Carl Simon Adorf, Ph.D.

Computational Scientist & Research Software Engineer

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Education

- **University of Michigan** 2014 – 2019
  Doctor of Philosophy in Chemical Engineering *Ann Arbor, MI*

  Dissertation: Inverse Design and Analysis of Crystallization Pathways of Colloidal Systems
  Advisor: Prof. Sharon C. Glotzer, member of the National Academy of Sciences (NAS)

- **RWTH Aachen University** 2008 – 2013
  Bachelor of Science in Engineering, Mechanical Engineering *Aachen, Germany*

Experience

- **Computational Materials Scientist / Software Scientist** 2019 – present
  In the group of Prof. Nicola Marzari at École Polytechnique Fédérale de Lausanne (EPFL) *Lausanne, Switzerland*
  - **Materials MarketPlace**: Work package manager and full-stack developer for the Horizon 2020 Materials MarketPlace project, a five-year international collaboration with 18 industrial and academic partners funded by the European Commission (9.2 M EUR budget). the-marketplace-project.eu
  - **AiiDA**: Maintainer for the NumFOCUS-affiliated open-source data and workflow infrastructure AiiDA (Python) – hundreds of users in academia and industry (500 citations). Responsible for managing dependencies, CI workflows, and spearheaded a successful project on a complete installation flow and documentation overhaul. aiida.net
  - **AiiDAlab**: Led successful effort to significantly increase the technical maturity and product stability of AiiDAlab, an open-source Jupyter-based web platform to run AiiDA in the cloud (simulation-as-a-service model). Leading technical development, managing collaborations, and maintaining deployments on Kubernetes clusters (AWS, DigitalOcean). In use by (among others) the Empa institute (Switzerland). www.aiidalab.net
  - **Machine Learning**: Supervised MARVEL INSPIRE graduate fellow (6 month fully-paid stipend) in a high-throughput machine learning study (publication in preparation).
  - **Recruitment**: Led successful hiring campaign for two post-doctoral research positions.

- **Graduate Student Researcher** 2014 – 2019
  Advised by Prof. Sharon C. Glotzer at the University of Michigan *Ann Arbor, MI*
  - **Data & Workflow Management**: Inventor, maintainer, and former lead developer of the open-source data and workflow management framework: signac (Python, NumFOCUS-affiliated). The project has since grown to over 50 contributors, more than 70 citations, and has been presented (20+ times) at conferences and meetings in various scientific domains. Co-mentored Google Summer of Code (GSoC) student interns (paid scholarship). signac.io
  - **Simulation**: Contributed features for data provenance tracking and integration of advanced sampling frameworks to HOOMD-blue, an open-source application for the high-performance simulation of multi-particle systems on GPUs (C++, CUDA, Python; >400 citations) and helped design a major API revision (v3). glotzerlab.engin.umich.edu/hoomd-blue
  - **High-performance computing**: Ran GPU-accelerated simulation and machine-learning studies on leadership class super computers including the OLCF Summit system (ranked first in the TOP500 at the time) using MPI, Tensorflow (Keras), and cuML. Hosted workshops and provided support in my role as XSEDE Student Champion.
  - **Publications**: Published six (*four first-author*) journal articles on soft matter physics, machine learning applications, inverse design, and software engineering in scientific computing and gave 13 (4 invited) oral presentations at national and international meetings. Google Scholar Profile
  - **Teaching & Mentorship**: Instructor for the CHE 330 Chemical & Engineering Thermodynamics class and mentored/supervised graduate (3) and undergraduate (2) students.

Technical Skills

- **Programming**: Python, Cython, C++, JavaScript, TypeScript, HTML, MPI, OpenMP, git, bash
- **Web development**: Docker, REACT, HTML, Node.js, RESTful APIs, OpenAPI, MongoDB, Selenium
- **Cloud Computing**: AWS, Kubernetes, Ansible, Terraform, JupyterHub, OAuth2
- **High-performance computing (HPC)**: Executed massively-parallel and GPU-accelerated campaigns on: OLCF Summit & Titan, SDSC Comet, PSC Bridges, and others.
- **Python libraries**: NumPy, Jupyter, Pandas, Matplotlib, SciPy, Scikit-Learn, RAPIDS, TensorFlow (Keras)