

List of Scientific Publications of Christof Schütte as of Jan., 2013

Recently submitted

1. Enciso, M. and Schütte, Ch. and Delle Site, L. (2012) *pH-dependent coarse-grained model of peptides*. *Soft Matter*. (Submitted)
2. Rath, B. A. and Yousef, K. P. and Katzenstein, D. K. and Shafer, R. W. and Schütte, Ch. and von Kleist, M. and Merigan, T. C. (2012) *HIV-1 Evolution in Response to Triple Reverse Transcriptase Inhibitor Induced Selective Pressure in vitro*. *PLoS ONE*. ISSN 1932-6203 (Submitted)
3. Wang, H. and Hartmann, C. and Delle Site, L. and Schütte, Ch. (2012) *The reliability of the adaptive resolution technique in performing grand canonical-like molecular dynamics simulations*. *Phys. Rev. X*. (Submitted)
4. Winkelmann, S. and Schütte, Ch. and von Kleist, M. (2012) *Markov Control Processes with Rare State Observation: Theory and Application to Treatment Scheduling in HIV-1*. *Communications in Mathematical Sciences*. (Submitted)
5. Winkelmann, S. and Schütte, Ch. and von Kleist, M. (2012) *Markov Control with Rare State Observation: Sensitivity Analysis with Respect to Optimal Treatment Strategies against HIV-1*. *International Journal of Biomathematics and Biostatistics*. (Submitted)

Complete List of Scientific Publications (excluding Technical Reports)

2012

6. Aiche, S. and Reinert, K. and Schütte, Ch. and Hildebrand, D. and Schlüter, H. and Conrad, T. O. F. (2012) *Inferring Proteolytic Processes from Mass Spectrometry Time Series Data Using Degradation Graphs*. *PLoS ONE*, 7 (7). e40656. ISSN 1932-6203
7. Djurdjevac, N. and Bruckner, S. and Conrad, T. O. F. and Schütte, Ch. (2012) *Random Walks on Complex Modular Networks*. *Journal of Numerical Analysis, Industrial and Applied Mathematics*, 6 (1-2). pp. 29-50. ISSN 1790-8140
8. Djurdjevac, N. and Sarich, M. and Schütte, Ch. (2012) *Estimating the eigenvalue error of Markov State Models*. *Multiscale Modeling & Simulation*, 10 (1). pp. 61-81.
9. Duwal, S. and Schütte, Ch. and von Kleist, M. (2012) *Pharmacokinetics and Pharmacodynamics of the Reverse Transcriptase Inhibitor Tenofovir & Prophylactic Efficacy against HIV-1 Infection*. *PLoS One*, 7 (7). e40382.
10. Hartmann, C. and Schütte, Ch. (2012) *Efficient rare event simulation by optimal nonequilibrium forcing*. *J. Stat. Mech. Theor. Exp.*, 2012. P11004.
11. Meerbach, E. and Latorre, J.C. and Schütte, Ch. (2012) *Sequential Change Point Detection in Molecular Dynamics Trajectories*. *Multiscale Model. Sim.*, 10 (4). pp. 1263-1291.
12. Menz, S. and Latorre, J.C. and Schütte, Ch. and Huisinga, W. (2012) *Hybrid Stochastic-Deterministic Solution of the Chemical Master Equation*. *SIAM Interdisciplinary Journal Multiscale Modeling and Simulation (MMS)*, 10 (4). pp. 1232-1262.
13. Sarich, M. and Djurdjevac, N. and Bruckner, S. and Conrad, T. O. F. and Schütte, Ch. (2012) *Modularity revisited: A novel dynamics-based concept for decomposing complex networks*. *Journal of Computational Dynamics*. (In Press)
14. Sarich, M. and Schütte, Ch. (2012) *Approximating Selected Non-dominant Timescales by Markov State Models*. *Comm. Math. Sci.*, 10 (3). pp. 1001-1013.
15. Schütte, Ch. and Winkelmann, S. and Hartmann, C. (2012) *Optimal control of molecular dynamics using Markov state models*. *Math. Program. (Series B)*, 134 (1). pp. 259-282.

16. Senne, M. and Trendelkamp-Schroer, B. and Mey, A.S.J.S. and Schütte, Ch. and Noé, F. (2012) *EMMA - A software package for Markov model building and analysis*. Journal of Chemical Theory and Computation, 8 . pp. 2223-2238.
17. von Kleist, M. and Metzner, Ph. and Marquet, R. and Schütte, Ch. (2012) *Polymerase Inhibition by Nucleoside Analogs: Cellular- and Kinetic Parameters of Efficacy, Susceptibility and Resistance Selection*. Plos Computational Biology, 8 (1). e1002359.
18. Wang, H. and Schütte, Ch. and Delle Site, L. (2012) *Adaptive Resolution Simulation (AdResS): A Smooth Thermodynamic and Structural Transition from Atomistic to Coarse Grained Resolution and Vice Versa in a Grand Canonical Fashion*. J. Chem. Theo. Comp., 8 (8). pp. 2878-2887.
19. Wang, H. and Schütte, Ch. and Zhang, P. (2012) *Error Estimate of Short-Range Force Calculation in the Inhomogeneous Molecular Systems*. Phys. Rev. E, 86 (02). 026704.
20. Wang, H. and Zhang, P. and Schütte, Ch. (2012) *On the Numerical Accuracy of Ewald, Smooth Particle Mesh Ewald, and Staggered Mesh Ewald Methods for Correlated Molecular Systems*. J. Chem. Theo. Comp., 8 (9). pp. 3243-3256.
21. Weiss, M. E. R. and Paulus, F. and Steinhilber, D. and Nikitin, A. and Haag, R. and Schütte, Ch. (2012) *Estimating Kinetic Parameters for the Spontaneous Polymerization of Glycidol at Elevated Temperatures*. MACROMOLECULAR THEORY and SIMULATIONS, 21 (7). pp. 470-481.

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22. Bernhard, S. and Al Zoukra, K. and Schütte, Ch. (2011) *Statistical parameter estimation and signal classification in cardiovascular diagnosis*. In: Modelling in Medicine and Biology. WIT Transactions on Biomedicine and Health, IX (15). WIT Press, Southampton & Boston. ISBN 978-1-84564-546-5
23. Frank, M. and von Kleist, M. and Kunz, A. and Harms, G. and Schütte, Ch. and Kloft, Ch. (2011) *Quantifying the impact of nevirapine-based prophylaxis strategies to prevent mother-to-child transmission of HIV-1: A combined pharmacokinetic, pharmaco- and viral dynamic analysis to predict clinical outcomes*. Antimicrob. Agents Chemother., 55 (12). pp. 5529-5540.
24. Latorre, J.C. and Metzner, Ph. and Hartmann, C. and Schütte, Ch. (2011) *A Structure-preserving numerical discretization of reversible diffusions*. Commun. Math. Sci. , 9 (4). pp. 1051-1072.
25. Prinz, J.-H. and Wu, H. and Sarich, M. and Keller, B. and Fischbach, M. and Held, M. and Chodera, J. D. and Schütte, Ch. and Noé, F. (2011) *Markov models of molecular kinetics: Generation and Validation*. J. Chem. Phys., 134 . p. 174105.
26. Schäfer-Bung, B. and Hartmann, C. and Schmidt, B. and Schütte, Ch. (2011) *Dimension reduction by balanced truncation: Application to light-induced control of open quantum systems*. J. Chem. Phys., 135 (1). 014112.
27. Schütte, Ch. and Noé, F. and Lu, Jianfeng and Sarich, M. and Vanden-Eijnden, E. (2011) *Markov State Models Based on Milestoning*. J. Chem. Phys., 134 (20). 204105 .
28. von Kleist, M. and Menz, S. and Stocker, H. and Arasteh, K. and Huisinga, W. and Schütte, Ch. (2011) *HIV Quasispecies Dynamics during Pro-active Treatment Switching: Impact on Multi-Drug Resistance and Resistance Archiving in Latent Reservoirs*. Plos One, 6 (3). e18204.

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29. Metzner, Ph. and Weber, M. and Schütte, Ch. (2010) *Observation Uncertainty in Reversible Markov Chains*. Phys. Rev. E, 82 (3). 031114.
30. Horenko, I. and Schütte, Ch. (2010) *On metastable conformational analysis of non-equilibrium biomolecular time series*. Multiscale Modeling & Simulation, 8 (2). pp. 701-716. ISSN 15403467
31. Hartmann, C. and Vulcanov, V.-M. and Schütte, Ch. (2010) *Balanced Truncation of Second Order Systems: a Hamiltonian approach*. Multiscale Model. Simul., 8 (4). pp. 1348-1367.

32. Latorre, J.C. and Hartmann, C. and Schütte, Ch. (2010) *Free energy computation by controlled Langevin processes*. Procedia Computer Science, 1 (1). pp. 1591-1600.
33. Schütte, Ch. and Wulkow, M. (2010) *A Hybrid Galerkin–Monte-Carlo Approach to Higher-Dimensional Population Balances in Polymerization Kinetics*. Macromol. React. Eng., 4 (9-10). pp. 562-577.
34. Marsalek, O. and Frigato, T. and VandeVondele, J. and Bradforth, P. E. and Schmidt, B. and Schütte, Ch. and Jungwirth, P. (2010) *Hydrogen Forms in Water by Proton Transfer to a Distorted Electron*. J. Phys. Chem. B, 114 (2). pp. 915-920.
35. Sarich, M. and Noé, F. and Schütte, Ch. (2010) *On the Approximation Quality of Markov State Models*. Multiscale Model. Simul., 8 (4). pp. 1154-1177.
36. Hartmann, C. and Schütte, Ch. and Ciccotti, G. (2010) *On the linear response of mechanical systems with constraints*. J. Chem. Phys. , 132 (11). p. 111103.
37. Djurdjevac, N. and Sarich, M. and Schütte, Ch. (2010) *On Markov State Models for Metastable Processes*. In: Proceedings of the International Congress of Mathematics, Hyderabad, India, Section Invited Talks. 2010.
38. Bernhard, S. and Al Zoukara, K. and Schütte, Ch. (2010) *From non-invasive hemodynamic measurements towards patient-specific cardiovascular diagnosis*. In: Quality Assurance in Healthcare Service Delivery, Nursing and Personalized Medicine. Hershey, PA: Medical Information Science Reference. (in press)
39. Sarich, M. and Schütte, Ch. and Vanden-Eijnden, E. (2010) *Optimal Fuzzy Aggregation of Networks*. Multiscale Modeling and Simulation, 8 (4). pp. 1535-1561.
40. Diederichs, E. and Juditski, A. and Spokoyny, V. and Schütte, Ch. (2009) *Sparse NonGaussian Component Analysis*. IEEE Transactions on Information Theory, Volume 56 Issue 6, 2010

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41. Frank Noé, Christof Schütte, Eric Vanden-Eijnden, Lothar Reich, and Thomas R. Weigl (2009) *Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations*, PNAS vol. 106 no. 45 19011-19016
42. Fiedler, G. M. and Leichtle, A. and Kase, J. and Baumann, S. and Ceglarek, U. and Felix, K. and Conrad, T. O. F. and Witzigmann, H. and Weimann, A. and Schütte, Ch. and Hauss, J. and Büchler, M. and Thiery, J. (2009) *Serum Peptidome Profiling Revealed Platelet Factor 4 as a Potential Discriminating Peptide Associated With Pancreatic Cancer*. Clinical Cancer Research, 15 (11). pp. 3812-3819. ISSN 1078-0432
43. Metzner, Ph. and Schütte, Ch. and Vanden-Eijnden, E. (2009) *Transition Path Theory for Markov Jump Processes*. Mult. Mod. Sim., 7 (3). pp. 1192-1219.
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46. Metzner, Ph. and Noé, F. and Schütte, Ch. (2009) *Estimating the Sampling Error: Distribution of Transition Matrices and Functions of Transition Matrices for Given Trajectory Data*. Phys. Rev. E 80, 021106 (2009) [13 pages]
47. Horenko, I. and Schütte, Ch. (2009) *Likelihood-Based Estimation of Multidimensional Langevin Models and its Application to Biomolecular Dynamics*. Mult. Mod. Sim.,7(2), 2009
48. Gräfe, Ch. and Schütte, Ch. and Nordmeier, V. (2009) *"Learner as creator" - SchülerInnen generieren eigene Lernspiele*. In: Didaktik der Physik - Bochum 2009. Lehmanns Media, Berlin. ISBN 978-3-86541-371-0
49. Schütte, Ch. and Noé, F. and Meerbach, E. and Metzner, Ph. and Hartmann, C. (2009) *Conformation Dynamics*. 6th International Congress on Industrial and Applied Mathematics, Zürich, Switzerland, 16-20 July 2007. Invited Lectures. Editor: R. Jeltsch, G. Wanner, ECM Publishing House

50. Schütte, Ch. and Jahnke, T. (2009) *Towards Effective Dynamics in Complex Systems by Markov Kernel Approximation*. Mathematical Modelling and Numerical Analysis, ESAIM: M2AN Volume 43, Number 4, Special issue on Numerical ODEs today, pages 721-742

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51. Frigato, T. and VandeVondele, J. and Schmidt, B. and Schütte, Ch. and Jungwirth, P. (2008) *Ab Initio Molecular Dynamics Simulation of a Medium-Sized Water Cluster Anion: From an Interior to a Surface Located Excess Electron via a Delocalized State*. J. Phys. Chem. A, 112 (27). pp. 6125-6133.
52. Horenko, I. and Dittmer, E. and Lankas, T. and Maddocks, J. and Metzner, Ph. and Schütte, Ch. (2008) *Macroscopic Dynamics of Complex Metastable Systems: Theory, Algorithms, and Application to B-DNA*. SIAM J. Appl. Dyn. Syst. Volume 7, Issue 2, pp. 532-560 (2008)
53. Horenko, I. and Klein, R. and Dolaptchiev, S. and Schütte, Ch. (2008) *Automated Generation of Reduced Stochastic Weather Models I: Simultaneous Dimension and Model reduction for Time Series Analysis*. Mult. Mod. Sim., 6 (4). pp. 1125-1145.
54. Hartmann, C. and Schütte, Ch. (2008) *Balancing for partially-observed stochastic differential equations*. 47th IEEE Conference on Decision and Control . pp. 4867-4872.
55. Gräfe, C. and Nordmeier, V. and Schütte, Ch. (2008) *Spielend lernen - ein Online Computerspiel zur Moleküldynamik*. DPG (Deutsche Physikalische Gesellschaft e.V.), CD zur Frühjahrstagung, DD_36_2

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56. Hartmann, C. and Schütte, Ch. (2007) *Comment on Two Distinct Notions of Free Energy*. Physica D, 228 (1). pp. 59-63.
57. Held, M. and Meerbach, E. and Hinderlich, S. and Reutter, W. and Schütte, Ch. (2007) *Conformational Studies of UDP-GlcNAc in Environments of Increasing Complexity*. In: From Computational Biophysics to Systems Biology.
58. Horenko, I. and Hartmann, C. and Schütte, Ch. and Noé, F. (2007) *Data-based Parameter Estimation of Generalized Multidimensional Langevin Processes*. Phys. Rev. E, 76 (01). 016706.
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60. Metzner, Ph. and Dittmer, E. and Jahnke, T. and Schütte, Ch. (2007) *Generator Estimation of Markov Jump Processes*. J. Comp. Phys., 227 (1). pp. 353-375.
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63. Meerbach, E. and Schütte, Ch. and Horenko, I. and Schmidt, B. (2007) *Metastable Conformational Structure and Dynamics: Peptides between Gas Phase and Aqueous Solution*. In: Analysis and Control of Ultrafast Photoinduced Reactions.
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65. Fischer, A. and Waldhausen, S. and Horenko, I. and Meerbach, E. and Schütte, Ch. (2007) *Identification of Biomolecular Conformations from Incomplete Torsion Angle Observations by Hidden Markov Models*. J. Comp. Chem., 28 (15). pp. 2453-2464.

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67. Conrad, T. O. F. and Leichtle, A. and Hagehülsmann, A. and Diederichs, E. and Baumann, S. and Thiery, J. and Schütte, Ch. (2006) *Beating the Noise: New Statistical Methods for Detecting Signals in MALDI-TOF Spectra Below Noise Level*. Lecture Notes in Computer Science, 4216 . pp. 119-128.
68. Metzner, Ph. and Schütte, Ch. and Vanden-Eijnden, E. (2006) *Illustration of Transition Path Theory on a Collection of Simple Examples*. J. Chem. Phys., 125 (8). 084110.
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71. Walter, J. and Schütte, Ch. (2006) *Conditional Averaging for Diffusive Fast-Slow Systems: A Sketch for Derivation*. In: Analysis, Modeling and Simulation of Multiscale Problems. Ed. A. Mielke
72. Dellnitz, M. and Molo, M. and Metzner, Ph. and Preis, R. and Schütte, Ch. (2006) *Graph Algorithms for Dynamical Systems*. In: Analysis, Modeling and Simulation of Multiscale Problems. Ed. A. Mielke

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75. Meerbach, E. and Schütte, Ch. and Fischer, A. (2005) *Eigenvalue Bounds on Restrictions of Reversible Nearly Uncoupled Markov Chains*. Lin. Alg. Appl., 398 . pp. 141-160.
76. Hartmann, C. and Schütte, Ch. (2005) *A Geometric Approach to Constrained Molecular Dynamics and Free Energy*. Comm. Math. Sci., 3 (1). pp. 1-20.
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79. Dellnitz, M. and Neumann, M. and Schütte, Ch. (2005) *Special Issue on Matrices and Mathematical Biology*. Lin. Alg. Appl., 398 . pp. 1-245.
80. Schütte, Ch. and Forster, R. and Meerbach, E. and Fischer, A. (2005) *Uncoupling-Coupling Techniques for Metastable Dynamical Systems*. In: Domain Decomposition Methods in Science and Engineering.
81. Chipot, C. and Elber, R. and Laaksonen, A. and Leimkuhler, B. and Mark, A. and Schlick, T. and Schütte, Ch. and Skeel, R., eds. (2005) *New Algorithms for Macromolecular Simulation*. Lecture Notes in Computational Science and Engineering, 49 . Springer.
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