

Christoph Junghans

Staff Scientist

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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 Simulation 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. Nagaraajan, **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.