Karsten Kreis

Computational & Statistical Physicist

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Education

10/2005–02/2011 **Studies of Physics**, *Friedrich-Alexander University Erlangen-Nürnberg*, Germany, Degree: Diploma of physics (Grade: 1.0 - "with distinction")
- Course specializations: Quantum Optics and Quantum Information Theory, Astronomy
- Diploma thesis: "Characterizing and Exploiting Hybrid Entanglement", performed at the Max Planck Institute for the Science of Light

10/2007–04/2008 **Semester Abroad**, *Imperial College London*, London, Great Britain
- Research project: Experimental test of a novel spatial light modulator (Grade: 93%)

Experience

since 06/2012 **Ph.D. Student**, *Max Planck Institute for Polymer Research*, Mainz, Germany
- Develop and apply new adaptive resolution methods for efficient computer simulations of molecular fluids

since 01/2013 **Software Developer**, *ESPResSo++*
- Implement parallel algorithms for efficient molecular dynamics simulations
  www.espresso-pp.de

01/2015–09/2015 **Visiting Research Scholar**, *New York University*, New York City, USA
- Performed research on novel adaptive quantum/classical simulation methodologies for molecular dynamics and Monte Carlo simulations of soft matter

02/2014–01/2015 **Freelancer & Student Assistant**, *Stratley AG & KPMG*, Cologne, Germany
- Carried out research work and performed analyses for a study on land use competition (Stratley AG was taken over by KPMG in summer 2014)

06/2012 **Visiting Researcher**, *Kavli Institute for Theoretical Physics*, Santa Barbara, USA
- Month-long participation in the program "Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter"

02/2012–04/2012 **Visiting Associate**, *Stratley AG*, Cologne, Germany
- Conducted a worldwide market study for a globally active, German chemical company

03/2009–01/2012 **Research and Teaching Assistant**, *Max Planck Institute for the Science of Light*, Erlangen & *Friedrich-Alexander University Erlangen-Nürnberg*, Germany
- Worked on publications of results of the diploma thesis
- Teaching assistant for experimental physics 2
- Performed experimental research on photonic networks

03/2011–05/2011 **Traveler**, backpacked through China, Thailand, Laos and Cambodia

Awards and Scholarships

10/2013 **Poster prize** for the best poster (1. place) at the "Meet-Your-Collegue-Day 2013" of the Max Planck Institute for Polymer Research

02/2013–08/2016 **PhD scholarship** of the Graduate School of Excellence Materials Science in Mainz

10/2011 **Ohm-Prize** of the Department for Physics of the Friedrich-Alexander University Erlangen-Nürnberg for an outstanding diploma thesis

10/2007–04/2008 **Erasmus grant** during the semester abroad in London

06/2005 **Book prize of the German Physical Society** for excellent achievements in the subject of physics in school

Advanced Training

11/2016 **Advanced C++ with Focus on Software Engineering**, four-day course of the High Performance Computing Center Stuttgart

07/2016–09/2016 **Machine Learning**, 11-week online course on Coursera taught by Andrew Ng of Stanford University

06/2015–09/2015 **Data Science**, *General Assembly*, New York, USA

- Three-month part-time course Data Science: Topics include data exploration and analysis, modeling and predicting, machine learning and statistics, visualization
- Final project: "Read Like You Tweet", a news article recommendation system for Twitter users, implemented at readlikeyoutweet.herokuapp.com

10/2014 **Basic techniques and tools for development and maintenance of atomic-scale software**, five-day CECAM workshop at the École polytechnique fédérale de Lausanne

06/2014 **Programming in C++ for C programmers**, six-day training course of the Forschungszentrum Jülich

05/2014 **Leadership and Management Skills**, two-day workshop of the Graduate School of Excellence Materials Science in Mainz

03/2014 **Parallelization with MPI and OpenMP**, three-day parallel programming workshop of the High Performance Computing Center Stuttgart

10/2013 **Cross-Cultural Communication and Leadership**, two-day workshop of the Graduate School of Excellence Materials Science in Mainz

06/2013 **Interpersonal Communication and Problem Resolution**, two-day workshop of the Graduate School of Excellence Materials Science in Mainz

01/2013 **MolSim-2013**, two-week school on molecular simulation techniques at the University of Amsterdam

10/2011 **Strategy School 2011**, two-day workshop of the Boston Consulting Group

IT Skills

Programming	Good knowledge of Python, C/C++ and Bash. Basic knowledge of MPI and OpenMP
Typesetting	Good knowledge of LaTeX
Operating Systems	Good knowledge of Linux/Unix and Windows
Microsoft Office	Good knowledge of Word, Powerpoint and Excel
Others	Basic knowledge of Gnuplot, Mathematica, GIMP and Inkscape

Language Skills

German Mother tongue

English Fluent in both spoken and written English

Publications

07/2016 **The relative entropy is fundamental to adaptive resolution simulations**, *K. Kreis* and *R. Potestio*, J. Chem. Phys. **145**, 044104 (2016)

07/2016 **Adaptive Resolution Simulations with Self-Adjusting High-Resolution Regions**, *K. Kreis, R. Potestio, K. Kremer,* and *A. C. Fogarty*, J. Chem. Theory Comput. **12**, 4067 (2016)

- *Featured on the journal cover,* Volume 12, Issue 10, October 2016

05/2016 **From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations**, *K. Kreis, M. E. Tuckerman, D. Donadio, K. Kremer,* and *R. Potestio*, J. Chem. Theory Comput. **12**, 3030 (2016)

09/2015 **Advantages and challenges in coupling an ideal gas to atomistic models in adaptive resolution simulations**, *K. Kreis, A. C. Fogarty, K. Kremer,* and *R. Potestio*, Eur. Phys. J. Special Topics **224**, 2289 (2015)

11/2014 **A unified framework for force-based and energy-based adaptive resolution simulations**, *K. Kreis, D. Donadio, K. Kremer,* and *R. Potestio*, EPL **108**, 30007 (2014)

03/2012 **Classifying, quantifying, and witnessing qudit-qumode hybrid entanglement**, *K. Kreis* and *P. van Loock*, Phys. Rev. A **85**, 032307 (2012)

Presentations

03/2016 **From classical to quantum and back: A Hamiltonian scheme for adaptive multiresolution classical/path integral simulations**, *K. Kreis, M. E. Tuckerman, D. Donadio, K. Kremer,* and *R. Potestio*, Spring Meeting of the German Physical Society, Regensburg, Germany

10/2015 **Quantum/Classical Adaptive Resolution Simulations**, *K. Kreis*, Student Seminar of the Graduate School of Excellence Materials Science in Mainz, Lisbon, Portugal

09/2015 **Adaptive Resolution: From Atomistic and Coarse-Grained Hybrid Simulations to Quantum-Classical Coupling**, *K. Kreis*, Invited Talk, D. E. Shaw Research, New York City, USA

08/2015 **Adaptive Resolution: From Atomistic and Coarse-Grained Hybrid Simulations to Quantum-Classical Coupling**, *K. Kreis*, Invited Talk, Pennsylvania State University, State College, USA

03/2015 **A Hamiltonian theory of adaptive resolution simulations of classical and quantum models of nuclei**, *K. Kreis, D. Donadio, K. Kremer,* and *R. Potestio*, APS March Meeting, San Antonio, USA

07/2014 **About Planets and Proteins - Computer Simulations in Materials Science**, *K. Kreis*, Student Seminar of the Graduate School of Excellence Materials Science in Mainz, Prague, Czech Republic

03/2011 **On Hybrid Entanglement**, *K. Kreis* and *P. van Loock*, Spring Meeting of the German Physical Society, Dresden, Germany

Posters

10/2014 **Quantum/Classical Adaptive Resolution Simulations**, *K. Kreis, D. Donadio, K. Kremer,* and *R. Potestio*, CECAM meeting: Multiscale simulation methods for soft matter systems, Mainz, Germany

10/2013 **Water in Adaptive Quantum/Classical Resolution**, *K. Kreis, S. Fritsch, R. Potestio, D. Donadio,* and *K. Kremer*, Retreat of the Graduate School of Excellence Materials Science in Mainz, Bad Dürkheim, Germany

10/2013 **Water in Adaptive Quantum/Classical Resolution**, *K. Kreis, S. Fritsch, R. Potestio, D. Donadio,* and *K. Kremer*, "Meet-Your-Collegue-Day 2013" of the Max Planck Institute for Polymer Research, Mainz, Germany

- Poster prize for the best poster (1. place)

08/2013 **Multiscale Simulations of Soft Matter with Adaptive Resolution Methods**, *K. Kreis, R. Potestio,* and *K. Kremer*, Student Seminar of the Graduate School of Excellence Materials Science in Mainz, Stockholm, Sweden

06/2013 **Adaptive resolution techniques for molecular simulation**, *K. Kreis, S. Fritsch, R. Potestio, D. Mukherji,* and *K. Kremer*, CECAM meeting: Mainz Materials Simulation Days 2013, Mainz, Germany

Teaching

10/2016 **Tutorial on Adaptive Resolution Simulations in ESPResSo++**, *CECAM school "Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA"*, Mainz, Germany

10/2015 **Tutorial on Adaptive Resolution Simulations in ESPResSo++**, *ESPResSo Summer School 2015*, Institute for Computational Physics, Stuttgart, Germany

10/2014 **Teaching Assistant for ESPResSo++**, *School on Multiscale Modeling and Use of Espresso++ and VOTCA*, Mainz, Germany

10/2013 **Tutorial on Adaptive Resolution Simulations in ESPResSo++**, *ESPResSo Summer School 2013*, Institute for Computational Physics, Stuttgart, Germany

10/2013–02/2014 **Teaching Assistant in Physics Lab for medical students**, Johannes Gutenberg University of Mainz, Germany

04/2013–07/2013 **Teaching Assistant in Physics Lab for medical students**, Johannes Gutenberg University of Mainz, Germany

10/2012–02/2013 **Teaching Assistant for Analytical Mechanics**, Johannes Gutenberg University of Mainz, Germany

04/2010–07/2010 **Teaching Assistant for Experimental Physics 2**, Friedrich-Alexander University Erlangen-Nürnberg, Germany