Christoph Junghans

Staff Scientist
Applied Computer Science Group
Computer, Computational, & Statistical Sciences Division
Los Alamos National Laboratory, NM, USA

Phone: ++1-505-695-2142
Email: junghans@lanl.gov
Web: www.lanl.gov/junghans

Research Interests

- **Currently:** Computational Co-Design
- Software design and management – core developer of the coarse-graining package VOTCA
- Porting and optimization of scientific codes (VOTCA, ESPReSo, GroMaCS)
- Performance optimization for Co-Design of molecular dynamics codes using discrete event simulations
- 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
Jan 2017 - Present	**Deputy Team Leader**, Co-Design Team, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
Feb 2016 - Present	**CNLS Affiliate**, The Center for Nonlinear Studies, Theoretical 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	Advanced Linux distribution	Developer
Fedora	Linux distribution	Contributor
OpenSuse	Linux distribution	Contributor
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	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 high 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

Representative

July 2015 - June 2016	Member of the Worker Safety & Security Team (WSST) for CCS-7
July 2007 - Dec 2008	PhD representative of the theory group, Max Planck Institute for Polymer Research, Mainz
Nov 2007 - Nov 2008	PhD representative of the MPI for Polymer Research
Oct 2002 - Sep 2005	Elected member of student government (Fachschaftsrates) of the Department for Physics and Earth Science, University of Leipzig - Extensive committee work in this period incl. spokesperson, treasurer and member of several faculty/university committees

Computer Skills

General	Linux, AIX, Mac OS, DOS, Windows
Programming	C, Fortran, MPI, OpenMP, C++
Scripting	Shell, awk, Perl, expect, PHP, tcl, Python
Markup Languages	HTML, latex, mediawiki, txt2tags

Teaching Experience

Teaching Assistant

Apr 2008 - Sep 2008	Theoretical physics III, Johannes Gutenberg University of Mainz
Oct 2007 - Mar 2008	Theoretical physics II, Johannes Gutenberg University of Mainz
Apr 2007 - Sep 2007	Theoretical physics I, Johannes Gutenberg University of Mainz
Apr 2006 - Sep 2006	Introduction to computer simulations I, University of Leipzig
Sep 2004 - Oct 2004	Mathematical preparation course for first-year students, University of Leipzig

Mentoring

Dec 2016 - Present	Postdoctoral research assistant, Los Alamos, National Laboratory
Aug 2016 - Present	Postdoctoral research assistant, Los Alamos, National Laboratory
Feb 2016 - Present	Postdoctoral research assistant, Los Alamos, National Laboratory
May 2015 - Present	Metropolis Postdoc Fellow, Los Alamos, National Laboratory
Jul 2016 - Sep 2016	CNLS Summer Student, Los Alamos, National Laboratory
Jun 2016 - Aug 2016	Co-Design Summer School (7 Students), Los Alamos, National Laboratory
Jul 2015 - Sep 2015	IC Summer Student, Los Alamos, National Laboratory
Jun 2015 - Aug 2015	Co-Design Summer School (6 Students), Los Alamos, National Laboratory
Jul 2014 - Sep 2014	CNLS Summer Student, Los Alamos, National Laboratory
Jun 2014 - Aug 2014	Co-Design Summer School (6 Students), Los Alamos, National Laboratory
Jul 2013 - Aug 2013	Co-Design Summer School (6 Students), Los Alamos, National Laboratory
Jun 2010 - Aug 2010	Summer Student, University of Mainz
Oct 2005 - Mar 2006	Simulation methods in generalized ensembles (2 Students), University of Leipzig

Tutorials (invited)

Oct. 2016	"Coarse-Graining with VOTCA" (Tutorial), CECAM Workshop "Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA", Mainz, Germany
May 2016	Gitlab Hands-On course, ASC/NGC Program, LANL
Oct. 2015	"Coarse-Graining with VOTCA" (Tutorial), CECAM Summer School "Simulating Soft and Active Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
Sep. 2015	Git Hands-On course, ASC/NGC Program, LANL
Nov. 2014	Git IC Tutorial, Institutional Computing, LANL
Oct. 2014	Hands-on: VOTCA, CECAM "School on Multiscale Modeling and Use of Espresso++ and VOTCA", Mainz, Germany
Aug. 2014	Gromacs Tutorial, The Eighth q-bio Summer School, Albuquerque, NM (LA-UR 14-26188)
June 2014	Gromacs IC Tutorial, Institutional Computing, LANL (LA-UR 14-24814)
Oct. 2013	"Systematic Coarse-Graining with VOTCA" (Tutorial), CECAM Summer School "Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
July 2013	Gromacs Tutorial, The Seventh q-bio Summer School, Santa Fe, NM
Oct. 2012	"Systematic Coarse-Graining with VOTCA" (Tutorial), CECAM Workshop "Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
July 2012	Gromacs Tutorial, The Sixth q-bio Summer School, Santa Fe, NM
Oct. 2011	Hands-on: VOTCA, CECAM Workshop "Coarse-grained Simulation of Biological Soft Matter Systems using ESPResSo", ICP Stuttgart
May 2010	Votca Workshop, CSI Darmstadt

Talks

Colloquium Talks

July 2011	"Locality Analysis via Adaptive Resolution Simulations", Theoriekolloquium, Faculty of Natural Sciences II, Martin Luther University Halle-Wittenberg

Invited Talks

Oct. 2016	"Recent developments in VOTCA", CECAM Workshop "Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA", Mainz, Germany
Oct. 2015	"Recent and Future Developments of VOTCA", CECAM Summer School "Simulating Soft and Active Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
Oct. 2014	"Introduction to coarse-graining of liquids and soft matter using VOTCA", CECAM "School on Multiscale Modeling and Use of Espresso++ and VOTCA", Mainz, Germany
Oct. 2013	"Recent and Future Developments of VOTCA", CECAM Summer School "Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
Oct. 2012	"Multi-scale modeling using AdResS", CECAM Workshop "Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA", ICP Stuttgart
June 2012	"Molecular Dynamics using Gromacs", Intel EPOCH, Workshop, Portland, OR
June 2012	"Towards a Unified Framework for Coarse-graining Particle-based Simulations", KITP Conference: "Modeling Soft Matter: Linking Multiple Length and Time Scales", UCSB
Oct. 2011	"Multi-scale modeling using AdResS", CECAM Workshop "Coarse-grained Simulation of Biological Soft Matter Systems using ESPResSo", ICP Stuttgart
Oct. 2010	"Multi-scale modeling using AdResS", CECAM Workshop "Simulating Soft Matter with ESPResSo", ICP Stuttgart
Nov. 2007	"Controlling material properties using a thermostat", CompPhys07, ITP Leipzig

Seminar Talks (invited)

Oct. 2016	"Co-Design at Los Alamos National Laboratory", MPCDF
June 2016	ASC/NGC Gitlab Tutorial, Parallel Computing Summer Research Internship Program, LANL
Sep. 2012	"Adaptive Resolution Simulations of C60 in Toluene", Biomolecular Modeling Group, UMD
Aug. 2012	"Multi-scale Modeling using the Adaptive Resolution Scheme", Sandia National Laboratory, Albuquerque, NM
May 2012	"Particle-based multi-scale simulations using the Adaptive Resolution Scheme", IBM Research, Almaden
May 2012	"Coarse-graining Using the VOTCA Package", KITP Program: "Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter", UCSB
July 2011	"Locality Analysis via Adaptive Resolution Simulations", DFH-UFA & TKM Seminar, Institut für Theoretische Physik, University of Leipzig
June 2011	"Versatile object-oriented toolkit for coarse-graining applications", Department of Materials and Environmental Chemistry, Stockholm University
Apr. 2011	"Adaptive resolution simulations of aqueous solutions", Séminaire de Physique, Biophysique et Physique Statistique, UPV Metz
Mar. 2011	"Adaptive resolution simulations of water", Theoretical and Computational Biophysics Group, UIUC
Mar. 2011	"Adaptive resolution simulations of aqueous solutions", Laufer Center for Physical and Quantitative Biology, Stony Brook University
Jan. 2011	"Versatile object-oriented toolkit for coarse-graining applications", Theoretical and Computational Biophysics Department, MPI-BPC
Nov. 2009	"Versatile object-oriented toolkit for coarse-graining applications", Computational Biology Cluster Seminar, IFF-2, FZ Jülich
July 2009	"New HPC libraries for performance improvements", HPC Seminar, IBM Systems & Technology Group
June 2007	"Extensions to Dissipative Particle Dynamics", Faculty of Science, Lund University

Contributed Talks

Feb. 2016	"Tabasco: A realistic multi-scale proxy app for Material science" (with S. Mniszewski), Programming Models and Co-Design Meeting, Los Alamos, NM
Feb. 2016	"Actually Using Runtimes for Meaningful Computation: Multiphysics, not Fibonacci" (with R. Pavel), Programming Models and Co-Design Meeting, Los Alamos, NM
Aug. 2015	"Coarse-graining using VOTCA and LAMMPS", August 2015 LAMMPS Users' Workshop and Symposium, Albuquerque, NM
May 2015	"Parallel Runtime Environments with Cloud Database: Performance Study for HMM with Adaptive Sampling", 13th Annual Workshop on Charm++ and its Applications, Champaign-Urbana
Mar. 2014	"Discrete Event-based Performance Prediction for Temperature Accelerated Dynamics", APS March Meeting 2014, Denver
Sep. 2013	"Adaptive Resolution Simulations of C60 in Toluene", Gromacs USA Workshop and Conference, UVA
Aug. 2013	"Introduction to coarse-graining of liquids and soft matter", August 2013 LAMMPS Users' Workshop and Symposium, Albuquerque, NM
Mar. 2013	"Recent developments in the VOTCA package for coarse-graining", APS March Meeting 2013, Baltimore

Sep. 2012	"Multi-scale simulations of fullerenes in aqueous solution employing the Adaptive Resolution Scheme", IWCMM XXII
Mar. 2012	"Structure formation of toluene around C60: Application of the Adaptive Resolution Scheme", APS March Meeting 2012, Boston
Feb. 2012	"Local structure formation of toluene around a C60 fullerene: An adaptive resolution study", 25th Annual CSP Workshop, Center for Simulational Physics, University of Georgia
Nov. 2009	"Versatile object-oriented toolkit for coarse-graining applications", CompPhys09, ITP Leipzig
Nov. 2008	"Comparative atomistic and coarse-grained study of water: simulation details vs. simulation feasibility", CompPhys08, ITP Leipzig
June 2008	"Adjusting dynamic material properties by a thermostat", ICMMES 2008, University of Amsterdam
Feb. 2008	"Controlling material properties using a thermostat", DPG Spring Meeting 2008 Berlin

Publications

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

Reviewed Papers

25. T. E. de Oliveira, P. A. Netz, K. Kremer, **C. Junghans**, and D. Mukherji, *C-IBI: Targeting cumulative coordination within an iterative protocol to derive coarse-grained models of (multi-component) complex fluids*, J. Chem. Phys. **144**, 174106 (2016).

24. R. S. Pavel, A. L. McPherson, T. C. Germann, and **C. Junghans**, *Database Assisted Distribution to Improve Fault Tolerance for Multiphysics Applications*, in: *Proceedings of the 2nd International Workshop on Hardware-Software Co-Design for High Performance Computing 2015* (Co-HPC '15), ACM, New York, NY, USA, Article 4.

23. S. Y. Mashayak, M. N. Jochum, K. Koschke, N. R. Aluru, V. Rühle, and **C. Junghans**, *Relative entropy and optimization-driven coarse-graining methods in VOTCA*, PLoS one **10**, e131754 (2015).

22. S. M. Mniszewski, **C. Junghans**, A. F. Voter, D. Perez, and S. J. Eidenbenz, *TADSim: Discrete Event-based Performance Prediction for Temperature Accelerated Dynamics*, Trans. Mod. Comp. Sim. **25**, 15 (2015).

21. D. G. Roehm, R. S. Pavel, K. Barros, B. Rouet-Leduc, A. L. McPherson, T. C. Germann, and **C. Junghans**, *Distributed Database Kriging for Adaptive Sampling*, Comp. Phys. Comm. **192**, 138 (2015).

22. S. Bevc, **C. Junghans**, and M. Praprotnik, *STOCK: Structure Mapper and Online Coarse-Graining Kit for Molecular Simulations*, J. Comp. Chem. **36**, 467 (2015).

19. **C. Junghans**, D. Perez and T. Vogel, *Molecular Dynamics in the Multicanonical Ensemble: Equivalence of Wang-Landau Sampling, Statistical Temperature Molecular Dynamics, and Metadynamics*, J. Chem. Theo. Comp. **10**, 1843 (2014).

18. B. Rouet-Leduc, K. Barros, E. Cieren, V. Elango, **C. Junghans**, T. Lookman, J. Mohd-Yusof, R. S. Pavel, A. Y. Rivera, D. Roehm, A. L. McPherson, T. C. Germann, *Spatial adaptive sampling in multiscale simulation*, Comp. Phys. Comm. **185**, 1857 (2014).

17. A. Nagarajan, **C. Junghans** and S. Matysiak, *Multiscale simulation of liquid water using a four-to-one mapping for coarse-graining*, J. Chem. Theo. Comp. **9**, 5168 (2013).

16. S. Bevc, **C. Junghans**, K. Kremer and M. Praprotnik, *Adaptive resolution simulation of salt solutions*, New J. Phys., **15**, 105007 (2013).

15. P. Ganguly, D. Mukherji, **C. Junghans** and N. F. A. van der Vegt, *Kirkwood-Buff coarse-grained force fields for aqueous solutions*, J. Chem. Theo. Comp., **8**, 1802 (2012).

14. S. Fritsch, S. Poblete, **C. Junghans**, G. Ciccotti, L. Delle Site and K. Kremer, *Adaptive resolution molecular dynamics simulation through coupling to an internal particle reservoir*, Phys. Rev. Lett. **108**, 170602 (2012).

13. S. Fritsch, **C. Junghans** and K. Kremer, *Structure formation of toluene around C60: Implementation of the Adaptive Resolution Scheme (AdResS) into GROMACS*, J. Chem. Theo. Comp. **8**, 398 (2012).

12. V. Rühle and **C. Junghans**, *Hybrid approaches to coarse-graining using the VOTCA package: liquid hexane*, Macromol. Theory Simul., **20**, 472 (2011).

11. **C. Junghans**, W. Janke and M. Bachmann, *Hierarchies in Nucleation Transitions*, Comp. Phys. Comm., **182**, 1937 (2011).

10. B. P. Lambeth, Jr., **C. Junghans**, K. Kremer, C. Clementi, and L. Delle Site, *Communication: On the Locality of Hydrogen Bond Networks at Hydrophobic Interface*, J. Chem. Phys. **133**, 221101 (2010).

9. **C. Junghans** and S. Poblete, *A reference implementation of the adaptive resolution scheme in ESPResSo*, Comp. Phys. Comm. **181**, 1449 (2010).

8. V. Rühle, **C. Junghans**, A. Lukyanov, K. Kremer and D. Andrienko, *Versatile Object-oriented Toolkit for Coarse-graining Applications*, J. Chem. Theo. Comp. **5**, 3211 (2009).

7. **C. Junghans**, M. Bachmann and W. Janke, *Statistical Mechanics of Aggregation and Crystallization for Semiflexible Polymers*, Europhys. Lett. **87**, 40002 (2009).

6. H. Wang, **C. Junghans** and K. Kremer, *Comparative atomistic and coarse-grained study of water: What do we lose by coarse-graining?*, Euro. Phys. J. E **28**, 221 (2009). "*Most cited article published in the journal in the past 5 years*" (2014)

5. M. Praprotnik, **C. Junghans**, L. Delle Site and K. Kremer, *Simulation approaches to soft matter: Generic statistical properties vs. chemical details*, Comp. Phys. Comm. **179**, 51 (2008).

4. **C. Junghans**, M. Bachmann and W. Janke, *Thermodynamics of Peptide Aggregation Processes: An Analysis from Perspectives of Three Statistical Ensembles*, J. Chem. Phys. **128**, 085103 (2008) .

3. **C. Junghans**, M. Praprotnik and K. Kremer, *Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat*, Soft Matter **4**, 156 (2008).

2. **C. Junghans**, M. Bachmann and W. Janke, *Microcanonical Analyses of Peptide Aggregation Processes*, Phys. Rev. Lett. **97**, 218103 (2006).

1. **C. Junghans** and U. H. E. Hansmann, *Numerical Comparison of Wang Landau Sampling and Parallel Tempering for Met-enkephalin*, Int. J. Mod. Phys. C **17**, 817 (2006).

More information can be found on my ResearcherID profile, my Google Scholar profile, my ORCID profile, my ResearchGate profile or my Impactstory profile.

Book Chapters

3. L. Delle Site, A. Agarwal, **C. Junghans**, and H. Wang, *Adaptive Resolution Simulation as a Grand Canonical Molecular Dynamics Scheme: Principles, Applications, Perspectives*, in: C. Clementi (Ed.), *Multiscale Methods in Molecular Biophysics*, Series in Computational Biophysics, CRC Press (2016), ISBN 1482225700.

2. E. Apol, R. Apostolov, H.J.C. Berendsen, A. van Buuren, P. Bjelkmar, R. van Drunen, A. Feenstra, S. Fritsch, G. Groenhof, **C. Junghans**, P. Kasson, P. Larsson, P. Meulenhoff, T. Murtola, S. Pall, S. Pronk, R. Schulz, M. Shirts, A. Sijbers, P. Tieleman, B. Hess, D. van der Spoel, and E. Lindahl, *Gromacs User Manual Version 4.6*, gromacs.org (2013).

1. **C. Junghans**, M. Praprotnik and L. Delle Site, *Adaptive Resolution Schemes*, in: J. Grotendorst, N. Attig, S. Blügel and D. Marx (Eds.), *Multiscale Simulation Methods in Molecular Sciences*, NIC Series Vol. 42, Jülich (2009), 359.

Other Publications

5. **C. Junghans**, A. K. Hüttel and U. Müller, *Gentoo Linux: Quelltexte und Rolling Releases*, c't Magazin **16**, 162 (2012).

4. S. Eidenbenz, K. Davis, A. Voter, H. Djidjev, L. Gurvits, **C. Junghans**, S. Mniszewski, D. Perez, N. Santhi and S. Thulasidasan, *Optimization Principles for Codesign applied to Molecular Dynamics: Design Space Exploration, Performance Prediction, and Optimization Strategies*, in: Proceedings of the DOE ASCR Exascale Research Conference, Portland, OR (2012), (LA-UR 12-20070).

3. T. Weidauer, **C. Junghans**, O. Pauluis, M. Pütz and J. Schumacher, *Shallow Moist Convection*, in: G. Münster, D. Wolf, M. Kremer (Eds.), NIC Symposium 2010, IAS Series Vol. 3, Jülich (2010), 373.

2. **C. Junghans**, M. Bachmann and W. Janke, *Phase Separation in Peptide Aggregation Processes - Multicanonical Study of a Mesoscopic Model*, in: U. H. E. Hansmann, J. Meinke, S. Mohanty and O. Zimmermann (Eds.), *From Computational Biophysics to Systems Biology 2007*, NIC Series Vol. 36, Jülich (2007), 169.

1. **C. Junghans** and U. H. E. Hansmann, *Cross-Check Methods in Protein Simulations*, in: U. H. E. Hansmann, J. Meinke, S. Mohanty and O. Zimmermann (Eds.), *From Computational Biophysics to Systems Biology 2006*, NIC Series Vol. 34, Jülich (2006), 157.