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 moleculare 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

Reseach assistent @ Ludwig-Maximilians-Universität München
04/2010 - 11/2010

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

Reseach assistent @ 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

- 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

- Representation Learning with Spherinator
  SPACE CoE: High-Performance Computing Visualization, 2025 in Barelona (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