**Methods of Computational Physics - 2022, Assignment No. 06**

(Date: 13 September, 2022; Due Date: 20 September, 2022)

Note: Print and file only the program listings and plots. Do not print output files of the programs, unless specifically asked in the question.

**Q1** Write a program for the Metropolis Monte Carlo simulation of a 1D Lennard-Jones fluid. Use the following parameters (in reduced units): box size $L = 40.0$, number of particles $n = 20$, temperature $T = 0.3$, number of MC cycles $n_{\rm mc} = 5000$, L-J potential cut-off $x_{\rm cut} = 3.0$. Displace particles randomly with an increment $\Delta x \in [-\delta, \delta]$, with $\delta = 0.3$. Use initial configuration where particles are placed on a 1D lattice with a lattice parameter $a$. Make two runs with $a = 0.95$ and $a = 1.12$, and plot the total potential energy $U$ Vs mcs (Monte Carlo cycles) in both cases on the same set of axis. Calculate the average value of $U$ after discarding the first 3000 mcs values.

Answer: Average value of potential energy $\overline{U} = -13.59$.