



# CURRICULUM VITAE

Bernd Doser

## EXPERIENCE

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### Senior Software Engineer @ HITS gGmbH

Since 08/2019

- Participation in EU Centre of Excellence project [Scalable Parallel Astrophysical Codes for Exascale \(SPACE-CoE\)](#).
- Implementation of [Random Acceleration Molecular Dynamics \(RAMD\)](#) within GROMACS (C++)
- Implementation of [Hyperspherical Variational Autoencoder \(Spherinator\)](#)
- Implementation of [Tools for Automated Characterisation of Oscillations \(TACO\)](#) (Python and R)
- Design und 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
- Validations studies to improve the accuracy of 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

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- 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
- 08/2003 - 02/2004 **Diplom**  
[Institute of Physical and Theoretical Chemistry](#)  
University of Tübingen

## CERTIFICATES

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- **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

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- K. L. Polsterer, B. Doser, A. Fehlner and S. Trujillo-Gomez  
Spheringator 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

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- [Poster: Machine-Learning Workflow for Morphology Classification of Galaxies] ([https://drive.google.com/file/d/1X8ztdw\\_echSe0TJIMJA5QgHWyHAnSoE0/view?usp=sharing](https://drive.google.com/file/d/1X8ztdw_echSe0TJIMJA5QgHWyHAnSoE0/view?usp=sharing)) 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