References and Suggestions for Further Reading

- Farid F. Abraham, "Computational statistical mechanics: Methodology, applications, and supercomputing," Adv. Phys. **35**, 1–111 (1986). The author discusses both molecular dynamics and Monte Carlo techniques.
- B. J. Alder and T. E. Wainwright, "Phase transition for a hard sphere system," J. Chem. Phys. 27, 1208-1209 (1957).
- M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon Press, 1987). A classic text on molecular dynamics and Monte Carlo methods.
- Jean-Louis Barrat and Jean-Pierre Hansen, *Basic Concepts for Simple and Complex Liquids* (Cambridge University Press, 2003). Also see Jean-Pierre Hansen and Ian R. McDonald, *Theory of Simple Liquids*, 2nd ed. (Academic Press, 1986). Excellent graduate level texts that derive most of the theoretical results mentioned in this chapter.
- Kurt Binder, Jürgen Horbach, Walter Kob, Wolfgang Paul, and Fathollah Varnik, "Molecular dynamics simulations," J. Phys.: Condens. Matter **16**, S429–S453 (2004).
- R. P. Bonomo and F. Riggi, "The evolution of the speed distribution for a two-dimensional ideal gas: A computer simulation," Am. J. Phys. **52**, 54–55 (1984). The authors consider a system of hard disks and show that the system evolves to the Maxwell–Boltzmann distribution.
- J. P. Boon and S. Yip, *Molecular Hydrodynamics* (Dover, 1991). Their discussion of transport properties is an excellent supplement to our brief discussion.
- Giovanni Ciccotti and William G. Hoover, eds., Molecular-Dynamics Simulation of Statistical-Mechanics Systems (North-Holland, 1986).
- Giovanni Ciccotti, Daan Frenkel, and Ian R. McDonald, eds., Simulation of Liquids and Solids (North-Holland, 1987). A collection of reprints on the simulation of many body systems. Of particular interest are B. J. Alder and T. E. Wainwright, "Phase transition in elastic disks," Phys. Rev. 127, 359–361 (1962) and earlier papers by the same authors; A. Rahman, "Correlations in the motion of atoms in liquid argon," Phys. Rev. 136, A405–A411 (1964), the first application of molecular dynamics to systems with continuous potentials; and Loup Verlet, "Computer 'experiments' on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules," Phys. Rev. 159, 98–103 (1967).
- Daan Frenkel and Berend Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, 2nd ed. (Academic Press, 2002). This monograph is one of the best on molecular dynamics and Monte Carlo simulations. It is particularly strong on simulations in various ensembles and on methods for computing free energies.
- J. M. Haile, *Molecular Dynamics Simulation* (John Wiley & Sons, 1992). A derivation of the mean pressure using periodic boundary conditions is given in Appendix B.
- J. P. Hansen, D. Levesque, and J. J. Weis, "Self-diffusion in the two-dimensional, classical electron gas," Phys. Rev. Lett. 43, 979–982 (1979).
- D. Hirchfeld, Y. Radzyner, and D. C. Rapaport, "Molecular dynamics studies of granular flow through an aperture," Phys. Rev. E **56**, 4404–4415 (1997).
- W. G. Hoover, *Molecular Dynamics* (Springer-Verlag, 1986) and W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, 1991).
- K. Kadau, T. C. Germann and P. S. Lomdahl, "Large-scale molecular-dynamics simulation of 19 billion particles," Int. J. Mod. Phys. C 15, 193–201 (2004).

- J. Krim, "Friction at macroscopic and microscopic length scales," Am. J. Phys. 70, 890–897 (2002).
- J. Kushick and B. J. Berne, "Molecular dynamics methods: Continuous potentials" in Statistical Mechanics Part B: Time-Dependent Processes, Bruce J. Berne, ed. (Plenum Press, 1977). Also see the article by Jerome J. Erpenbeck and William Wood on "Molecular dynamics techniques for hard-core systems" in the same volume.
- Shang-keng Ma, "Calculation of entropy from data of motion," J. Stat. Phys. 26, 221 (1981). Also see Chapter 25 of Ma's graduate level text, Statistical Mechanics (World Scientific, 1985). Ma discusses a novel approach for computing the entropy directly from the trajectories. Note that the coincidence rate in Ma's approach is related to the recurrence time for a finite system to return to an arbitrarily small neighborhood of almost any given initial state. The approach is intriguing, but is practical only for small systems.
- A. McDonough, S. P. Russo, and I. K. Snook, "Long-time behavior of the velocity autocorrelation function for moderately dense, soft-repulsive, and Lennard–Jones fluids," Phys. Rev. E 63, 026109-1–9 (2001).
- S. Ranganathan, G. S. Dubey, and K. N. Pathak, "Molecular-dynamics study of two-dimensional Lennard-Jones fluids," Phys. Rev. A 45, 5793-5797 (1992).
- Dennis Rapaport, *The Art of Molecular Dynamics Simulation*, 2nd ed. (Cambridge University Press, 2004). The most complete text on molecular dynamics written by one of its leading practitioners.
- John R. Ray and H. W. Graben, "Direct calculation of fluctuation formulae in the microcanonical ensemble," Mol. Phys. 43, 1293 (1981).
- F. Reif, Fundamentals of Statistical and Thermal Physics (McGraw-Hill, 1965.) An intermediate level text on statistical physics with a more thorough discussion of kinetic theory than found in most undergraduate texts. Statistical Physics, Vol. 5 of the Berkeley Physics Course (McGraw-Hill, 1965), by Reif was one of the first texts to use computer simulations to illustrate the approach of macroscopic systems to equilibrium.
- Marco Ronchetti and Gianni Jacucci, eds., Simulation Approach to Solids (Kluwer Academic Publishers, 1990). Another excellent collection of classic reprints.
- James Ringlein and Mark O. Robbins, "Understanding and illustrating the atomic origins of friction," Am. J. Phys. **72** (7), 884–891 (2004). A very readable paper on the microscopic origins of sliding friction.
- Duncan A. Sanders, Michael R. Swift, R. M. Bowley, and P. J. King, "Are Brazil nuts attractive?," Phys. Rev. Lett. 93, 208002 (2004). An example of a simulation of granular matter.
- Tamar Schlick, *Molecular Modeling and Simulation* (Springer-Verlag, 2002). Although the book is at the graduate level, it is an accessible introduction to computational molecular biology.
- Leonardo E. Silbert, Deniz Ertas, Gary S. Grest, Thomas C. Halsey, Dov Levine, and Steven J. Plimpton, "Granular flow down an inclined plane: Bagnold scaling and rheology," Phys. Rev. E **64**, 051302-1-14 (2001). This paper discusses the contact force model, which captures the major features of granular interactions.
- R. M. Sperandeo Mineo and R. Madonia, "The equation of state of a hard-particle system: A model experiment on a microcomputer," Eur. J. Phys. 7, 124–129 (1986).