



CURRICULUM VITAE

Bernd Doser

EXPERIENCE

Senior Software Engineer @ HITS gGmbH

Since 08/2019

- Participation in the EU Centre of Excellence project [Scalable Parallel Astrophysical Codes for Exascale \(SPACE-CoE\)](#).
- Implementation of [Random Acceleration Molecular Dynamics \(RAMD\)](#) within GRO-MACS (C++)
- Implementation of [Hyperspherical Variational Autoencoder \(Spherinator\)](#)
- Implementation of [Tools for Automated Characterisation of Oscillations \(TACO\)](#) (Python and R)
- Design and implementation of a coarse-grained collagen simulation program (C++20)
- Implementation of a container-based development environment

Software Engineer @ HITS gGmbH

08/2014 - 07/2019

- Implementation of [Parallelized rotation and flipping INvariant Kohonen maps \(PINK\)](#) (C++, CUDA)
- Implementation of [Force Distribution Analysis \(FDA\)](#) in GROMACS (C++)
- Implementation of [algebraic multigrid methods in HiFlow3](#) (C++)
- Bonsai code extension [War Of Galaxies](#) for [ESO Supernova](#)
- Project-oriented support for scientific groups
- In-house training of modern software development techniques
- Implementation and support of continuous integration services
- Advisory service in high-performance computing, C++, Docker, continuous integration and deployment, ...
- Requirement analysis

Scientific Software Engineer @ AMS GmbH

12/2010 - 06/2014

- Implementation of a C++ library for automatic differentiation
- Implementation of molecular structure fragmentation for the automated force field fitting
- Contract research and validation studies for the chemical and pharmaceutical industry
- Integration of third-party software
- Validation studies to improve the accuracy of the crystal structure prediction

Research assistant @ Ludwig-Maximilians-Universität München

04/2010 - 11/2010

- Implementation of sparse algebra routines using multi-core CPU and GPU architectures

Research assistant @ Eberhard-Karls-Universität Tübingen

03/2009 - 03/2010

- Development and implementation of ab initio methods for high-accuracy calculations of large biochemical systems.



EDUCATION

- 02/2004 - 02/2009 **PhD** (summa cum laude)
Linear-scaling Møller-Plesset Perturbation Theory for the Calculation of Electron Correlation in Large Molecules
Institute of Physical and Theoretical Chemistry
University of Tübingen
- 10/1998 - 02/2004 **Chemistry Diploma**
Institute of Physical and Theoretical Chemistry
University of Tübingen

CERTIFICATES

- **Encoder-Decoder Architecture** (Google, 2023)
- **Introduction to Generative AI** (Google, 2023)
- **Introduction to Large Language Models** (Google, 2023)
- **Jenkins Engineer** (CloudBees, 2017)
- **Embedded Smart Home** (OpenHPI, 2016)
- **Concurrency- and Multi-Threading in C++11/14** (Nicolai Josuttis, 2015)
- **C++ für Fortgeschrittene** (Peter Gottschling, 2013)
- **High-Performance Computing with GPGPUs** (Leibniz-RZ, 2010)

PUBLICATIONS

- B. Doser, K. L. Polsterer, A. Fehlner, and S. Trujillo-Gomez
Machine Learning Workflow for Morphological Classification of Galaxies
[Astronomical Data Analysis Software and Systems XXXIV \(2025\)](#).
- K. L. Polsterer, B. Doser, A. Fehlner, and S. Trujillo-Gomez
Spherinator and HiPster: Representation Learning for Unbiased Knowledge Discovery from Simulations
[Astronomical Data Analysis Software and Systems XXXIII \(2024\)](#).
- D. B. Kokh, B. Doser, S. Richter, F. Ormersbach, X. Cheng, and R. C. Wade
A workflow for exploring ligand dissociation from a macromolecule: Efficient random acceleration molecular dynamics simulation and interaction fingerprint analysis of ligand trajectories
[J. Chem. Phys. 153, 125102 \(2020\)](#).
- K. L. Posterer, F. Gieseke, C. Igel, B. Doser, and N. Gianniotis
Parallelized rotation and flipping INvariant Kohonen maps (PINK) on GPUs
[ESANN \(2016\)](#).
- B. Doser, D. S. Lambrecht, J. Kussmann, and C. Ochsenfeld
Linear-Scaling Atomic Orbital-Based Second-Order Møller-Plesset Perturbation Theory by Rigorous Integral Screening Criteria
[J. Chem. Phys. 130, 064107 \(2009\)](#).
- [Complete list](#)



TALKS

- [Poster: Representation Learning for Gaia XP DR3](#)
ADASS XXXV, 2025 in Görlitz
- [Representation Learning with Spherinator \(Video\)](#)
SPACE CoE: High-Performance Computing Visualization, 2025 in Barcelona (Spain)
- [Poster: Machine-Learning Workflow for Morphology Classification of Galaxies](#)
ADASS XXXIV, 2024 in Valetta (Malta)
- [Seminar: Machine Learning Workflow Orchestration](#)
HITS gGmbH, 2024 in Heidelberg
- [Machine learning prototype for SPACE applications \(Video\)](#)
SPACE CoE, May 2024
- [Workshop: The New ISO Standard C++20](#)
HITS gGmbH, 2022 in Heidelberg
- [Demo: Parallelized rotation and flipping INvariant Kohonen maps \(PINK\)](#)
ADASS 2019 in Groningen, the Netherlands
- [Workshop: Dependency management](#)
HITS gGmbH, 2019 in Heidelberg
- [Workshop: Continuous Integration and Deployment](#)
HITS gGmbH, 2017 in Heidelberg
- [HiFlow3: Classification regarding new C++ techniques](#)
EMCL-Klausurtagung, 2015 in Trier
- [Workshop: Modern Software Development with C++](#)
HITS gGmbH, 2015 in Heidelberg
- [Assessment of a Variety of Dispersion-corrected Density Functional Theory Calculations Used in Molecular Crystal Structure Prediction](#)
7th German Conference on Chemoinformatics, 2011 in Goslar