List of Scientific Publications of Christof Schütte as of Jan., 2012

Recently submitted

1. Senne, M., Schuette, Ch., Noé, F. (2012) *EMMA - A software package for Markov model building and analysis,* Submitted to Journal of Chemical Theory and Computation
2. Wang, H., Schuette, Ch.; Zhang, P. (2012) *The Error Estimate of Force Calculation in the Inhomogeneous Molecular Systems*, Submitted to Journal of Chemical Theory and Computation
3. Weiss, M., Paulus' F., Steinhilber' D., Nikitin, A., Haag, R., Schuette' C. (2012) *Estimating Kinetic Parameters for the Spontaneous Polymerization of Glycidol at High Temperatures*, Submitted to MACROMOLECULAR THEORY and SIMULATIONS
4. M. Sarich, M., Djurdjevac, N., Bruckner, Sh., Conrad, T., Schuette, Ch. (2012) *Use multilevel random walks to find modules and hubs in complex networks* Submitted to Journal of Computational Dynamics
5. Menz, S. and Latorre, J.C. and Schütte, Ch. and Huisinga, W. (2011) *Hybrid Stochastic–Deterministic Solution of the Chemical Master Equation.* SIAM Interdisciplinary Journal Multiscale Modeling and Simulation (MMS) . (Submitted)
6. Latorre, J.C, Meerbach, E. and Schütte, Ch. (2011) *Sequential Change Point Detection in Molecular Dynamics Trajectories.* Multiscale Modeling & Simulation (Submitted).

Complete List of Scientific Publications (excluding Technical Reports)

2011

7. Sarich, M. and Schütte, Ch. (2011) *Approximating Selected Non-dominant Timescales by Markov State Models.* CPAM (Accepted)
8. Djurdjevac, N. and Sarich, M. and Schütte, Ch. (2010) *Estimating the Eigenvalue Error of Markov State Models.* Multiscale Modeling & Simulation . (Accepted)
9. von Kleist, M. and Metzner, P. and Marquit, R. and Schütte, Ch. (2011) *Polymerase inhibition by nucleoside analogs: Cellularand kinetic parameters of efficacy, susceptibility and resistance selection.* Plos Comp. Biol. (Accepted)
10. 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.
11. Latorre, J.C. and Metzner, Ph. and Hartmann, C. and Schütte, Ch. (2010) *A Structure-preserving numerical discretization of reversible diffusions.* Commun. Math. Sci. . (In Press)
12. 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 .
13. Djurdjevac, N. and Bruckner, Sh and Conrad, T. and Schütte, Ch (2011) *Random walks on complex modular networks*, Journal of Numerical Analysis, Industrial and Applied Mathematics (In press)
14. 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.
15. 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.

2010

16. Metzner, Ph. and Weber, M. and Schütte, Ch. (2010) *Observation Uncertainty in Reversible Markov Chains.* Phys. Rev. E, 82 (3). 031114.
17. 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

18. 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.
19. 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.
20. 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.
21. 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.
22. 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.
23. 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.
24. 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.
25. Bernhard, S. and Al Zoukra, 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)
26. Sarich, M. and Schütte, Ch. and Vanden-Eijnden, E. (2010) *Optimal Fuzzy Aggregation of Networks.* Multiscale Modeling and Simulation, 8 (4). pp. 1535-1561.
27. Diederichs, E. and Juditski, A. and Spokoiny, V. and Schütte, Ch. (2009) *Sparse NonGaussian Component Analysis.* IEEE Transactions on Information Theory, Volume 56 Issue 6, 2010

2009

28. Frank Noé, Christof Schütte, Eric Vanden-Eijnden, Lothar Reich, and Thomas R. Weikl (2009) *Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations,* PNAS vol. 106 no. 45 19011-19016
29. 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
30. 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.
31. Gräfe, C. and Nordmeier, V. and Schütte, Ch. (2009) *Computerspiel zum Thema Moleküldynamik für Schüler der 7.-10. Klasse, Experimentelles Prototyping zur Entwicklung eines Lernspiels.* Jahrestagung 2008 der GDCP (Gesellschaft für Didaktik der Chemie und Physik), 1 . pp. 77-79. ISSN 978-3-643-10010-8
32. 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]
33. 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
34. 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
35. 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. Jeltzsch, G. Wanner, ECM Publishing House
36. 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

2008

37. 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.
38. 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)
39. 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.
40. Hartmann, C. and Schütte, Ch. (2008) *Balancing for partially-observed stochastic differential equations.* 47th IEEE Conference on Decision and Control . pp. 4867-4872.
41. 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

2007

42. Hartmann, C. and Schütte, Ch. (2007) *Comment on Two Distinct Notions of Free Energy.* Physica D, 228 (1). pp. 59-63.
43. 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.
44. 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.
45. Lorenz, S. and Diederichs, E. and Telgmann, R. and Schütte, Ch. (2007) *Discrimination of Dynamical System Models for Biological and Chemical Processes.* J. Comp. Chem., 28 (8). pp. 1384-1399.
46. 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.
47. Metzner, Ph. and Horenko, I. and Schütte, Ch. (2007) *Generator Estimation of Markov Jump Processes Based on Incomplete Observations Nonequidistant in Time.* Phys. Rev. E, 76 (06). 066702.
48. Noé, F. and Horenko, I. and Schütte, Ch. and Smith, J. C. (2007) *Hierarchical Analysis of Conformational Dynamics in Biomolecules: Transition Networks of Metastable States.* J. Chem. Phys., 126 (15). p. 155102.
49. 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.
50. Noé, F. and Smith, J. C. and Schütte, Ch. (2007) *A network-based approach to biomolecular dynamics.* From Computational Biophysics to Systems Biology (CBSB07). Editors: U. H. E. Hansmann, J. Meinke, S. Mohanty and O. Zimmermann, NIC Series 36
51. 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.

2006

52. Horenko, I. and Dittmer, E. and Fischer, A. and Schütte, Ch. (2006) *Automated Model Reduction for Complex Systems exhibiting Metastability.* Mult. Mod. Sim., 5 (3). pp. 802-827.
53. 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.
54. 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.

55. Meerbach, E. and Dittmer, E. and Horenko, I. and Schütte, Ch. (2006) *Multiscale Modelling in Molecular Dynamics: Biomolecular Conformations as Metastable States.* In: Computer Simulations in Condensed Matter: Systems: From Materials to Chemical Biology. Volume I.
56. Horenko, I. and Schmidt-Ehrenberg, J. and Schütte, Ch. (2006) *Set-Oriented Dimension Reduction: Localizing Principal Component Analysis via Hidden Markov Models.* In: Proc. Computational Life Sciences II.
57. 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
58. 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

1992-2005

59. Horenko, I. and Lorenz, S. and Schütte, Ch. and Huisinga, W. (2005) *Adaptive Approach for Non-Linear Sensitivity Analysis of Reaction Kinetics.* J. Comp. Chem., 26 (9). pp. 941-948.
60. Hartmann, C. and Schütte, Ch. (2005) *A Constrained Hybrid Monte-Carlo Algorithm and the Problem of Calculating the Free Energy in Several Variables.* Z. Angew. Math. Mech., 85 (10). pp. 700-710.
61. 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.
62. Hartmann, C. and Schütte, Ch. (2005) *A Geometric Approach to Constrained Molecular Dynamics and Free Energy.* Comm. Math. Sci., 3 (1). pp. 1-20.
63. Antony, J. and Schmidt, B. and Schütte, Ch. (2005) *Nonadiabatic Effects on Peptide Vibrational Dynamics Induced by Conformational Changes.* J. Chem. Phys., 122 (1). 014309.
64. Horenko, I. and Dittmer, E. and Schütte, Ch. (2005) *Reduced Stochastic Models for Complex Molecular Systems.* Comp. Vis. Sci., 9 (2). pp. 89-102.
65. Dellnitz, M. and Neumann, M. and Schütte, Ch. (2005) *Special Issue on Matrices and Mathematical Biology.* Lin. Alg. Appl., 398 . pp. 1-245.
66. 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.
67. 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.
68. Walter, J. and Schütte, Ch. and Pavliotis, G. A. and Stuart, A. (2004) *Averaging of Stochastic Differential Equations: Kurtz's Theorem Revisited.* In: Analysis, Modeling and Simulation of Multiscale Problems. Ed. A. Mielke
69. Schütte, Ch. and Walter, J. and Hartmann, C. and Huisinga, W. (2004) *An Averaging Principle for Fast Degrees of Freedom Exhibiting Long-Term Correlations.* Multiscale Model. Simul., 2 (3). pp. 501-526.
70. Horenko, I. and Weiser, M. and Schmidt, B. and Schütte, Ch. (2004) *Fully Adaptive Propagation of the Quantum-Classical Liouville Equation.* J. Chem. Phys., 120 (19). pp. 8913-8923.
71. Deuflhard, P. and Schütte, Ch. (2004) *Molecular Conformation Dynamics and Computational Drug Design.* In: Applied Mathematics Entering the 21st Century.
72. Huisinga, W. and Meyn, S. and Schütte, Ch. (2004) *Phase Transitions and Metastability in Markovian and Molecular Systems.* Ann. Appl. Prob., 14 (1). pp. 419-458.
73. Schütte, Ch. and Huisinga, W. (2003) *Biomolecular Conformations can be Identified as Metastable Sets of Molecular Dynamics.* In: Special Volume: Computational Chemistry.
74. Huisinga, W. and Schütte, Ch. and Stuart, A. M. (2003) *Extracting Macroscopic Stochastic Dynamics: Model Problems.* Comm. Pure Appl. Math., 56 (2). pp. 234-269.
75. Schütte, Ch. and Huisinga, W. and Meyn, S. (2003) *Metastability of Diffusion Processes.* In: Nonlinear Stochastic Dynamics.
76. Fischer, A. and Schütte, Ch. and Deuflhard, P. and Cordes, F. (2002) *Hierarchical Uncoupling-Coupling of Metastable Conformations.* In: Computational Methods for Macromolecules: Challenges and Applications.

77. Horenko, I. and Schmidt, B. and Schütte, Ch. (2002) *Multidimensional Classical Liouville Dynamics with Quantum Initial Conditions.* J. Chem. Phys., 117 (10). pp. 4643-4650.
78. Horenko, I. and Salzmann, Ch. and Schmidt, B. and Schütte, Ch. (2002) *Quantum-Classical Liouville Approach to Molecular Dynamics: Surface Hopping Gaussian Phase-Space Packets.* J. Chem. Phys., 117 (24). pp. 11075-11088.
79. Horenko, I. and Schmidt, B. and Schütte, Ch. (2001) *A Theoretical Model for Molecules Interacting with Intense Laser Pulses: The Floquet-based Quantum-Classical Liouville Equation.* J. Chem. Phys., 115 (13). pp. 5733-5743.
80. Schütte, Ch. and Huisinga, W. and Deuflhard, P. (2001) *Transfer Operator Approach to Conformational Dynamics in Biomolecular Systems.* In: Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems.
81. Schütte, Ch. and Huisinga, W. (2000) *Biomolecular Conformations as Metastable Sets of Markov Chains.* In: Proceedings of the 38th Annual Allerton Conference on Communication, Control, and Computing, Monticello, Illinoins/USA.
82. Deuflhard, P. and Huisinga, W. and Fischer, A. and Schütte, Ch. (2000) *Identification of Almost Invariant Aggregates in Reversible Nearly Uncoupled Markov Chains.* Lin. Alg. Appl., 315 (1-3). pp. 39-59.
83. Schütte, Ch. and Huisinga, W. (2000) *On Conformational Dynamics induced by Langevin Processes.* In: Equadiff 99.
84. Schütte, Ch. and Cordes, F. (2000) *On Dynamical Transitions between Conformational Ensembles.* In: Molecular Dynamics on Parallel Computers.
85. Bornemann, F. A. and Schütte, Ch. (1999) *Adaptive Accuracy Control for Car-Parrinello Simulations.* Num. Math., 83 (2). pp. 179-186.
86. Deuflhard, P. and Dellnitz, M. and Junge, O. and Schütte, Ch. (1999) *Computation of Essential Molecular Dynamics by Subdivision Techniques.* In: Computational Molecular Dynamics: Challenges, Methods, Ideas.
87. Schütte, Ch. (1999) *Conformational Dynamics: Modelling, Theory, Algorithm, and Application to Biomolecules.* Habilitation Thesis, FU Berlin, 1999
88. Schütte, Ch. and Fischer, A. and Huisinga, W. and Deuflhard, P. (1999) *A Direct Approach to Conformational Dynamics based on Hybrid Monte Carlo.* J. Comp. Phys, 151 (1). pp. 146-168.
89. Huisinga, W. and Best, Ch. and Roitzsch, R. and Schütte, Ch. and Cordes, F. (1999) *From Simulation Data to Conformational Ensembles: Structure and Dynamics based Methods.* J. Comp. Chem., 20 (16). pp. 1760-1774.
90. Fischer, A. and Cordes, F. and Schütte, Ch. (1999) *Hybrid Monte Carlo with adaptive temperature choice: Efficient conformational analysis of RNA.* Comp. Phys. Comm., 121 . pp. 37-39.
91. Bornemann, F. A. and Schütte, Ch. (1999) *On the Singular Limit of the Quantum-Classical Molecular Dynamics Model.* J. Appl. Math., 59 (4). pp. 1208-1224.
92. Schütte, Ch. (1999) *Partial Wigner transforms and the quantum-classical Liouville equation.* In: Computational Molecular Dynamics: Challenges, Methods, Ideas.
93. Schütte, Ch. and Bornemann, F. A. (1999) *Approximation Properties and Limits of the Quantum-Classical Molecular Dynamics Model.* In: Computational Molecular Dynamics: Challenges, Methods, Ideas.
94. Schütte, Ch. and Nettesheim, P. (1999) *Nonadiabatic Effects in Quantum-Classical Molecular Dynamics.* In: Scientific Computing in Chemical Engineering II.
95. Nettesheim, P. and Schütte, Ch. (1999) *Numerical Integrators for Quantum-Classical Molecular Dynamics.* In: Computational Molecular Dynamics: Challenges, Methods, Ideas.
96. Fischer, A. and Cordes, F. and Schütte, Ch. (1998) *Hybrid Monte Carlo with adaptive temperature in mixed-canonical ensemble: Efficient conformational analysis of RNA.* J. Comp. Chem., 19 (15). pp. 1689-1697.
97. Bornemann, F. A. and Schütte, Ch. (1998) *A mathematical investigation of the Car-Parrinello Method.* Num. Math., 78 (3). pp. 359-376.
98. Schütte, Ch. and Bornemann, F. A. (1997) *Homogenization Approach to Smoothed Molecular Dynamics.* Nonlinear Analysis, 30 (3). pp. 1805-1814.
99. Bornemann, F. A. and Schütte, Ch. (1997) *Homogenization of Hamiltonian Systems with a Strong Constraining Potential.* Physica D, 102 (1-2). pp. 57-77.

100. Nettesheim, P. and Bornemann, F. A. and Schmidt, B. and Schütte, Ch. (1996) *An Explicit and Symplectic Integrator for Quantum-Classical Molecular Dynamics.* Chem. Phys. Lett., 256 (6). pp. 581-588.
101. Bornemann, F. A. and Nettesheim, P. and Schütte, Ch. (1996) *Quantum-classical molecular dynamics as an approximation to full quantum dynamics.* J. Chem. Phys., 105 (3). pp. 1074-1083.
102. Schütte, Ch. and Zumbusch, M. D. G and Brinkmann, R. (1995) *Dynamics of Erbium-doped Waveguide Lasers: Modelling, Reliable Simulation, and Comparison with Experiments.* Lightw. Techn., 14 (2)
103. Schütte, Ch. and Dinand , M. (1995) *Theoretical Modeling of Relaxation Oscillations in Er-Doped Wave-Guide Lasers.* J. Lightw. Techn., 13 (1). pp. 14-23
104. Schütte, Christof (1994) *A Quasiresonant Smoothing Algorithm for Solving Large Highly Differential Equations from Quantum Chemistry*, Freie Universität Berlin, Dissertation, 1994. Shaker, ISBN 3-8265-0181-0.
105. Manz, J. and Paramonov, G. K. and Polasek, M. and Schütte, Ch. (1994) *Overtone State-Selective Isomerization by a Series of Picosecond Infrared Laser Pulses - Model Simulations for Be2H3D.* Isr. J. Chem., 34 (1). pp. 115-125.
106. Schütte, Ch. (1993) *A Quasiresonant Smoothing Algorithm for the Fast Analysis of Selective Vibrational Excitation.* Impact of Computing in Sci. Eng., 5 (3). pp. 176-200.