypotheses. One of these tools is ModeScore [4] whose purpose is the understanding of metabolic functions through expression profiles. A crucial aspect of my work is the integration of different types of large-scale data — for the metabolic modeling metabolite concentrations, flux data, proteome data of the enzymes and transporters, and the expression of genes coding and controlling them.

Visualization is an integral part of my computational work in systems biology. It is based on the notion that derivatization of measured data should not be taken too far, instead, raw data should be visualized in the context of computed results. In molecular geometry I created images with pymol and rasmol [9,32], the figure in [31] was chosen for the title page of the conference proceedings. For metabolic networks I developed a plugin faBiNA [6] to draw network diagrams with visual elements showing computed results. For the visulization of expression data I intrduced a special diagram type used in [2].

In my future career I plan a stronger focus on Bioinformatics and closer connection to the process of experimental investigation.