Maximilian Saller, Ph.D.

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Date of Birth: 5/1/1991 • Citizenship: German • Visa Status: Green Card Holder

Skills

Software Stack

Python, Fortran, C/C++, PyData stack (numpy, scipy, matplotlib, etc.), MPI, OpenMP, numba, BLAS/LAPACK, Linux, bash, SLURM, git, github, make, cmake, LaTeX, Q-Chem, Gaussian, Orca, Cadpac, vmd, Mathematica

Computational and Technical

- 10 years software development experience.
- 8 years experience in data analysis and visualization.
- 8 years experience in software development for HPC environments.
- 8 years experience in version control and good software development practices.
- 8 years experience with workstation and server-grade HPC hardware.
- 4 years experience in system administration for HPC Linux systems.

Communication and Languages

- 8 years experience presenting complicated scientific concepts to both specialist and general audiences.
- 8 years experience in scientific and technical writing for the purpose of publication and presentation.
- 4 years experience taking part in and leading collaborations with teams from a variety of fields.
- Fluent speaking, reading and writing English and German. Intermediate conversational skills in Japanese.

Research and Teaching

- 10 years experience combining analytical and theoretical work with computational methods.
- 6 years experience designing and leading research projects involving multiple team members.
- 8 years experience independently developing and pursuing novel research avenues.
- 10 years experience teaching scientific and technical skills to specialist and general audiences.

Experience

Kent State University, Kent, OH, USA

Postdoctoral Research Fellow *2022–present*

Working in the group of Prof. Barry Dunietz. Scientific software development and application with a focus on the Q-Chem package for electronic structure. Applying screened range separated hybrid functionals within density functional theory to energy and charge transfer in biologically interesting systems. Development Experience: Python, C/C++

University of Michigan, Ann Arbor, MI, USA

Visiting Scholar *2022–present*

Postdoctoral Research Fellow *2020–2022*

Working in the group of Prof. Eitan Geva in the Department of Chemistry. Scientific software development and application of the improved dynamics methods to light-matter interactions. Work has been published in *The Journal of Physical Chemistry Letters* and *The Journal of Physical Chemistry C*. Purchase, installation and management of a cluster of high performance scientific workstations. Development Experience: Python, FORTRAN, C/C++

Swiss Federal Institute of Technology (ETH Zurich), Zurich, Switzerland

ETH Postdoctoral Fellow *2018–2020*

Competitive 24-month postdoctoral fellowship financed through the European Commission (valued at $250,000). Awarded based on a grant application including a detailed research proposal and interview panel. Continuing the project with Prof. Jeremy Richardson. Development Experience: Python, FORTRAN, C/C++

Postdoctoral Researcher *2017–2018*

Working in the group of Prof. Jeremy Richardson. Development of improved quantum dynamics methods with a particular focus on computational efficiency. Leading a team of researchers in the development of a general-purpose, extendable scientific software package focused on scalability on high performance hardware. Work has been published in *The Journal of Chemical Physics* and *Faraday Discussions* Development Experience: Python, FORTRAN

Education

University of Warwick, Coventry, United Kingdom

PhD in Theoretical Chemistry *2013–2017*

PhD Thesis: Sampling minimal, adaptive basis sets for multidimensional, nuclear quantum dynamics using simple, semi-classical trajectories.

Working in the group of Prof. Scott Habershon. Research was focused on development of new quantum dynamics methods with a particular focus on computational efficiency. After a rapid prototyping stage of theoretical work, focus shifted to scientific software development as well as optimization for HPC environments. Work has been published in *The Journal of Chemical Theory and Computation* and won the 2016 RSC Coulson Prize. Development Experience: Python, FORTRAN

Durham University, Durham, United Kingdom

MChem (Integrated Master's with Hons equivalent to a BS and MS) in Chemistry, 2:1 *2009–2013*

Masters thesis: *Electron affinities and overlap dispersion in density functional theory.*

Supervised by Prof. David Tozer. Investigated links between spurious overlap dispersion and trends in electron affinities and ionization potentials within density functional theory.

Open Source Projects

PyMap

https://github.com/maxsaller/pymap

Software package for running quantum dynamics simulations intended for students and new researchers. Focus on accessibility for non-expert users and a low threshold for implementing new methods and systems. Scalable due to embarrassingly parallel nature and optimization through low-level routines in C/C++ (Cython).

Publications

- Cavity-Modified Fermi's Golden Rule Rate Constants from Cavity-Free Inputs, M.A.C. Saller, Y. Lai and E. Geva, *J. Phys. Chem. C*, **127** 3154-3164 (2023)
- Quasiclassical approaches to the generalized quantum master equation, G. Amati, M.A.C. Saller, A. Kelly and J.O. Richardson, *J. Chem. Phys.*, **23**, 234103 (2022)
- An Accurate Linearized Semiclassical Approach for Calculating Cavity-Modified Charge Transfer Rate Constants, M.A.C. Saller, Y. Lai and E. Geva, *J. Chem. Phys. Lett.*, **13**, 2330–2337 (2022)
- Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Cavity-Modified Molecular Dynamics, M.A.C. Saller, A. Kelly and E. Geva, *J. Chem. Phys. Lett.*, **12**, 3163-3170 (2021)
- Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Electronically Nonadiabatic Molecular Dynamics, X. Gao, M.A.C. Saller, Y. Liu, A. Kelly, J.O. Richardson and E. Geva, *J. Chem. Theo. Comput.*, **16**, 2883-2895 (2020)
- Path-integral approaches to nonadiabatic dynamics, Book Chapter in *Quantum Chemistry and Excited States: Methods and Applications*, M.A.C. Saller, J.E. Runeson and J.O. Richardson, Wiley, 629–653 (2020)
- Emerging opportunities and future directions: general discussion, *Faraday Discuss.*, **221**, 564–581 (2019)
- Quantum coherence in complex environments: general discussion, *Faraday Discuss.*, **221**, 168-201 (2019)
- Improved population operators for multi-state nonadiabatic dynamics with the mixed quantum-classical mapping approach, M.A.C. Saller, A. Kelly and J.O. Richardson, *Faraday Discuss.*, **221**, 150–167 (2019)
- On the identity of the identity operator in nonadiabatic linearized semiclassical dynamics, M.A.C. Saller, A. Kelly and J.O. Richardson, *J. Chem. Phys.*, **150**, 071101 (2019)
- Quantum Dynamics with Short-Time Trajectories and Minimal Adaptive Basis Sets, M.A.C. Saller and S. Habershon, *J. Chem. Theo. Comput.*, **13**, 3085–3096 (2017)
- Basis Set Generation for Quantum Dynamics Simulations Using Simple Trajectory-Based Methods, M.A.C. Saller and S. Habershon, *J. Chem. Theo. Comput.*, **11**, 8–16 (2015)

Awards and Grants

- **ETH Postdoctoral Fellowship 2018–2020** Competitive 24-month postdoctoral fellowship at ETH Zurich.
- **Warwick University Award for Teaching Excellence 2017** Postgraduate teaching commendation.
- **2016 Coulson Prize** Best graduate talk at the RSC Theoretical Chemistry Group Conference 2016.
- **2016 Contributed Talk Prize** RSC Spectroscopy and Dynamics Group Meeting 2016.
- **2016 Talk Prize** University of Warwick, Department of Chemistry Postgraduate Symposium 2016.

Conferences

- **52nd Midwest Theoretical Chemistry Conference**
  Ohio State University, Jun 2022. Contributed talk
- **Faraday Discussion: Quantum effects in complex systems**
  University of Warwick, Sep 2019. Presenting invited article and panel member for general discussion.
- **Recent developments in quantum dynamics, an E-CAM state-of-the-art workshop**
  Lyon, June 2019
- **C4 Computational Workshop**
  University of Zurich, June 2019. Invited talk
- **Computational Molecular Science**
  University of Warwick, March 2019
- **CECAM Workshop: Non-adiabatic quantum dynamics: From theory to experiment**
  University of Lausanne, July 2018

Teaching and Service

- **Lecture Courses**, *University of Michigan*
  Teaching undergraduate lecture courses, CHEM 262 - Mathematical Methods for Physical Scientists and CHEM 461 - Physical Chemistry I (Quantum Mechanics), on a substitute basis.
- **Mathematica Workshops**, *ETH Zurich*
  Developing and teaching an introductory undergraduate workshop for the Mathematica software and Wolfram language. Focus on numerical and analytical approaches to scientific problems.
- **Programming Skills for Chemists**, *ETH Zurich*
  Introduction to programming in C/C++, compilation and working in Linux. Focus on establishing programming as a tool first year students can use to solve problems over the course of their degree.
- **Physical Chemistry Tutorials**, *ETH Zurich*
  Leading problem classes with small groups of undergraduate students. Working through topics covered in lectures, contextualizing and deepening understanding. Providing support solving typical exam problems.
- **Masters Research Projects** *University of Warwick*
  Coordinating and supervising 6-month undergraduate research projects. Introduction to programming, working in high-performance computing environments and scientific writing (LaTeX).
- **Computational Chemistry Laboratory Projects**, *University of Warwick*
  Supervising and developing undergraduate computer laboratory projects. Crash course in Linux and terminal environments. Introduction to computational chemistry software culminating in a research project.
- **Spectroscopy in Schools**, *University of Warwick/Royal Society of Chemistry*
  Providing high school students with hands-on experience using portable, research-grade spectroscopy equipment. Providing advice on higher education, particularly in STEM fields.