

Homework 3

1. Monte Carlo (MC) simulations of Lennard-Jones argon

Use the Metropolis Monte Carlo method to calculate the radial distribution function (RDF) in the homework 2. Discuss how to choose a good trial displacement. Is the RDF obtained by MC consistent with the one from MD? Which method is more efficient according to your experience? Why?

12:31 Monday 26th September, 2022