Darius Schaub

Billhorner Kanalstraße 22, 20539 Hamburg, Germany
+49 159 0197 0346 schaub.darius@gmail.com linkedin.com/dschaub github.com/dschaub95

Objective

My goal is to contribute to the understanding of biological life and to solving the stabilization problem underlying medicine. To achieve this, I am especially interested in establishing a communication channel with biological matter to enable top-down control of the system, as proposed by Prof. Michael Levin. Technically, this includes modeling multi-cellular collectives using frameworks such as Graph Neural Cellular automata and analyzing how they process information and make decisions.

Education

University Medical Center Hamburg-Eppendorf, Center for Biomedical AI **Dec. 2022 – Present**
Ph.D. student in the lab of Prof. Stefan Bonn *Hamburg, Germany*

- Focus: describing and modeling spatial organization of cells in health and disease

Harvard Medical School, Channing Division of Network Medicine **Feb. 2021 – Jun. 2023**
Remote visiting student in the lab of Prof. Yang-Yu Liu *Boston, MA*

- Focus: deep reinforcement learning, combinatorial optimization, graph neural networks, multi-omics integration, microbiome modeling
- Successful participation in the VDAART disease outcome prediction challenge hosted by the Channing Division of Network Medicine

University of Hamburg & Hamburg University of Technology **Oct. 2019 – Jun. 2022**
Master of Science in Industrial Mathematics *Hamburg, Germany*

- Grade 1.05 (passed with distinction)
- Relevant courses: partial differential equations, systems theory, mathematics of neural networks, machine learning, optimization
- Projects: mathematical data analysis on the approximate inverse for linear problems, "Project: Machine Learning" in image classification as team leader
- Thesis: *Solving the traveling salesman problem via deep reinforcement learning* (supervised by Prof. Yang-Yu Liu)

University of Hamburg **Oct. 2017 – Sep. 2019**
Bachelor of Science in Nanoscience *Hamburg, Germany*

- Grade 1.35 (excellent)
- Relevant courses: quantum/statistical/solid-state physics, optimization, numerical mathematics, statistics
- Thesis: *Ionization dynamics of H_2O - a Matrix Product State study* (supervised by Prof. Daniela Pfannkuche)

University of Hamburg **Oct. 2015 – Sep. 2017**
Bachelor of Science in Chemistry *Hamburg, Germany*

- Successfully attended 80% of the B.Sc. Chemistry curriculum, including courses in biochemistry and organic chemistry

Experience

SICK AG **Jan. 2020 – Nov. 2022**
Data Science working student *Hamburg, Germany*

- Achieved an 80% reduction in scheduled maintenances by predicting sensor contamination
- Developed and deployed a predictive maintenance and time-series forecasting framework for various sensor species (scikit-learn, unittest, TypeScript)
- Gained experience with rare event prediction, time series forecasting, anomaly detection, and software engineering best practices (CI/CD)

SICK AG **Oct. 2020 – Dec. 2020**
Data Science intern *Hamburg, Germany*

- Tested various machine learning algorithms for predicting device errors and maintenance events (scikit-learn)

University of Hamburg **Sep. 2016 – Jul. 2020**

Assistant teacher *Hamburg, Germany*

- Supervised exercise classes for mathematical courses in the chemistry department

Publications

[1] **Darius P Schaub***, Behnam Yousefi*, Nico Kaiser, Robin Khatri, Victor G Puelles, Christian F Krebs, Ulf Panzer, Stefan Bonn, "PCA-based spatial domain identification with state-of-the-art performance," *Bioinformatics*, vol. 41, no. 1, btaf005, Jan. 1, 2025, ISSN: 1367-4811. DOI: 10.1093/bioinformatics/btaf005.

[2] Huiying Wang, Jonas Engesser, Robin Khatri, **Darius P. Schaub**, Hans-Joachim Paust, Zeba Sultana, Saskia-Larissa Jauch-Speer, Anett Peters, Anna Kaffke, Stefan Bonn, "Type I interferon drives T cell cytotoxicity by upregulation of interferon regulatory factor 7 in autoimmune kidney diseases in mice," *Nature Communications*, vol. 16, no. 1, p. 4686, May 20, 2025, ISSN: 2041-1723. DOI: 10.1038/s41467-025-59819-7.

[3] Behnam Yousefi*, **Darius P. Schaub***, Robin Khatri, Nico Kaiser, Malte Kuehl, Cedric Ly, Victor G. Puelles, Tobias B. Huber, Immo Prinz, Christian F. Krebs, "SCALE: Unsupervised Multi-Scale Domain Identification in Spatial Omics Data." (May 27, 2025), [Online]. Available: https://www.biorxiv.org/content/10.1101/2025.05.21.653987v1, pre-published.

[4] Sina Abdollahi, **Darius P. Schaub**, Madalena Barroso, Nora C. Laubach, Wiebke Hutwelker, Ulf Panzer, S.øren W. Gersting, Stefan Bonn, "A comprehensive comparison of deep learning-based compound-target interaction prediction models to unveil guiding design principles," *Journal of Cheminformatics*, vol. 16, no. 1, p. 118, Oct. 28, 2024, ISSN: 1758-2946. DOI: 10.1186/s13321-024-00913-1.

[5] Jonas Engesser*, Robin Khatri*, **Darius P. Schaub***, Yu Zhao, Hans-Joachim Paust, Zeba Sultana, Nariaki Asada, Jan-Hendrik Riedel, Varshi Sivayoganathan, Anett Peters, "Immune profiling-based targeting of pathogenic T cells with ustekinumab in ANCA-associated glomerulonephritis," *Nature Communications*, vol. 15, no. 1, p. 8220, Sep. 19, 2024, ISSN: 2041-1723. DOI: 10.1038/s41467-024-52525-w.

[6] Zeba Sultana, Robin Khatri, Behnam Yousefi, Nikhat Shaikh, Saskia L. Jauch-Speer, **Darius P. Schaub**, Jonas Engesser, Malte Hellmig, Arthur L. Hube, Varshi Sivayoganathan, "Spatio-temporal interaction of immune and renal cells determines glomerular crescent formation in autoimmune kidney disease." (Dec. 21, 2024), [Online]. Available: http://biorxiv.org/lookup/doi/10.1101/2024.12.18.629206, pre-published.

[7] Zeba Sultana, Robin Khatri, Behnam Yousefi, Nikhat Shaikh, Saskia L. Jauch-Speer, **Darius P. Schaub**, Jonas Engesser, Malte Hellmig, Arthur L. Hube, Varshi Sivayoganathan, "Spatio-temporal interaction of immune and renal cells determines glomerular crescent formation in autoimmune kidney disease." (Dec. 21, 2024), [Online]. Available: http://biorxiv.org/lookup/doi/10.1101/2024.12.18.629206, pre-published.

[8] Xu-Wen Wang, Tong Wang, **Darius P. Schaub**, Can Chen, Zheng Sun, Shanlin Ke, Julian Hecker, Anna Maaser-Hecker, Oana A. Zeleznik, Roman Zeleznik, "Benchmarking omics-based prediction of asthma development in children," *Respiratory Research*, vol. 24, no. 1, p. 63, Feb. 26, 2023, ISSN: 1465-993X. DOI: 10.1186/s12931-023-02368-8.

Conferences, Hackathons, and Summer schools

scverse Hackathon, Paris, France **Mar. 2025**

- Accelerated point filter implementation in the spatialdata package by several orders of magnitude

ESSB Conference, Berlin, Germany **Dec. 2024**

- Discussed spatial domain identification methods and nomenclature

scverse Conference, Munich, Germany **Sep. 2024**

- Presented a poster on the paper "PCA-based spatial domain identification with state-of-the-art performance"

Oxford Machine Learning Summer School, Oxford, UK **Jun. 2023**

- Winner of the MLx Cases team challenge among 30 competing teams, with the task to classify histology images of breast carcinoma under limited data constraints (PyTorch)
- Learned about and gained hands-on experience with state-of-the-art deep learning approaches to various medical and biological problem settings both from ML and clinical experts (self-supervised learning, geometric deep learning, causal ML, bayesian deep learning)

*Equal contribution.

Skills and interests

Languages/Frameworks: Python (professional), PyTorch (professional), TensorFlow (advanced), C/C++ (intermediate), TypeScript (basic), SQL (basic)
Technologies: Linux, Github, Gitlab, Docker, Kubernetes, Jira
Other interests: science-fiction, fitness, nutrition, dancing, politics, philosophy, learning