Christoph Junghans

Group Leader
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:** Applied computer science
- Software design and management – core developer of the coarse-graining package VOTCA
- Porting and optimization of scientific codes (VOTCA, Cabana, FleCSI)
- Novel software development workflow for Exascale computing
- 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**, *magna cum laude*,
Johannes Gutenberg University, 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**, *summa cum laude*, University of Leipzig, Germany
Aggregation of Mesoscopic Protein-like Heteropolymers
A generalized ensemble Monte Carlo study using multicanonical techniques

Work Experience

Feb 2021 - Present	**Group Leader**, Applied Computer Science Group, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
Feb 2016 - Present	**CNLS Affiliate**, Center for Nonlinear Studies, Theoretical Division, Los Alamos National Lab
July 2018 - Feb 2021	**Deputy Group Leader**, Applied Computer Science Group, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
Jan 2017 - July 2018	**Deputy Team Leader**, Co-Design Team, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
May 2014 - July 2018	**Staff Scientist**, Computer, Computational, and Statistical Sciences Division, Los Alamos National Lab
Mar 2013 – Apr 2014	**Director's Postdoc. Fellow**, Theoretical Division, Los Alamos National Lab
Nov 2011 – Feb 2013	**Postdoc. 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	**Postdoc. 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
Cabana	Performance-portable library for particle-based simulations	Core Developer
FleCSI	Flexible Computer Science Infrastructure	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

Nov 2019	Top 10% most cited PLOS ONE papers published in 2015
Sep 2017	LAAP Award in recognition of outstanding contributions to the ISTI Summer School Program
Feb 2017	Postdoc. Distinguished Mentor Award, LANL
July 2016	LAAP Achievement Award in appreciation for active service on the WSST team
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

Managerial

- Line management, since July 2018, Group of 65+ staff scientists and Postdocs, $50M+ budget
- Team management, 2 years, technical management of 12+ team member
- Project management, multiple lead roles in Exascale Computing Project (ECP), Laboratory Directed Research & Development (LDRD) and Advanced Simulation & Computing (ASC) projects

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

Conferences

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

Representative

Nov 2018 - Sep 2022	Member of the Information Science and Technology Institute (ISTI) council, LANL
July 2015 - June 2016	Member of the Worker Safety & Security Team (WSST) for CCS-7, LANL
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 (Fachschaftsrat) 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

Aug 2021	"VOTCA and LAMMPS for electronic spectroscopy and transport" (Tutorial), LAMMPS Workshop and Symposium, Virtual
Aug 2019	"VOTCA and LAMMPS for electronic spectroscopy and transport" (Tutorial), LAMMPS Workshop and Symposium, Albuquerque, NM
May 2018 - Aug 2018	Co-Design Summer School (6 Students), Los Alamos National Laboratory
May 2017 - Jul 2017	Co-Design Summer School (6 Students), Los Alamos National Laboratory
Oct 2016	"Coarse-Graining with VOTCA" (Tutorial), CECAM Workshop "Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA", Mainz, Germany
Jun 2016 - Aug 2016	Co-Design Summer School (7 Students), Los Alamos National Laboratory
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
Jun 2015 - Aug 2015	Co-Design Summer School (6 Students), Los Alamos National Laboratory
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
Jun 2014 - Aug. 2014	Co-Design Summer School (6 Students), Los Alamos National Laboratory
Aug 2014	Gromacs Tutorial, The Eighth q-bio Summer School, Albuquerque, NM (LA-UR 14-26188)

Jun 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
Jul 2013 - Aug 2013	Co-Design Summer School (6 Students), Los Alamos National Laboratory
Jul 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
Jul 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
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

Feb 2022 - present	Postdoc. Research Assistant, Los Alamos National Laboratory
Jun 2019 - Mar 2021	Postdoc. Research Assistant, Los Alamos National Laboratory
Feb 2018 - Apr 2020	Postdoc. Research Assistant (now Staff Scientist), Los Alamos National Laboratory
May 2018 - Feb 2019	Postdoc. Research Assistant (now Staff Scientist), Los Alamos National Laboratory
Feb 2017 - Jan 2019	Postdoc. Research Assistant (now Staff Scientist), Los Alamos National Laboratory
Sep 2018	Member of PhD committee, University of Reims Champagne-Ardenne
Jun 2018 - Aug 2018	ECP Summer Student, Los Alamos National Laboratory
May 2018 - Aug 2018	Co-Design Summer School (6 Students), Los Alamos National Laboratory
May 2018 - Aug 2018	ASC Summer Student, Los Alamos National Laboratory
Feb 2016 - May 2018	Postdoc. Research Assistant (now Staff Scientist), Los Alamos National Laboratory
Dec 2016 - Apr 2018	Postdoc. Research Assistant (now Staff Scientist), Los Alamos National Laboratory
Jun 2017 - Aug 2017	High School Internship Student, Los Alamos National Laboratory
Apr 2017 - Jun 2017	ASC Summer Student, Los Alamos National Laboratory
May 2017 - Jul 2017	Data-Science at Scale Summer Student, Los Alamos National Laboratory
May 2017 - Jul 2017	Co-Design Summer School (6 Students), Los Alamos National Laboratory
May 2015 - May 2017	Metropolis Postdoc. Fellow (now Staff Scientist), Los Alamos National Laboratory
Aug 2016 - Apr 2017	Postdoc. Research Assistant (now Staff Scientist), 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

Talks

Over 50 invited and contributed talks

Selected Talks

Sep. 2018	Lecture: "Co-Design at Los Alamos National Laboratory", University of Reims Champagne-Ardenne
Oct. 2016	Talk: "Recent developments in VOTCA", CECAM Workshop "Multiscale Simulations of Soft Matter with Hands-On Tutorials on ESPResSo++ and VOTCA", Mainz, Germany
May 2012	Seminar: "Particle-based multi-scale simulations using the Adaptive Resolution Scheme", IBM Research, Almaden
July 2011	Colloquium: "Locality Analysis via Adaptive Resolution Simulations", Theoriekolloquium, Faculty of Natural Sciences II, Martin Luther University Halle-Wittenberg

Publications

h-index: 23 (Google Scholar), 19 (ResearcherID)

Reviewed Papers

44. S. Karra, M. Mehana, N. Lubbers, Y. Chen, A. Diaw, J. E. Santos, A. Pachalieva, R. S. Pavel, J. R. Haack, M. McKerns, **C. Junghans**, Q. Kang, D. Livescu, T. C. Germann, and H. S. Viswanathan, *Predictive Scale-Bridging Simulations through Active Learning*, Sci. Rep. **13**, 16262 (2023).

43. S. Wijesinghe, **C. Junghans**, D. Perahia, and G. S. Grest, *Polydots, soft nanoparticles, at membrane interfaces*, RSC Adv. **13**, 19227 (2023).

42. R. Halver, **C. Junghans**, and G. Sutmann, *Using heterogeneous GPU nodes with a Cabana-based implementation of MPCD*, Paral. Comp. **117**, 103033 (2023).

41. J. Vance, Z.-H. Xu, N. Tretyakov, T. Stuehn, M. Rampp, S. Eibl, **C. Junghans**, and A. Brinkmann, *Code modernization strategies for short-range non-bonded molecular dynamics simulations*, Comp. Phys. Comm. **290**, 108760 (2023).

40. R. Halver, **C. Junghans**, and G. Sutmann, *Kokkos-Based Implementation of MPCD on Heterogeneous Nodes*, in: R. Wyrzykowski, J. Dongarra, E. Deelman, and K. Karczewski (Eds.), Parallel Processing and Applied Mathematics. PPAM 2022. Lecture Notes in Computer Science, Vol. 13827 (2023).

39. A. Pachalieva, R. S. Pavel, J. E. Santos, A. Diaw, N. Lubbers, M. Mehana, J. R. Haack, H. S. Viswanathan, D. Livescu, T. C. Germann, and **C. Junghans**, *GLUE Code: A framework handling communication and interfaces between scales*, J. Open Source Softw. **7**, 4822 (2022).

38. P. Grete, J. C. Dolence, J. M. Miller, J. Brown, B. Ryan, A. Gaspar, F. Glines, S. Swaminarayan, J. Lippuner, C. J. Solomon, G. Shipman, **C. Junghans**, D. Holladay, and J. M. Stone, *Parthenon - a performance portable block-structured adaptive mesh refinement framework*, Int. J. High Perf. Comp. App. **37**, 465 (2023).

37. S. Slattery, S. T. Reeve, **C. Junghans**, D. Lebrun-Grandie, R. Bird, G. Chen, S. Fogerty, Y. Qiu, S. Schulz, A. Scheinberg, A. Isner, K. Chong, S. Moore, T. Germann, J. Belak, and S. Mniszewski, *Cabana: A Performance Portable Library for Particle-Based Simulations*, J. Open Source Softw. **7**, 4115 (2022).

36. J. Bakosi, R. Bird, F. Gonzalez, **C. Junghans**, W. Li, H. Luo, A. Pandare, and J. Waltz, *Asynchronous distributed-memory task-parallel algorithm for compressible flows on unstructured 3D Eulerian grids*, Adv. Eng. Softw. **160**, 102962 (2021).

35. S. M. Mniszewski, J. Belak, J.-L. Fattebert, C. F. A. Negre, S. R. Slattery, A. A. Adedoyin, R. F. Bird, C.S. Chang, G. Chen, S. Ethier, S. Fogerty, S. Habib, **C. Junghans**, D. Lebrun-Grandie, J. Mohd-Yusof, S. G. Moore, D. Osei-Kuffuor, S. J. Plimpton, A. Pope, S. T. Reeve, L. Ricketson, A. Scheinberg, A. Y. Sharma, and M. E. Wall, *Enabling Particle Applications for Exascale Computing Platforms*, Int. J. High Perf. Comp. App. **35**, 572 (2021).

34. A. Diaw, K. Barros, J. Haack, **C. Junghans**, B. Keenan, Y. W. Li, D. Livescu, N. Lubbers, M. McKerns, R. S. Pavel, D. Rosenberger, I. Sagert, and T. C. Germann, *Multiscale simulation of plasma flows using active learning*, Phys. Rev. E **102**, 023310 (2020).

33. N. Lubbers, A. Agarwal, Y. Chen, S. Son, M. Mehana, Q. Kang, S. Karra, **C. Junghans**, T. C. Germann, and H. S. Viswanathan, *Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media*, Sci. Rep. **10**, 13312 (2020).

32. G. Tirimbo, V. Sundaram, O. Caylak, W. Scharpach, J. Sijen, **C. Junghans**, J. Brown, F. Zapata Ruiz, N. Renaud, J. Wehner, and B. Baumeier, *Excited-State Electronic Structure of Molecules Using Many-Body Green's Functions: Quasiparticles and Electron-Hole Excitations with VOTCA-XTP*, J. Chem. Phys. **152**, 114103 (2020).

31. H. V. Guzman, N. Tretyakov, H. Kobayashi, A. C. Fogarty, K. Kreis, J. Krajniak, **C. Junghans**, K. Kremer, and T. Stuehn, *ESPResSo++ 2.0: Advanced methods for multiscale molecular simulation*, Comp. Phys. Comm. **238**, 66 (2019).

30. J. Wehner, L. Brombacher, J. Brown, **C. Junghans**, O. Caylak, Y. Khalak, P. Madhikar, G. Tirimbo, and B. Baumeier, *Electronic Excitations in Complex Molecular Environments: Many-Body Green's Functions Theory in VOTCA-XTP*, J. Chem. Theo. Comp. **14**, 6253 (2018).

29. C. Krekeler, A. Agarwal, **C. Junghans**, M. Praprotnik, and L. Delle Site, *Adaptive Resolution Molecular Dynamics Technique: Down to the Essential*, J. Chem. Phys. **149**, 024104 (2018).

28. H. V. Guzman, **C. Junghans**, K. Kremer, and T. Stuehn, *Scalable and fast heterogeneous molecular simulation with predictive parallelization schemes*, Phys. Rev. E **96**, 053311 (2017).

27. S. K. Gutierrez, K. Davis, D. Arnold, R. S. Baker, R. W. Robey, P. McCormick, D. Holladay, J. A. Dahl, J. Zerr, F. Weik, and **C. Junghans**, *Accommodating Thread-Level Heterogeneity in Coupled Parallel Applications*, in: *Proceedings of 2017 IEEE International Parallel and Distributed Processing Symposium* (IPDPS), Orlando, FL, USA, 469 (2017).

26. **C. Junghans**, A. Agarwal, and L. Delle Site, *Computational efficiency and Amdahl's law for the adaptive resolution simulation technique*, Comp. Phys. Comm. **215**, 20 (2017).

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). "*Among the top 10% most cited PLoS ONE papers published in 2015.*" (2019)

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).

20. 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

6. *Balancing the load: Los Alamos researchers develop code to distribute computation more efficiently and across increasing numbers of supercomputer processors.* ASCR Discovery Story, HPCwire, insideHPC and LANL Science Brief (2018).

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.