Boulder lecture
Computer simulations of glass-forming liquids

Ludovic Berthier, July 2017

LECTURE 1 – The classic book for molecular dynamics simulations of liquids is "Computer simulations of liquids" by Allen and Tildesley (OUP). The historical figures came from the following papers: 1) Roux, Barrat, Hansen, J. Phys.: Condens. Matter **1**, 7171 (1989). 2) Kob and Andersen, Phys. Rev. Lett. **73**, 1376 (1994). 3) Brambilla, El Masri, Pierno, Petekidis, Schofield, Berthier, and Cipelletti, Phys. Rev. Lett. **102**, 085703 (2009). The figure containing the 4 estimates of the configurational entropy comes from the preprint: Berthier, Charbonneau, Coslovich, Ninarello, Ozawa, and Yaida, arXiv:1704.08257 Classic textbooks that I like for liquid state theory and statistical mechanics are: "Theory of simple liquids" by Hansen and McDonald, and "Introduction to Modern Statistical Mechanics" by Chandler.

LECTURE 2 – A book I like for Monte Carlo simulations is "Monte Carlo methods in statistical physics" by Newman and Barkema (OUP). A review on the potential energy landscape approach is: Sciortino, J. Stat. Mech: Theory and experiments P05015 (2005). The mysteries of the mixing entropy in the glass context are in Ozawa, Berthier, J. Chem. Phys. **146**, 014502 (2017). The event-chain algorithm is Bernard, Krauth, Wilson, Phys. Rev. E **80**, 056704 (2009). The swap algorithm is explained and optimised in Ninarello, Berthier, and Coslovich, Phys. Rev. X **7**, 021039 (2017).

LECTURE 3 – The Wang Landau algorithm is reviewed in Landau, Tsai, and Exler, Am. J. Phys. **72**, 1294 (2004). The Franz Parisi potential is in Franz and Parisi, Phys. Rev. Lett. **79**, 2486 (1997), and its equilibrium measurement is in Berthier, Phys. Rev. E **88**, 022313 (2013). Umbrella sampling and histogram reweighting are explained in Newman and Barkema. Another classic textbook for these topics is "Understanding molecular simulations" by Frenkel and Smit (Academic Press). A physical discussion of the point-to-set lengthscale is in Biroli, Bouchaud, J. Chem. Phys. **121**, 7347 (2004). The numerical method to get it using parallel tempering is explained in Berthier, Charbonneau, and Yaida, J. Chem. Phys. **144**, 024501 (2016).