

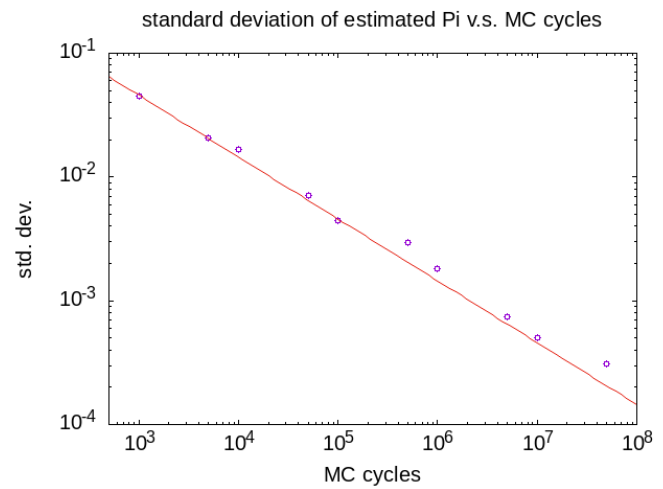
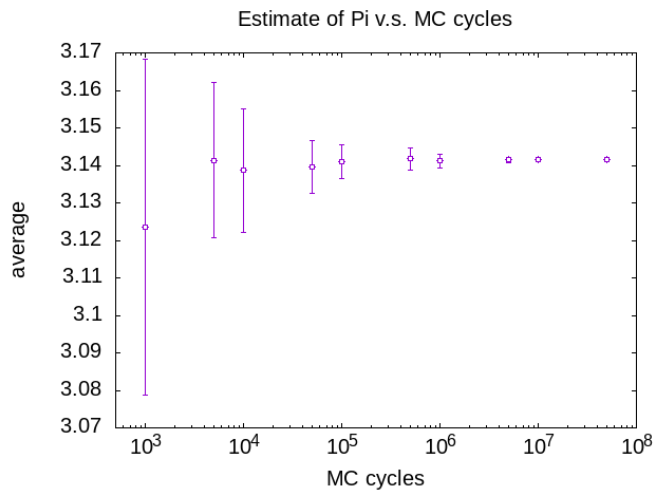
复杂体系分子模拟导论 课程汇报

221505023 张牧原

case study 1

Fig.1 (left) Estimate of π vs MC cycles

Fig.2 (right) Standard deviation of the estimation of π vs MC cycles



case study 2

Fig.1 (left) Pressure vs density for L-J fluid at $T=1.2$ and $2.0 \epsilon/k_B T$

Fig.2 (right) Pressure vs density at $T=2.0 \epsilon/k_B T$ with and without detailed balance

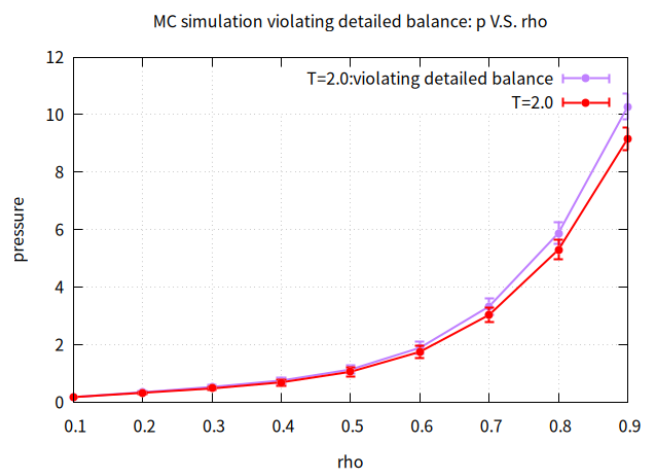
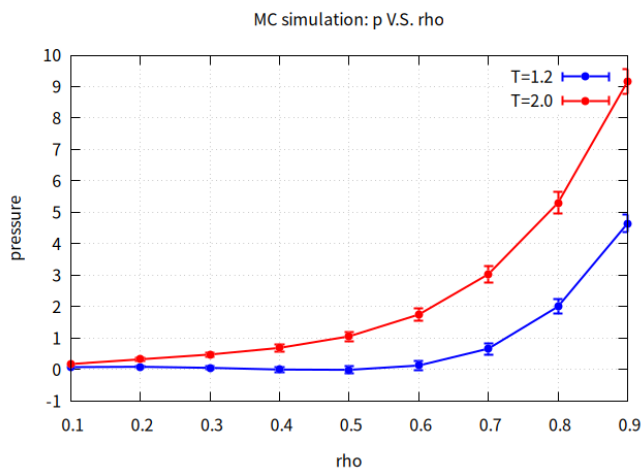
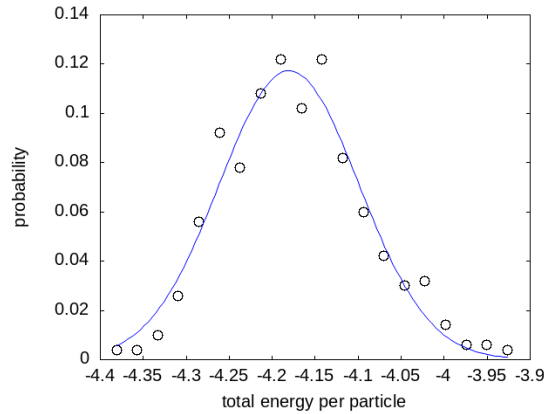


Fig.3 Distribution of the total potential energy per particle at $T=2.0 \epsilon/k_B T$, $\rho=0.9 \sigma^{-3}$



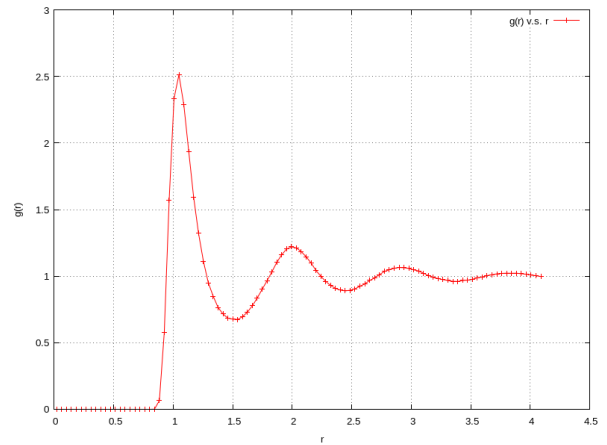
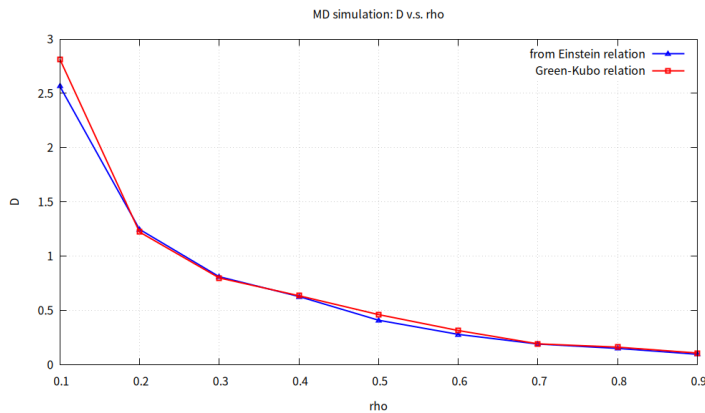
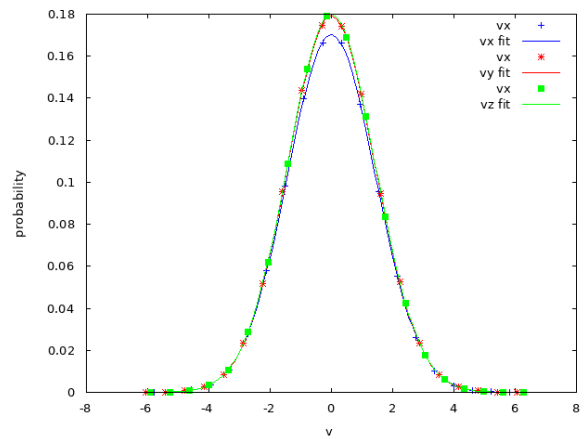
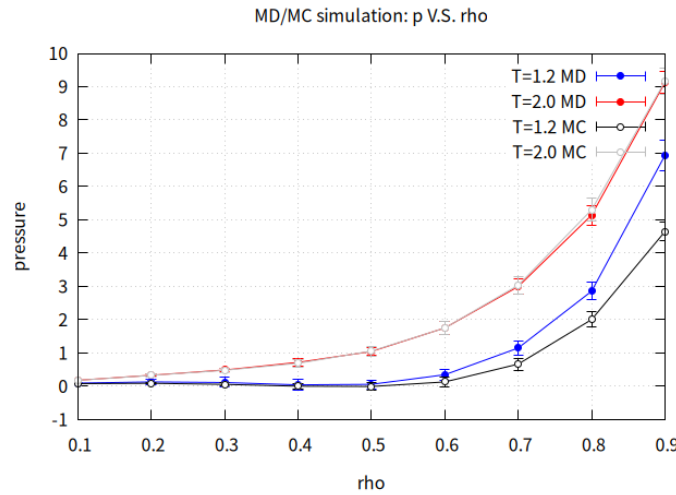
case study 3

Fig.1 (top left) Pressure vs density for L-J fluid obtained from MD & MC simulation at $T=1.2$ and $2.0 \epsilon/k_B T$

Fig.2 (top right) Distributions of v_x , v_y , v_z for L-J fluid at $T=2.0 \epsilon/k_B T$, $\rho=0.9 \sigma^{-3}$

Fig.3 (bottom right) Radial distribution function for L-J fluid at $T=2.0 \epsilon/k_B T$, $\rho=0.9 \sigma^{-3}$

Fig.4 (bottom left) Diffusion coefficient D vs density for L-J fluid at $T=2.0 \epsilon/k_B T$, $\rho=0.9 \sigma^{-3}$ from MSD and auto-correlation function



case study 5

Fig.1 (left) Excess pressure of water vs density obtained from dissipative particle dynamics simulation of pure water system

case study 6

Fig. 1 (right) Tension of DMP bilayers as a function of area per particle

