End Semester Examination
Methods of Computational Physics (MCP, PH5730)
Dt-12/01/2021

Note:

1a. If you think the question has errors, justify the error, make changes and proceed.

1b. Similarly, if you think the question is incomplete and lack information, then you are free to include additional information with proper justification.

This paper has two parts. Part-A is the written paper. Duration: 2Hrs. To be submitted by 6 PM.

Part-B is the coding part. Write codes for the given questions. Should be submitted by 6 PM on 13/01/2021. Some important points for writing the codes.

(i) Very limited information is provided to write the code. So, this should allow you to apply your own thought process and write a code as universal as possible.
(ii) Write enough comments in your code so that it is understandable.
(iii) Make sure you have output in the form of data or plots. Put them in a separate pdf file.

Mention your output in the form of data or plots (as asked in the question) in a separate pdf file and submit that as well. Compress all the codes and pdf files in a single zip file.

Name the Part-A file as "Part-A- 'Roll-No".pdf

Name the Part-B file as "Part-B- 'Roll-No".zip

Part-A

1. In the class, we have discussed both discrete and fast Fourier transform. Provide a quantitative picture of the time that you save by carrying out fast Fourier transform. Write an algorithm for fast Fourier transform.

2. How will you justify the random walk model and metropolis algorithm to carry out Monte Carlo integration?

3. How can the Crank-Nicolson scheme serve as a predictor-corrector method? Derive the error associated with this scheme.

4. The temperature of a unit square metal plate is subject to the following conditions U (0, y) = $e^{-10(y-0.5)^2}$, 0 < y < 1; U (x, 0) = U (x, 1) = 100x and the right-hand side boundary is insulated. We have to find the steady state temperature of the plate. How will you solve this problem computationally? Write the algorithm.

5. (a) In Molecular Dynamics Simulations, what are the errors if we calculate both velocity and position as a function of time using the standard equations:

$$v_i(t + \delta t) = v_i(t) + a_i(t)\delta t$$

$$r_i(t + \delta t) = r_i(t) + v_i(t)\delta t + \frac{1}{2}a_i(t)\delta t^2$$

Explain the origin of these errors.

How does the accuracy improve through Verlet algorithm? Do you think the Verlet algorithm is free from errors? If not elaborate.

(b) If we want to make a move from NVE ensemble to NVT ensemble, what changes we need to introduce in a MD simulation? What are the quantities conserved in the case of NVT ensemble?

Part-B

Code-1: The Lennard-Jones potential describes the approximate interaction between a neutral pair of atoms and has the form $V_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$, where r is the distance between the atoms, and ε and σ are properties of the potential to be determined. At what value of r, does the potential V_{LJ} equal zero? At what value of r, do the force balance between the atoms, and what is the value of V_{LJ} at this point? Confirm these results writing a root finding program. As a bonus question, what is the minimum energy required to tear the atom pair apart according to the Lennard-Jones potential?]

Code-2: Consider the differential equation y'' + 3y' – 5y = 7x, subject to the boundary conditions y(0) = -20, y(1) = 100. Find a numerical solution to this equation using a direct finite difference method. Ensure at least 4 significant figures of accuracy.

Code-3: Write a code that uses the L-J potential to perform molecular dynamics simulations with NVE conserved. [Microcanonical ensemble]. Apply appropriate boundary conditions and any other restrictions that come to your mind.

Code-4: Part-I: Write a code that produces random walk using normal distribution and Gaussian distribution. Compare you results. Restrict to one dimension.

Part-II: Use the above distribution to calculate $\int_{-\infty}^{\infty} dx\, e^{\left(\frac{-x^2}{4}\right)} x^2$ and estimate the uncertainty in your answer. Study how your results depend upon where the random walker is started and on how thermalization steps you take before beginning the sampling.