Christoph Junghans

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Research Interests

- **Currently:** Computational Co-Design
- Extending the time-scale of bio-simulations using accelerated molecular dynamics
- Performance optimization for codesign of molecular dynamics codes using discrete event simulations
- Porting and optimization of scientific codes (VOTCA, ESPReSo, GroMaCS)
- Software design and management – core developer of the coarse-graining package VOTCA
- Systematic coarse-graining of liquids and implementation of new methodologies (e.g. thermostats)
- Development of adaptive resolution simulation approaches (changing the degrees of freedom on the fly)
- Generalized ensemble methods to study phase transitions (multicanonical techniques)

Education

Oct 2010	**Dr. rer. nat. (Ph.D.) in Physics**, Johannes Gutenberg University of Mainz, Germany *Between the Scales: Water from different Perspectives* An adaptive resolution molecular dynamics study using various coarse-graining methods
Nov 2006	**Diploma (M.Sc.) in Physics**, University of Leipzig, Germany *Aggregation of Mesoscopic Protein-like Heteropolymers* A generalized ensemble Monte Carlo study using multicanonical techniques

Work Experience

May 2014 – Present	**Staff Scientist**, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
Mar 2013 – Apr 2014	**Director's Postdoctoral Fellow**, Theoretical Division, Los Alamos National Lab
Nov 2011 – Feb 2013	**Postdoctoral research assistant**, Theoretical Division, Los Alamos National Lab
May 2012 – June 2012	**Member**, The Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA
Nov 2010 – Oct 2011	**Postdoctoral research assistant**, Polymer Theory Group, Max Planck Institute for Polymer Research, Mainz, Germany
Jan 2007 – Oct 2010	**Ph.D. Student**, Polymer Theory Group, Max Planck Institute for Polymer Research, Mainz, Germany
Jan 2009 – July 2009	**Specialist for Application Performance & Deep Computing**, Internship, IBM Systems & Technology Group Europe
Oct 2003 – Sept 2006	**Student assistant**, Institute for Theoretical Physics, University of Leipzig
Aug 2005 – Oct 2005	**Research student** in the "Scientific Computing" program, Jülich Supercomputing Centre, Germany
Sep 2004	**Student assistant**, Institute for Meteorology, University of Leipzig
Feb 2003 – April 2003	**Research student**, Chair for Fluid Mechanics, Martin Luther University of Halle-Wittenberg, Germany

Open Source Projects

VOTCA	Versatile Toolkit for coarse-graining applications	Core Developer
Gentoo	An advanced linux distribution	Developer
ESPReSo++	Successor of the ESPResSo simulation package	Developer
GroMaCS	Versatile package to perform molecular dynamics	Developer (inactive)
ESPReSo	Extensible Simulation Package for Research on Soft matter	Developer (inactive)

More information can be found on my GitHub profile and my OpenHUB profile.

Awards

Jan 2015	Classified as outstanding researcher, USCIS
Jan 2014	The most cited article published in EPJE in the past 5 years
Mar 2013	Los Alamos National Laboratory Director's Post-Doctoral Fellowship
May 2012	Member of the Kavli Institute for Theoretical Physics
June 2010	Participant of the 60th Lindau Nobel Laureate Meeting
Nov 2006	Diploma with honor (highest possible grade)
Nov 2005	Wolfgang Natonek award, University of Leipzig
Oct 2003	Teubner award, Department for Physics and Earth Science, University of Leipzig
July 2000	Book award of the German Physical Society (DPG) for school graduates

Professional Skills

Referee for Scientific Journals

- ACS: J. Chem. Inf. Model. & J. Phys. Chem.
- AIP: J. Chem. Phys.
- Elsevier: Comp. Phys. Comm.
- RSC: Phys. Chem. Chem. Phys.
- and others

Code Review

- Gromacs
- OpenSuse Build Service
- Gentoo Science Project

Conferences

- Member of the Organization Committee for the Salishan Conference on High Speed Computing
- Chairman for APS annual meetings

Publications

h-index: 15 (Google Scholar), 12 (ResearcherID)

- 25 reviewed papers
- 3 book chapters
- 7 proceedings and other publications
- over 50 invited and contributed talks