



CURRICULUM VITAE

Bernd Doser

EXPERIENCE

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

- 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

- **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

- 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

- **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