

# Bibliography

- [1] Alves, N.A., Berg, B.A. and Villanova, R. (1990). *Ising-Model Monte Carlo Simulations: Density of States and Mass Gap*, Phys. Rev. B **41**: 383–394.
- [2] Berg, B.A. and Neuhaus, T. (1991). *Multicanonical Algorithms for First Order Phase Transitions*, Phys. Lett. B **267**: 249–253.
- [3] Berg, B.A. and Neuhaus, T. (1992). *Multicanonical Ensemble: A New Approach to Simulate First-Order Phase Transitions*, Phys. Rev. Lett. **68**: 9–12.
- [4] Berg, B.A. and Celik, T. (1992). *A New Approach to Spin Glass Simulations*, Phys. Rev. Lett. **69**: 2292–2295.
- [5] Berg, B.A., Hansmann, U.H. and Neuhaus, T. (1993). *Properties of Interfaces in the Two and Three Dimensional Ising Model*, Z. Phys. B **90**: 229–239.
- [6] Berg, B.A., Celik T. and Hansmann, U.H. (1994). *Groundstate Properties of the 3D Ising spin glass*, Phys. Rev. B **50**: 16444–16452.
- [7] Berg, B.A., Hansmann, U.H. and Okamoto, Y. (1995). *Comment on “Monte Carlo Simulation of a First Order Transition for Protein Folding”*, J. Phys. Chem. **99**: 2236–2237.
- [8] Berg, B.A. (1996). *Multicanonical Recursions*, J. Stat. Phys. **82**: 323–342.
- [9] Berg, B.A., Muguruma, C. and Okamoto, Y. (2006). *Residual Entropy of Ordinary Ice from Multicanonical Simulations*, cond-mat/0609211.
- [10] Berg, B.A. and Janke, W. (2006). *Wang-Landau Recursion for Cluster Algorithms*, cond-mat/0610647.
- [11] Binder, K. (1982). *The Monte Carlo Calculation of the Surface Tensions for Two- and Three-Dimensional Lattice-Gas Models*, Phys. Rev. A **25**: 1699–1709.
- [12] Borgs, C. and Janke, W. (1992). *An explicit formula for the interface tension of the 2D Potts model*, J. Phys. I France **2**: 2011–2018.

- [13] Chandler, D. (1987). *Introduction to Modern Statistical Mechanics*, Oxford University Press (chapter 6.3).
- [14] Dinner, A.R., Lazaridis, T. and Karplus, M. (1999). *Understanding  $\beta$ -hairpin formation*, Proc. Nat. Acad. Sci. USA **96**: 9068–9073.
- [15] Falcioni, M., Marinari, E., Paciello, L., Parisi, G. and Taglienti, B. (1982). *Complex Zeros in the Partition Function of Four-Dimensional SU(2) Lattice Gauge Model*. Phys. Lett. B **108**: 331–332.
- [16] Ferrenberg, A.M. and Swendsen, R.H. (1988). *New Monte Carlo Technique for Studying Phase Transitions*, Phys. Rev. Lett. **61**: 2635–2638; **63**: 1658.
- [17] Ferrenberg, A.M. and Swendsen, R.H. (1989). *Optimized Monte Carlo Data Analysis*, Phys. Rev. Lett. **63**: 1195–1198.
- [18] Frantz, D.D., Freemann, D.L. and Doll, J.D. (1990). *Reducing quasi-ergodic behavior in Monte Carlo simulations by J-walking: Applications to atomic clusters*, J. Chem. Phys. **93**: 2769–2784.
- [19] Fukunishi, H., Watanabe, O., and Takada, S. (2000). *On the Hamiltonian replica exchange method for efficient sampling of biomolecular systems: Application to protein structure prediction*, J. Chem. Phys. **116**: 9058–9067.
- [20] Geyer, G.J. (1991). *Markov Chain Monte Carlo Maximum Likelihood*, in *Computing Science and Statistics*, Proceedings of the 23rd Symposium on the Interface, Keramidas, E.M. (editor), Interface Foundation, Fairfax, Virginia, pp. 156–163.
- [21] Hansmann, U.H. and Okamoto, Y. (1993). *Prediction of Peptide Conformation by Multicanonical Algorithm: New Approach to the Multiple-Minima Problem*, J. Comp. Chem. **14**: 1333–1338.
- [22] Hansmann, U.H. (1997). *Parallel tempering algorithm for conformational studies of biological molecules*, Chem. Phys. Lett. **281**: 140–150.
- [23] Hansmann, U.H. and Okamoto, Y. (1999). *Finite-size scaling of helix-coil transitions in poly-alanine studied by multicanonical simulations*, J. Chem. Phys. **110**: 1267–1276; erratum **111**: 1339.
- [24] Hao, M.-H. and H.A. Scheraga, H.A. (1994). *Monte Carlo Simulations of a First-Order Transition for Protein Folding*, J. Phys. Chem. **98**: 4940–4948.
- [25] Jang, S., Shin, S. and Pak, Y. (2003). *Replica-Exchange Method Using the Generalized Effective Potential*, Phys. Rev. Lett. **91**: 058305.
- [26] Janke, W., Berg, B.A. and Katoott, M. (1992). *Monte Carlo calculation of the surface free energy for the two-dimensional 7-state Potts model, and an estimate for four-dimensional SU(3) gauge theory*, Nucl. Phys. B **382**: 649–661.

- [27] Li, H., Fajer, M. and Yang, W. (2006). *Simulated Scaling Method for Localized Enhanced Sampling and Simultaneous “Alchemical” Free Energy Simulations: A General Method for MM, QM, and QM/MM Simulations*, J. Chem. Phys, in press.
- [28] Li, Z. and Scheraga, H.A. (1988). *Structure and Free Energy of Complex Thermodynamic Systems*, J. Mol. Struct. (Theochem) **179**: 333–352.
- [29] Liu, P., Kim, B., Friesner, A., and Berne, B.J. (2005). *Replica exchange with solute tempering: A method for sampling biological systems in explicit water*, Proc. Nat. Acad. Sci. USA **102**: 13749–13754.
- [30] Lyubartsev, A.P., Martsinovski, A.A., Shevkanov, S.V. and Vorontsov-Velyaminov, P.N. (1992). *New Approach to Monte Carlo Calculation of the Free Energy: Method of Expanded Ensembles*, J. Chem. Phys. **96**: 1776–1783.
- [31] Marinari, E. and Parisi, G. (1992). *Simulated Tempering: A New Monte Carlo Scheme*, Europhys. Lett. **19**: 451–458.
- [32] Min, D., Li, H., Li, G., Bitteti-Putzer, and Yang, W. (2006). *A Synergistic Approach to Improve “Alchemical” Free Energy Calculations in Rough Energy Landscapes*, J. Chem. Phys, in press.
- [33] McDonald, I.R. and Singer, K. (1967). *Calculation of Thermodynamic Properties of Liquid Argon from Lennard-Jones Parameters by a Monte Carlo Method*, Discussions Faraday Soc. **43**: 40–49.
- [34] Neidigh, J.W., Fesinmeyer, R.M. and Andersen, N.H. (2002). *Designing a 20-Residue Protein*. Nat. Struct. Biol. **9**: 425–430.
- [35] Hukusima, K. and Nemoto, K. (1996). *Exchange Monte Carlo Method and Applications to Spin Glass Simulations*, J. Phys. Soc. Japan **65**: 1604–1608.
- [36] Neuhaus, T. and Hager, J.S. (2003). *2D Crystal Shapes, Droplet Condensation and Supercritical Slowing Down in Simulations of First Order Phase Transitions*, J. Stat. Phys. **113**: 47–83.
- [37] Pascheck, D., Nymeyer, H. and Garcia, A.E. (2006), *Replica Exchange Simulation of Reversible Folding/Unfolding of the Trp-Cage Miniprotein in Explicit Solvent: On the the Structure and Possible Role of Internal Water*, J. Struct. Biol. In Press.
- [38] Pelissetto, A. and Vicari, E. (2002). *Critical Phenomena and Renormalization Group Theory*, Phys. Rep. **368**: 549–727.
- [39] Qiu, L.L, Pabic, S.A., Roitberg, A.E. and Hagen. S.J. (2002). *Smaller and Faster: The 20-Residue Trp-Cage Folds within 4μs*, J. Am. Chem. Soc. **124**: 12952–12953.

- [40] Salsburg, Z.W., Jacobson, J.D., Fickett, W.S. and Wood, W.W. (1959). *Applications of the Monte Carlo Method to the Lattice-Gas Model. I. Two-Dimensional Triangular Lattice*, J. Chem. Phys. **30**: 65–72.
- [41] Sugita, Y. and Okamoto, Y. (1999). *Replica-exchange molecular dynamics method for protein folding*, Chem. Phys. Lett. **314**: 141–151.
- [42] Swendsen, R.H. and Wang, J.-S. (1986). *Replica Monte Carlo Simulations of Spin Glasses*, Phys. Rev. Lett. **57**: 2607–2609.
- [43] Swendsen, R.H. and Wang, J.-S. (1987). *Nonuniversal Critical Dynamics in Monte Carlo Simulations*, Phys. Rev. Lett. **58**: 86–88.
- [44] Wang, J.-S. and Swendsen, R.H. (2002). *Transition Matrix Monte Carlo Method*, J. Stat. Phys. **106**: 245–285.
- [45] Torrie, G.M. and Valleau, J.P. (1977). *Nonphysical Sampling Distributions in Monte Carlo Free-energy Estimation: Umbrella Sampling*, J. Comp. Phys. **23**: 187–199.
- [46] Trebst, S., Huse, D.A. and Troyer, M. (2004). *Optimizing the ensemble for equilibration in broad-histogram Monte Carlo simulations*, Phys. Rev. E **70**: 046701.
- [47] Valleau, J.P. and Card, D.N. (1972). *Monte Carlo Estimation of the Free Energy by Multistage Sampling*, J. Chem. Phys. **37**: 5457–5462.
- [48] Wang, F. and Landau, D.P. (2001). *Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States*, Phys. Rev. Lett. **86**: 2050–2053.
- [49] Wolff, U. (1989). *Collective Monte Carlo Updating for Spin Systems*, Phys. Rev. Lett. **62**: 361–363.
- [50] Yan, Q. and de Pablo, J.J. (1999). *Hyper-parallel tempering Monte Carlo: Application to the Lennard-Jones fluid and the restrictive primitive model*, J. Chem. Phys. **111**: 9509–9516; *Hyper-parallel tempering simulation of polymeric systems*, J. Chem. Phys. **113**: 1276–1282.