

# PHY 612 Assignment 1

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## Problem

Write the general Molecular Dynamics code using Verlet algorithm and Velocity-Verlet algorithm. Plot the total momentum (in each direction), total force (in each direction) and temperature as a function of time for both.

## Solution

Codes can be accessed at : MD Code

### Parameters:

- Number of particles = 50
- Size of the box =  $10 \times 10 \times 10$
- Diameter of each particle = 1
- Timestep = 0.001
- Number of timesteps = 100000
- Final temperature = 0.5

# 1 Verlet Algorithm

verlet\_final.f90

## Results

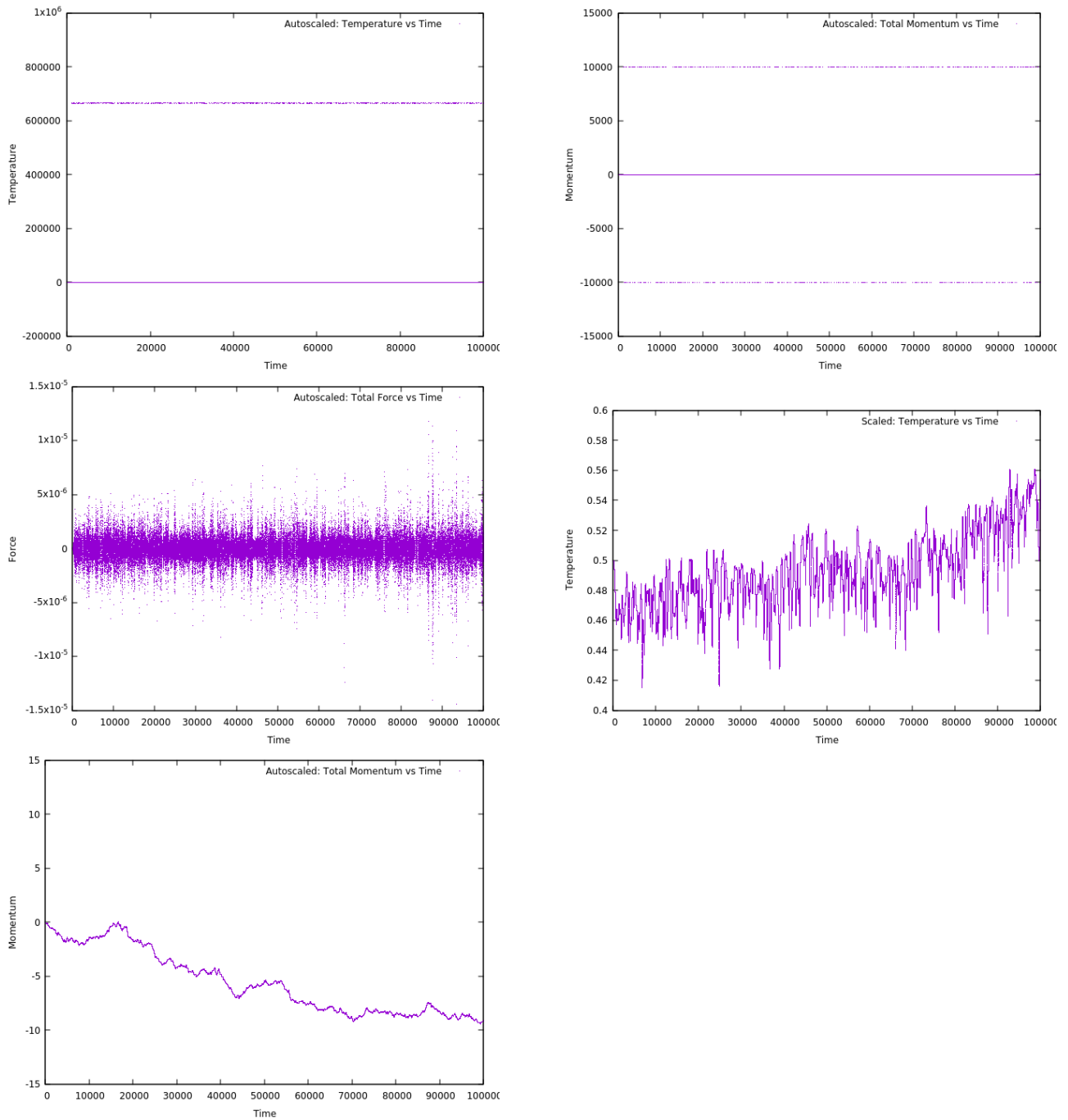


Figure 1: Results for Verlet Algorithm

## 2 Velocity Verlet Algorithm

velocity\_verlet\_final.f90

### Results

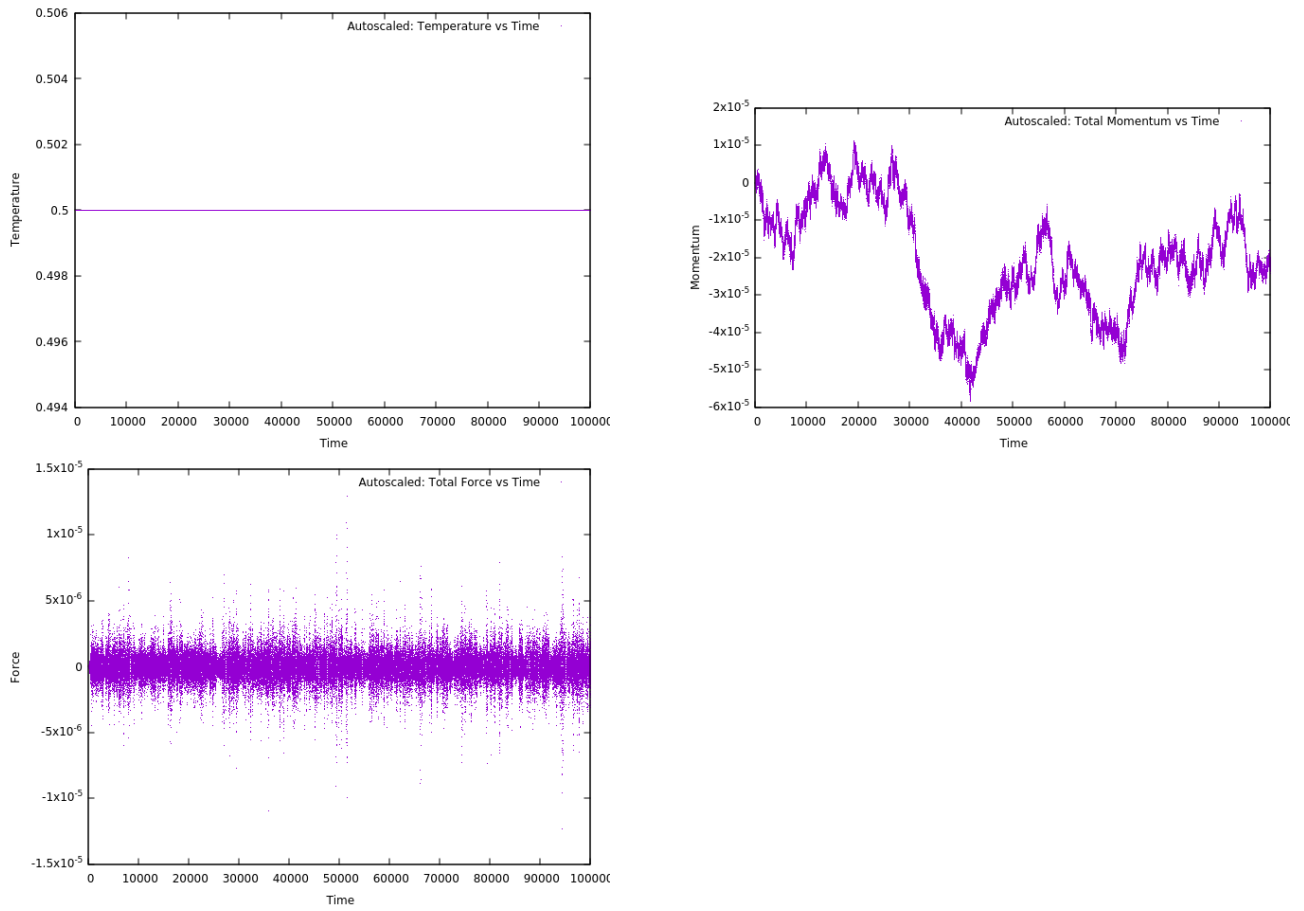


Figure 2: Results for Velocity Verlet Algorithm