References for techniques and derivations cited in the course

Recommended texts:

- Frenkel and Smit: Understanding Molecular Simulation: From Algorithms to Applications (Academic Press, 2002).
- Tuckerman: Statistical Mechanics: Theory and Molecular Simulation (Oxford, 1987).
- Allen and Tildesley: Computer Simulation of Liquids (Oxford, 2010).
- Huang: Statistical Mechanics (2^{nd} Ed.) (John Wiley and sons, 1987).
- Van Kampen: Stochastic Processes in Physics and Chemistry (3^{rd} Ed.) (Elsevier, 2007).
- Krauth: Algorithms and Computations (Oxford, 2006).
- Rapaport: The Art of Molecular Dynamics Simulation (Cambridge, 1995).
- Newman and Barkema: Monte Carlo Methods in Statistical Physics (Oxford,1999).
- Press et al.: Numerical Recipes in ?: The Art of Scientific Computing, (Cambridge).

References

[1] Newtonian and Lagrangian mechanics: Tuckerman Ch. 1; Frenkel Ap. A
[2] Statistical mechanics and ensembles: Huang Ch. 6-7, Frenkel Ch. 2, 5.4, 5.6; Tucker 3.1-3, 4.1-4, 5.1-3, 6.1-4 . Allen Ch. 2
[3] Equivalence of ensembles: Huang 7.2; Allen 2.3
[4] Conservation of shadow Hamiltonians: Tuckerman 3.13, Frenkel 4.3
[5] Equipartition and Virial Theorems: Huang 6.4, Allen 2.4, Tuckerman 3.3
[6] Averages with a Nose thermostat: Frenkel 6.1, Tuckerman 4.8
[7] Averages with a Nose-Hoover thermostat: Frenkel App B.2.1; Tuckerman 4.9.4
[8] Constant pressure Molecular Dynamics: Frenkel 6.2 and B3, Tuckerman 5.8-9
[9] Steady state of a Langevin Equation: Van Kampen, chapter 9
[10] Quaternions: Tuckerman 1.11, 3.12
[11] Shake: Tuckerman 3.9 Frenkel 15.1
[12] Multiple timestep algorithms: Tuckerman 3.11, Frenkel 15.3
[13] Evaluation of momentum integral in partition function: Tuckerman 4.6
[14] Indistinguishability: Huang 6.6
[15] Heat capacity: Haung 7.2, Allen 4.4
[16] Multi-histogram reweighting: Ferrenberg and Swensden, Phys. Rev. Lett. 63, 1195-1198 (1989)
[17] Configurational bias Monte Carlo: Frenkel 13.2
[18] Cluster moves in general: Frenkel 14.3
Examples include [19] and Whitelam and Geissler, J. Chem. Phys. 127, 154101 (2007)
[19] Troisi cluster algorithm: Bhattacharyay and Troisi, Chem. Phys. Lett. 458, 210-213 (2008)

[20] Modifying association bias Monte Carlo: Wierzchowski and Kofke, J. Chem. Phys. 114, 8752 (2001).
[21] Clausius-Clapeyron relation: Frenkel 9.2
[22] Combining windowed umbrellas: Tuckerman 8.8
[23] Rosenbluth Forward Flux Sampling: Allen, Frenkel and ten Wolde, J. Chem. Phys. 124, 024102 (2006).
[24] Non-stationary Forward Flux Sampling: Becker, Allen and ten Wolde, J. Chem. Phys. 136, 174118 (2012).
[25] Transition Path Sampling acceptance factors: Tuckerman 7.7; Frenkel 16.4.2; Dellago, Bolhuis and Geissler, "Transition Path Sampling", Advances in Chemical Physics, 2002.
[26] Transition Interface Sampling acceptance factors: van Erp and Bolhuis, J. Comp. Phys. 205, 157-181 (2005)
[27] Truncation of potentials: Frenkel Ch. 12
[28] Ewald sums and long-range interactions: Tuckerman Ap. B Frenkel Ch. 12; Allen 5.5
[29] Neighbour and cell lists: Tuckerman Ap. B; Frenkel Ap. F; Allen 5.3
[30] Nose and Nose-Hoover problems in periodic boundary conditions: Tuckerman 4.9.4 Frenkel Ap. B.2; Cho, Joannopouluos and Kleinman, Phys. Rev. E 47, 31345-3151 (1993)
[31] Nose-Hoover chains: Tuckerman 4.10 Frenkel 6.1.3
[32] Virial pressure correction in periodic boundary conditions: Louwerse and Jan Baerends, Chem. Phys. Lett. 421, 138-141 (2006)
[33] Dissipative Particle Dynamics: Frenkel Ch. 17