Axel W. Fischer, Ph.D.

Curriculum Vitae
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Major Projects and Contributions

- **BioChemical Library, software suite for molecular modeling and drug design**
  From 2012 to 2018, I have been the lead developer on algorithms for protein ensemble prediction and *in silico* simulation of spectroscopic data. The project follows a highly modular design, which is implemented in C++14 with about 600k LOC. My specific contributions included:
  - Redesign of the optimization framework according object-oriented standards to achieve an integration of probabilistic sampling and data mining methods
  - Development of algorithms for sampling loop regions in proteins, using probabilistic sampling through a Monte Carlo Metropolis algorithm in conjunction with knowledge-based potentials
  - Development of an abstraction layer for multi-processing and integration of MPI
  - Development of a CUDA application to simulate spectroscopic data from electron paramagnetic resonance experiments
  - Development of methods using statistical analysis to determine a proteins equilibrium constitution from experimentally determined and simulated spectroscopic data

- **Dedoop, software suite for entity resolution using MapReduce**
  This project was part of my Bachelor thesis and was primarily worked on by me and my thesis adviser. The software suite uses a distributed MapReduce approach for entity resolution and was implemented in Java with about 80k LOC. My specific tasks included:
  - Development of a submission component for MapReduce workflows, including a scheduler
  - Development of a file management system for the Hadoop Distributed File System, including handling of inconsistencies between clients and read/write errors

- **FAnToM, software suite for field analysis using topological methods**
  I worked on this project as undergraduate researcher in a team consisting of four developers. The software suite employs topological methods to simulate and visualize air and liquid flows. It was implemented using C++11 and Python with about 60k LOC. My specific tasks included:
  - Development of algorithms for vector field analysis
  - Implementation of file handlers to read/write and convert field data from and to binary format

My publications are listed on page 3.

Technical Skills

Programming languages	C++ (11, 14, 17, 20), Java, Python, Perl, R, Emacs Lisp, CUDA
Tools	CMake, GNU autotools, Git, SVN, boost, STL, MPI, Emacs
Software design	Object-oriented software design, functional software design

Education & Experience

2018–present Computer Research Scientist Renaissance Technologies LLC, NY, USA

2012–2018 Ph.D. (Chemistry) Vanderbilt University, Nashville, USA

- *Development of a software suite and algorithms for protein ensemble prediction*
- *Integration of experimental data into computational methods*

2009–2012 B.Sc. (Computer Science) Universität Leipzig, Leipzig, Germany

- *Development of algorithms for flow simulation and visualization*
- *Development of submission components for MapReduce workflows*
- *Development of a file management system for Hadoop Distributed File System*

Experience and Skills

- Since 2012, I have authored twelve research articles on algorithm development of methods for the prediction of protein ensembles from limited experimental data.
- I have experience in developing medium to large applications using object-oriented software design approaches and the programming languages C++, Java and Python. Notable projects I contributed to:
  - BioChemical Library (Molecular modeling and drug design): C++14, 600k LOC
  - FAnToM (Field analysis using topological methods): C++11, 60k LOC
  - Dedoop (Entity resolution using Hadoop): Java, 80k LOC
- From 2012 to 2018, I have been a key developer of Vanderbilt University's *BioChemical Library*, which is an integrated software suite for molecular modeling and computer-aided drug design. Besides the development of algorithms for protein ensemble prediction and structure optimization, my work encompassed improving parallelization and GPU acceleration (CUDA).
- I have substantiated knowledge of machine learning through Artificial Neural Networks, Hidden Markov Models, and Support Vector Machines, which I employed to evaluate thermodynamic properties of macro-molecules.
- From 2015 to 2018, I have refereed research articles for *IEEE Transactions on Evolutionary Computing* and *Nature Protocols*.
- I am proficient in statistical data analysis and visualization with R and Python.

- During my graduate studies I mentored five graduate and four undergraduate students on projects involving software design and object-oriented programming using C++ and Python.
- During my graduate and undergraduate studies I was employed as teaching assistant for object-oriented design and programming, algorithms and data structures, computer engineering, and thermodynamics of chemical systems.

Publications and Presentations

Invited Talks

- In silico *prediction of protein structures and ensembles*, Chemistry Forum, 2016, Nashville, USA
- *Prediction of protein structures from limited experimental data*, MBTP/CSB, 2016, Nashville, USA
- De novo *protein structure prediction from cross-linking data*, 5th Symposium on Structural Proteomics, 2015, Halle, Germany

Peer-reviewed Research Articles

[1] Diego del Alamo, Axel W Fischer, Rocco Moretti, Nathan S Alexander, Jeffrey Mendenhall, Nicholas J Hyman, and Jens Meiler. "Efficient Sampling of Protein Loop Regions Using Conformational Hashing Complemented with Random Coordinate Descent". In: *Journal of Structural Biology* (Dec. 2020). DOI: 10.1016/j.jsb.2016.04.014.

[2] Yan Xia, Axel Walter Fischer, and Jens Meiler. "Integrated Structural Biology for Alpha-Helical Membrane Protein Structure Determination". In: *Structure* 26.1 (Apr. 2018), pp. 657–666. DOI: 10.1016/j.str.2018.02.006.

[3] Bian Li, Jeffrey Mendenhall, Elizabeth Dong Nguyen, Brian E. Weiner, Axel W. Fischer, and Jens Meiler. "Improving prediction of helix-helix packing in membrane proteins using predicted contact numbers as restraints". In: *Proteins: Structure, Function, and Bioinformatics* 85.7 (July 2017), pp. 1212–1221. DOI: 10.1002/prot.25281.

[4] Axel Walter Fischer, David M Anderson, Maxx H Tessmer, Dara W. Frank, Jimmy B Feix, and Jens Meiler. "Structure and Dynamics of Type III Secretion Effector Protein ExoU As determined by SDSL-EPR Spectroscopy in Conjunction with De Novo Protein Folding". In: *ACS Omega* 2.6 (June 2017), pp. 2977–2984. DOI: 10.1021/acsomega.7b00349.

[5] Maximiliano Figueroa, Mike Sleutel, Marylene Vandevenne, Gregory Parvizi, Sophie Attout, Olivier Jacquin, Julie Vandenameele, Axel W. Fischer, Christian Damblon, Erik Goormaghtigh, Marie Valerio-Lepiniec, Agathe Urvoas, Dominique Durand, Els Pardon, Jan Steyaert, Philippe Minard, Dominique Maes, Jens Meiler, André Matagne, Joseph A. Martial, and Cécile Van de Weerdt. "The unexpected structure of the designed protein Octarellin V.1 forms a challenge for protein structure prediction tools". In: *Journal of Structural Biology* 195.1 (July 2016), pp. 19–30. DOI: 10.1016/j.jsb.2016.05.004.

[6] Axel W Fischer, Enrica Bordignon, Stephanie Bleicken, Ana J. García-Sáez, Gunnar Jeschke, and Jens Meiler. "Pushing the size limit of de novo structure ensemble prediction guided by sparse SDSL-EPR restraints to 200 residues: The monomeric and homodimeric forms of BAX". In: *Journal of Structural Biology* 195.1 (July 2016), pp. 62–71. DOI: 10.1016/j.jsb.2016.04.014.

[7] Axel Walter Fischer, Sten Heinze, Daniel K. Putnam, Bian Li, James C Pino, Yan Xia, Carlos F Lopez, and Jens Meiler. "CASP11 – An Evaluation of a Modular BCL::Fold-Based Protein Structure Prediction Pipeline". In: *PLOS ONE* 11.4 (Apr. 2016). Ed. by Yang Zhang, e0152517. DOI: 10.1371/journal.pone.0152517.

[8] Reza Dastvan, Axel W Fischer, Smriti Mishra, Jens Meiler, and Hassane S Mchaourab. "Protonation-dependent conformational dynamics of the multidrug transporter EmrE". In: *Proceedings of the National Academy of Sciences* 113.5 (Feb. 2016), pp. 1220–1225. DOI: 10.1073/pnas.1520431113.

[9] Bian Li, Jeffrey Mendenhall, Elizabeth Dong Nguyen, Brian E Weiner, Axel Walter Fischer, and Jens Meiler. "Accurate Prediction of Contact Numbers for Multi-Spanning Helical Membrane Proteins". In: *Journal of Chemical Information and Modeling* 56.2 (Feb. 2016), pp. 423–434. DOI: 10.1021/acs.jcim.5b00517.

[10] Tommy Hofmann, Axel W Fischer, Jens Meiler, and Stefan Kalkhof. "Protein structure prediction guided by crosslinking restraints – A systematic evaluation of the impact of the crosslinking spacer length". In: *Methods* 89 (Nov. 2015), pp. 79–90. DOI: 10.1016/j.ymeth.2015.05.014.

[11] Axel Walter Fischer, Nathan Scott Alexander, Nils Woetzel, Mert Karakas, Brian E. Weiner, and Jens Meiler. "BCL::MP-Fold: Membrane protein structure prediction guided by EPR restraints". In: *Proteins: Structure, Function, and Bioinformatics* 83.11 (Nov. 2015), pp. 1947–1962. DOI: 10.1002/prot.24801.

[12] Sten Heinze, Daniel K. Putnam, Axel W. Fischer, Tim Kohlmann, Brian E. Weiner, and Jens Meiler. "CASP10 – BCL::Fold efficiently samples topologies of large proteins". In: *Proteins: Structure, Function, and Bioinformatics* 83.3 (Mar. 2015), pp. 547–563. DOI: 10.1002/prot.24733.