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BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

(I Semester 2022-23)

Assignment-01

Computational Physics (PHY F313) **Date: 28-11-2022**

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Important:

1. It is expected that each group will work on the assignment independently. *Learning is more important than copying!*
2. Submit your assignment by 10-12-22 at the latest. Submission after this date will be treated as late submission. In any case after 12-12-22, the codes will not be executed.
3. Upload the assignments on link shared with you. Do not send through email.
4. Compress all the files in one directory as *grpxx_asgtyy.zip*, where, *xx* is the group number, *yy* is the assignment number.

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1. Simulate a random walk in 3D allowing the walker to make steps of unit length in random directions. Don't restrict the walker to sites on a discrete lattice. Show that the motion is diffusive, that is $\langle r^2 \rangle \sim t$. Find the value of the proportionality constant.

2. The potential given between a comet and Sun is given by

$$V(r) = -G\frac{M_S m_c}{r}$$

where r is the distance between the comet and Sun, M_S and m_c are the masses of Sun and comet respectively and G is the gravitational constant. The dynamics of the comet is governed by

$$\mu\frac{d^2\boldsymbol{r}}{dt^2} = f = -GM_S m_c\frac{\boldsymbol{r}}{r^3} \qquad \mu = \frac{M_S m_c}{M_S + m_c} \approx m_c$$

Take the aphelion as the starting point and obtain the comet's whole orbit with Verlet's algorithm. Some data: $x_0 = r_{max} = 5.28 \times 10^{12}$ m, $v_{x0} = 0$, $y_0 = 0$, $v_{y0} = v_{min} = 9.13 \times 10^2$ m/s. If we assume that semi major axis of the orbit, $a = 2.68 \times 10^{12}$ m and time unit as 76 years, in reduced units, we have, $r_{max} = 1.97$, $v_{min} = 0.816$, $\kappa = 39.5$, where $\kappa = -\frac{GMm}{\mu}$.

3. The equipartition theoram states that for a classical system the average energy of each quadratic degree of freedom is $\frac{k_B T}{2}$. Consider the speed of a particle in a classical gas. The distributions of velocity is given by Maxwell distribution as,

$$P(v) = C\frac{v^2}{k_B T}\exp\left(-\frac{mv^2}{k_B T}\right)$$

where $P(v)$ is the probability per unit v of finding a particle with speed v, and C is a constant that depends on the mass of the particle. It is said that if the molecular dynamic method describes the behaviour of a real gas, it should yield velocity and speed distributions that have Maxwell form.

Calculate the speed distributions for a dilute gas and compare your results with the Maxwell distributions. Follow the steps:

   (a) Consider all particles with initial speed as $v = 1$ (in reduced units).

   (b) Run your simulation and after every 10 time steps record the speed distribution by dividing the v range into bins.

   (c) Tabulate the number of atoms whose speed is in the range corresponding to each bin.