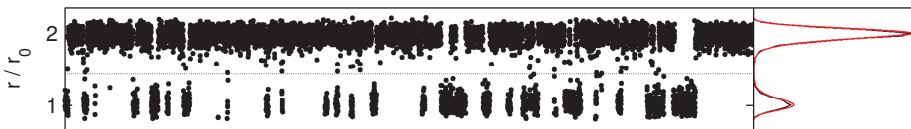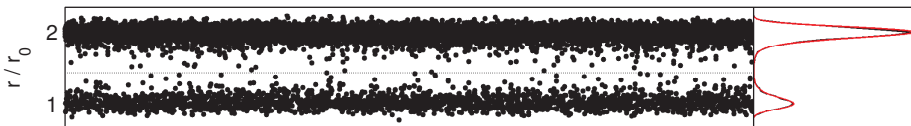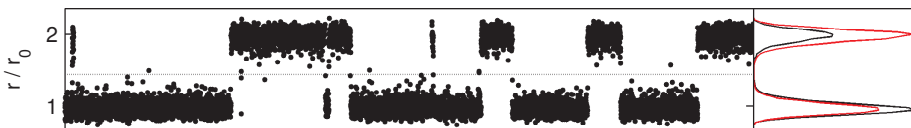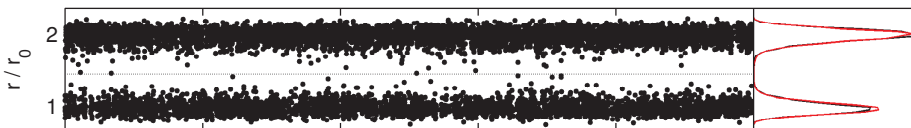vacuum MD ($\tau = 59.2$)

vacuum MD + MC ($\tau = 0.0$)

solvent MD ($\tau = 299.8$)

solvent MD + MC ($\tau = 355.0$)

solvent MD + 2048−step NCMC ($\tau = 4.0$)

MC iteration