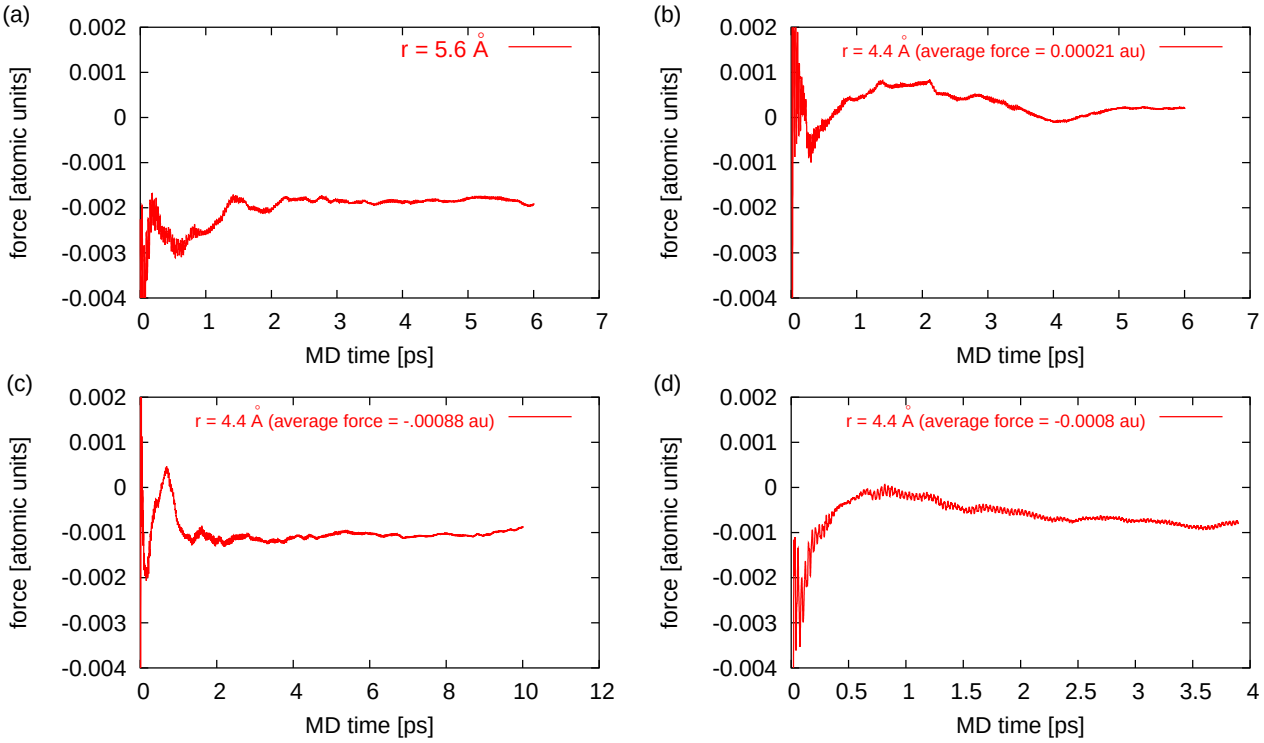
(a)
r = 5.6 Å
force [atomic units]
MD time [ps]
(b)
r = 4.4 Å (average force = 0.00021 au)
force [atomic units]
MD time [ps]
(c)
r = 4.4 Å (average force = -.00088 au)
force [atomic units]
MD time [ps]
(d)
r = 4.4 Å (average force = -0.0008 au)
force [atomic units]
MD time [ps]