

References

- [1] A. Amadei, A. B. M. Linssen, and H. J. C. Berendsen. Essential dynamics of proteins. *Proteins*, 17:412–425, 1993.
- [2] H. Andersen. Molecular dynamics simulations at constant pressure and/or temperature. *J. Chem. Phys.*, 72:2384, 1980.
- [3] F. A. Bornemann and C. Schütte. Homogenization of Hamiltonian systems with a strong constraining potential. *Physica D*, 102:57–77, 1997.
- [4] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein. Metastability in stochastic dynamics of disordered mean-field models. *Probab. Theor. Rel. Fields*, 119:99–161, 2001.
- [5] F. E. Browder. On the spectral theory of elliptic differential operators I. *Math. Ann.*, 142:22–131, 1961.
- [6] J. B. Conway. *A Course in Functional Analysis*. Springer, New York, 1990.
- [7] F. Cordes and T. Galliat, 2001. Details to [27] (private communication).
- [8] E. B. Davies. *One-Parameter Semigroups*. Academic Press, London, 1980.
- [9] E. B. Davies. Metastable states of symmetric Markov semigroups I. *Proc. London Math. Soc.*, 45(3):133–150, 1982.
- [10] E. B. Davies. Metastable states of symmetric Markov semigroups II. *J. London Math. Soc.*, 26(2):541–556, 1982.
- [11] E. B. Davies. *Heat Kernels and Spectral Theory*. Cambridge Uni. Press, Cambridge, 1989.
- [12] M. Dellnitz and O. Junge. An adaptive subdivision technique for the approximation of attractors and invariant measures. *Comput. Visual. Sci.*, 1:63–68, 1998.
- [13] M. Dellnitz and O. Junge. On the approximation of complicated dynamical behavior. *SIAM J. Num. Anal.*, 36(2):491–515, 1999.
- [14] P. Deuflhard, M. Dellnitz, O. Junge, and C. Schütte. Computation of essential molecular dynamics by subdivision techniques. In [15], pages 98–115, 1999.
- [15] P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, and R. D. Skeel, editors. *Computational Molecular Dynamics: Challenges, Methods, Ideas*, volume 4 of *Lecture Notes in Computational Science and Engineering*. Springer, 1999.
- [16] P. Deuflhard and A. Hohmann. *Numerische Mathematik I*. de Gruyter, Berlin, 1993.
- [17] P. Deuflhard, W. Huisings, A. Fischer, and C. Schütte. Identification of almost invariant aggregates in reversible nearly uncoupled Markov chains. *Lin. Alg. Appl.*, 315:39–59, 2000.
- [18] J. L. Doob. *Stochastic Processes*. John Wiley & Sons, Inc., New York, 1953.
- [19] N. Dunford and J. T. Schwartz. *Linear Operators, Part I: General Theory*, volume VII of *Pure and Applied Mathematics*. Interscience, New York, 1957.
- [20] A. Fischer. An uncoupling–coupling technique for Markov chains Monte Carlo methods. Konrad-Zuse-Zentrum, Berlin. Report 00-04, 2000.
- [21] A. Fischer, F. Cordes, and C. Schütte. Hybrid Monte Carlo with adaptive temperature in a mixed–canonical ensemble: Efficient conformational analysis of RNA. *J. Comput. Chem.*, 19:1689–1697, 1998.
- [22] A. Fischer, C. Schütte, P. Deuflhard, and F. Cordes. Hierarchical uncoupling–coupling of metastable conformations. In T. Schlick and H. H. Gan, editors, *Computational Methods for Macromolecules: Challenges and Applications—Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modelling*, Lecture Notes in Computational Science and Engineering. Springer, 2002.

- [23] M. Freidlin and A. Wentzell. *Random Perturbations of Dynamical Systems*. Springer, New York, 1984. Series in Comprehensive Studies in Mathematics.
- [24] G. Froyland. Private communication. Feb. 2001.
- [25] G. Froyland and M. Dellnitz. Statistically optimal almost-invariant sets: Efficient detection and adaptive resolution. Preliminary work, 2001.
- [26] T. Galliat and P. Deuflhard. Adaptive hierarchical cluster analysis by self-organizing box maps. Konrad-Zuse-Zentrum, Berlin. Report SC-00-13, 2000.
- [27] T. Galliat, P. Deuflhard, R. Roitzsch, and F. Cordes. Automatic identification of metastable conformations via self-organized neural networks. In T. Schlick and H. H. Gan, editors, *Computational Methods for Macromolecules: Challenges and Applications—Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modelling*, Lecture Notes in Computational Science and Engineering. Springer, 2002.
- [28] T. Galliat, W. Huiszinga, and P. Deuflhard. Self-organizing maps combined with eigenmode analysis for automated cluster identification. In H. Bothe and R. Rojas, editors, *Neural Computation*, pages 227–232. ICSC Academic Press, 2000.
- [29] W. Gilks, S. Richardson, and D. Spiegelhalter, editors. *Markov chain Monte-Carlo in Practice*. Chapman and Hall, London, 1997.
- [30] R. Haberlandt, S. Fritzsche, G. Peinl, and K. Heinzinger. *Molekulardynamik - Grundlagen und Anwendungen*. Vieweg, 1995.
- [31] D. W. Heermann. *Computer Simulation Methods*. Springer, Berlin, 2nd edition, 1990.
- [32] H. Heuser. *Funktionalanalysis*. Teubner, Stuttgart, 1986.
- [33] W. Huiszinga. Impression resulting from discussions with J. Mattingly, C. Schütte and A. Stuart during the Workshop on "Computational Stochastic Differential Equations", March 2001, Warwick.
- [34] W. Huiszinga. The essential spectral radius and asymptotic properties of transfer operators in L^1 . *submitted to Dynam. Systems Appl.*, 2000. Available via <http://www.math.fu-berlin.de/~huiszinga>.
- [35] W. Huiszinga, C. Best, R. Roitzsch, C. Schütte, and F. Cordes. From simulation data to conformational ensembles: Structure and dynamic based methods. *J. Comp. Chem.*, 20(16):1760–1774, 1999.
- [36] K. Ichihara and H. Kunita. A classification of the second order degenerate elliptic operators and its probabilistic characterization. *Z. Wahrscheinlichkeitstheorie verw. Gebiete*, 30:235–254, 1974.
- [37] A. K. Jain and R. C. Dubes. *Algorithms for Clustering Data*. Prentice Hall, New Jersey, Advanced Reference Series edition, 1988.
- [38] I. Karatzas and S. E. Shreve. *Brownian Motion and Stochastic Calculus*. Graduate Texts in Mathematics. Springer, New York, 1991.
- [39] T. Kato. Perturbation theory of nullity, deficiency and other quantities of linear operators. *J. d'Analyse Math.*, 6:261–322, 1958.
- [40] T. Kato. *Perturbation Theory for Linear Operators*. Springer, Berlin, 1995. Reprint of the 1980 edition.
- [41] P. E. Kloeden and E. Platen. *Numerical Solution of Stochastic Differential Equations*. Springer, New York, 1991.
- [42] Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), Indeed-Visual Concepts GmbH and TGS Template Graphics Software Inc. *Amira—Advanced Visualization, Data Analysis and Geometry Reconstruction, User's Guide and Reference Manual*, 2000.

- [43] M. A. Krasnoselskii, P. P. Zabreiko, E. I. Pustylnik, and P. E. Sboloevskii. *Integral Operators in Spaces of Summable Functions*. Noordhoff Int. Pub., Leyden, 1976.
- [44] D. P. Landau and K. Binder. *Monte Carlo Simulations in Statistical Physics*. Cambridge Uni. Press, Cambridge, 2000.
- [45] K. Lange. Decomposition of substochastic transition functions. *Proc. Amer. Math. Soc.*, 37:575–580, 1973.
- [46] A. Lasota and M. C. Mackey. *Chaos, Fractals and Noise*, volume 97 of *Applied Mathematical Sciences*. Springer, New York, 2nd edition, 1994.
- [47] A. Lebow and M. Schechter. Semigroups of operators and measures of noncompactness. *J. Funct. Anal.*, 7:1–26, 1971.
- [48] E. Leontidis, B. M. Forrest, A. H. Widmann, and U. W. Suter. Monte Carlo algorithms for the atomistic simulation of condensed polymer phases. *J. Chem. Soc. Faraday Trans.*, 91(16):2355–2368, 1995.
- [49] S. Lorenz. Asymptotic behavior of perturbed dynamical systems in the context of modelling biomolecules. Diploma thesis, Department of Mathematics and Computer Science, Free University Berlin, 2001.
- [50] L. Maligranda. Weakly compact operators and interpolation. *Acta Appl. Math.*, 72:79–89, 1992.
- [51] J. Mattingly, A. M. Stuart, and D. J. Higham. Ergodicity for SDEs and approximations: Locally Lipschitz vector fields and degenerated noise. Submitted, 2001.
- [52] S. Meyn and R. Tweedie. *Markov Chains and Stochastic Stability*. Springer, Berlin, 1993.
- [53] E. Nelson. *Dynamical Theories of Brownian Motion*. Mathematical Notes. Princeton Uni. Press, 1967.
- [54] S. Nosé. A unified formulation of the constant temperature molecular dynamics methods. *J. Chem. Phys.*, 81(1):511–519, 1984.
- [55] E. Nummelin. *General Irreducible Markov Chains and Non-Negative Operators*. Cambridge Uni. Press, Cambridge, London, New York, New Rochelle, 1984.
- [56] R. D. Nussbaum. The radius of the essential spectrum. *Duke Math. J.*, 37:473–478, 1970.
- [57] B. Øksendal. *Stochastic Differential Equations*. Universitext. Springer, Berlin, Heidelberg, fifth edition, 1998.
- [58] W. K. Olson and B. Victor. Modeling DNA deformations. *Current Opinion in Structural Biology*, 10:286–297, 2000.
- [59] M. Reed and B. Simon. *Methods of Modern Mathematical Physics IV, Analysis of Operators*. Academic Press, New York, 1978.
- [60] D. Revuz. *Markov Chains*. North-Holland, Amsterdam, Oxford, 1975.
- [61] H. Risken. *The Fokker-Planck Equation*. Springer, New York, 2nd edition, 1996.
- [62] G. O. Roberts and J. S. Rosenthal. Geometric ergodicity and hybrid Markov chains. *Elect. Comm. in Probab.*, 2:13–25, 1997.
- [63] G. O. Roberts and R. L. Tweedie. L^2 and L^1 convergence are equivalent for reversible Markov chains. *Accepted in J. Appl. Probab.*, 2000. Preprint.
- [64] Y. Saad. *Numerical Methods for Large Eigenvalue Problems*. Manchester Uni. Press, Manchester, 1992.
- [65] J. M. Sanz-Serna and M. P. Calvo. *Numerical Hamiltonian Problems*, volume 7 of *Applied Mathematics and Mathematical Computation*. Chapman & Hall, London, 1994.

- [66] M. Schechter. On the essential spectrum of an arbitrary operator I. *J. Math. Anal. Appl.*, 13:205–215, 1966.
- [67] M. Schechter. Quantities related to strictly singular operators. *Indiana Math. J.*, 21:1061–1071, 1972.
- [68] C. Schütte. *Conformational Dynamics: Modelling, Theory, Algorithm, and Application to Biomolecules*. Habilitation Thesis, Fachbereich Mathematik und Informatik, Freie Universität Berlin, 1998.
- [69] C. Schütte, A. Fischer, W. Huisenga, and P. Deuflhard. A direct approach to conformational dynamics based on hybrid Monte Carlo. *J. Comput. Phys., Special Issue on Computational Biophysics*, 151:146–168, 1999.
- [70] C. Schütte and W. Huisenga. Von Mehrskaligkeit zur effektiven Dynamik: Ein Transfer–Operator–Zugang über essentielle Freiheitsgrade. Schwerpunktprogramm der Deutschen Forschungsgesellschaft: "Analysis, Modellierung und Simulation von Mehrskalenproblemen".
- [71] C. Schütte and W. Huisenga. On conformational dynamics induced by Langevin processes. In B. Fiedler, K. Gröger, and J. Sprekels, editors, *EQUADIFF 99 - International Conference on Differential Equations*, volume 2, pages 1247–1262, Singapore, 2000. World Scientific.
- [72] C. Schütte, W. Huisenga, and P. Deuflhard. Transfer operator approach to conformational dynamics in biomolecular systems. In B. Fiedler, editor, *Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems*, pages 191–223. Springer, 2001.
- [73] G. Singleton. Asymptotically exact estimates for metastable Markov semigroups. *Quart. J. Math. Oxford*, 35(2):321–329, 1984.
- [74] G. Singleton. *Some Properties of Metastable Semigroups*. PhD thesis, King's College London, 1986.
- [75] A. D. Sokal. Monte Carlo methods in statistical mechanics: Foundations and new algorithms. Lecture Notes, Cours de Troisième Cycle de la Physique en Suisse Romande, Lausanne, 1989.
- [76] A. M. Stuart. Geometric ergodicity for SDEs arising in statistical physics. Warwick University preprint, April 2001.
- [77] W. F. van Gunsteren, S. R. Billeter, A. A. Eising, P. H. Hünenberger, P. Krüger, A. E. Mark, W. R. P. Scott, and I. G. Tironi. *Biomolecular Simulation: The GROMOS96 Manual and User Guide*. vdf Hochschulverlag AG, ETH Zürich, 1996.
- [78] J. Walter. Preparatory studies. Diploma thesis, Department of Mathematics and Computer Science, Free University Berlin, 2001.
- [79] L. Weis. On perturbations of Fredholm operators in $L_p(\mu)$ -spaces. *Proc. Amer. Math. Soc.*, 67:287–292, 1977.
- [80] L. Weis. Integral operators and changes of density. *Indiana Univ. Math. J.*, 31(1):83–96, 1982.
- [81] L. Weis. Decompositions of positive operators and some of their applications. In K. D. Bierstedt and B. Fuchssteiner, editors, *Functional Analysis: Surveys and Recent Results III*, pages 95–115. North-Holland, 1983.
- [82] L. Weis. Approximation by weakly compact operators in L_1 . *Math. Nachr.*, 118:321–326, 1984.
- [83] L. Weis. On the computation of some quantities in the theory of Fredholm operators. *Rend. Circ. Mat. Palermo, II (Supplemento)*, 5:109–133, 1984.
- [84] D. Werner. *Funktionalanalysis*. Springer, Berlin, 2nd edition, 1997.

- [85] K. Yosida and S. Kakutani. Operator-theoretical treatment of Markoff's process and mean ergodic theorem. *Ann. of Math.*, 42(1):188–228, 1941.
- [86] H. X. Zhou, S. T. Wlodec, and J. A. McCammon. Conformation gating as a mechanism for enzyme specificity. *Proc. Nat. Acad. Sci. USA*, 95(9280–9283), 1998.
- [87] R. Zwanzig. Problems in nonlinear transport theory. In J. Ehlers et al., editor, *Systems Far From Equilibrium*, Lecture Notes in Physics, pages 198–225. Springer, 1980.