Winfried Ripken

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Google scholar
GitHub
LinkedIn

COURSEWORK

GRADUATE
Machine Learning on Graphs
Probabilistic Graphical Models
Big Data and Visualization
Predictive Analytics
NLP using word vectors

UNDERGRADUATE
Linear Algebra
Probability Theory
ML & Computer Vision
Physics

SKILLS

ML tools:
Jax • PyTorch • Numpy • SciPy •
Pandas • OpenCV
MLOps:
Docker • Kubernetes • Terraform •
GCP • Weights & Biases • Slurm
Coding:
Python (proficient) • C++ (working
knowledge) • C#
Molecular Simulation:
E3x • Atomic Simulation Environment
(ASE) • SchNetPack • RDKit
Languages:
German • English • French (basic)

EXPERIENCE

TECHNICAL UNIVERSITY BERLIN | PhD Student
Apr 2024 - present | Berlin, Germany

I am a 2nd-year PhD student in the BIFOLD graduate school, supervised by Stefan Chmiela and Klaus-Robert Müller.

- My most recent project enables Molecular Dynamics (MD) simulations with variable time steps, at least an order of magnitude larger than typical integration steps. The operator is trained without trajectory supervision using a tailored consistency loss and independent pairs of positions and forces.
- I co-developed an efficient generative modeling architecture for molecular modeling based on (equivariant) diffusion transformers (DiTs). Using flow matching, we reach SOTA results on several molecular conformer generation benchmarks, significantly shifting the speed-accuracy pareto front.
- I co-developed a novel framework for diffusion-based generative modeling for molecules and images. It disentangles signal to noise ratio (SNR) from total variance (TV) to enable more efficient diffusion schedules, reaching high quality results with as few as 4 sampling step. Currently in submission.

MERANTIX MOMENTUM GMBH | Machine Learning Researcher
Nov 2021 - Mar 2024 | AI Campus Berlin, Germany

Merantix Momentum is one of the few startups in Berlin with a dedicated research department engaging in publicly funded research projects.

- I was the lead in two research projects, where we collaborated with Volkswagen to improve electric motor design via automated simulation of PDEs via surrogate models, and with other German manufacturing players to introduce ML-based decisions into their assembly lines.
- Learning a solution operator for Partial Differential Equations (PDEs) using Graph Neural Networks (GNNs): I developed a novel augmentation technique that improved generalization performance by more than one order of magnitude, as well as a graph rewiring strategy that enables to train solution operators for very high-resolution data (more than 30K nodes).

TERAKI GMBH | Video Deep Learning Intern & Working student
Jul 2020 - Mar 2021 | Berlin, Germany

Teraki provides software for teleoperated and autonomous driving.

- Trained a very lightweight yet accurate semantic segmentation network for road scenes (60 FPS on Jetson Nano, false negative rate < 2%).
- Pruned 50% of the weights to increase FPS by another 30%.
- I contributed to client projects & presented my results in client calls.

HASSO-PLATTNER-INSTITUTE | Teaching (Design Thinking)
Sep 2019 - Jun 2020 | Potsdam, Germany
I supervised 2 student ML projects, resulted in one filed patent.

TAKATA (NOW JOYSON SAFETY SYSTEMS) | Working student
Aug 2014 - Jul 2017 | Elterlein, Germany

EDUCATION

HASSO PLATTNER INSTITUTE MSc in Computer Science
Oct 2017-Oct 2021 | Potsdam, Germany | Grade: 1.1 (1.0 = best, 4.0 = pass)
Master thesis: User-controllable Neural Style Transfer (Published at ECCV 2022).
Master project: Self-supervised learning for 3D data (Published at NeurIPS 2020).

EFREI PARIS SUD Erasmus+ Semester
Aug 2018-Feb 2019 | Villejuif, France
Best grade for ML research project with Orange in Paris.

STANFORD UNIVERSITY ME310 | Global Team-based innovation
Oct 2017-Jun 2018 | Stanford, CA, USA
Co-created ML-based product prototype in a global team.

CHEMNITZ UNIVERSITY BSc in Computer Science
Oct 2014-Sep 2017 | Chemnitz, Germany | Grade: 1.1 (1.0 = best, 4.0 = pass)
Bachelor thesis about asynchronous Deep Reinforcement Learning (best grade 1.0).

PREPRINTS

Ripken, Winfried*, Michael Plainer*, Gregor Lied*, Thorben Frank*, Oliver T Unke, Stefan Chmiela, Frank Noé, and Klaus Robert Müller (2026). "Learning Hamiltonian Flow Maps: Mean Flow Consistency for Large-Timestep Molecular Dynamics". In: *arXiv preprint arXiv:2601.22123*.

Kahouli, Khaled, **Winfried Ripken**, Stefan Gugler, Oliver T Unke, Klaus-Robert Müller, and Shinichi Nakajima (2025). "Enhancing Diffusion Models Efficiency by Disentangling Total-Variance and Signal-to-Noise Ratio". In: *arXiv preprint arXiv:2502.08598*.

SELECTED PUBLICATIONS

Frank, J. Thorben*, **Winfried Ripken***, Gregor Lied*, Klaus-Robert Müller, Oliver T. Unke, and Stefan Chmiela (2025). "Sampling 3D Molecular Conformers with Diffusion Transformers". In: *NeurIPS*.

Ohler, Simon, Daniel Brady, Patrick Mischke, Jana Bender, Herwig Ott, Thomas Niederprüm, **Winfried Ripken**, Johannes S. Otterbach, and Michael Fleischhauer (2025). "Nonequilibrium universality of Rydberg-excitation spreading on a dynamic network". In: *Phys. Rev. Res.*

Siems, Julien*, Konstantin Ditschuneit*, **Winfried Ripken***, Alma Lindborg*, Maximilian Schambach, Johannes S Otterbach, and Martin Genzel (2023). "Curve Your Enthusiasm: Concurvity Regularization in Differentiable Generalized Additive Models". In: *NeurIPS*.

Lötzsch, Winfried*, Max Reimann*, Martin Büssemeyer, Amir Semmo, Jürgen Döllner, and Matthias Trapp (2022). "WISE: Whitebox Image Stylization by Example-Based Learning". In: *ECCV*.

Taleb, Aiham, **Winfried Lötzsch**, Noel Danz, Julius Severin, Thomas Gaertner, Benjamin Bergner, and Christoph Lippert (2020). "3D Self-Supervised Methods for Medical Imaging". In: *NeurIPS*.

* indicates equal contribution
See **scholar** for the full list of publications.