Science-2
End-semester examinations
(Spring 2025)
Total Marks: 32
Time: 3hrs.

Q1. For a certain class of distributions, it is possible to create pseudo-random numbers from uniformly distributed random numbers by finding a mathematical transformation (inverse transform method). If z (drawn from uniform distribution) is the random element chosen from 0 to 1, and the target distribution is $f = c\, y^{-\alpha}$, then find the relation between y and z. c is constant. What will happen if $\alpha \leq 1$?

3.5+0.5

Q2a. It is known that pollen grains suspended in water, instead of remaining stationary or falling downwards, would trace out a random zig-zagging pattern. Using Langevin's approach, write down (with explanation) the equation of motion of a pollen grain.

Specify which principles/axioms (of statistical thermodynamics) are required for solving the equation of motion of a large number of pollen grains (particularly, for the calculation of mean-squared displacement ($\langle x^2 \rangle$)).

2+1=3

Q2b. Using these axioms, calculate the mean-squared displacement ($\langle x^2 \rangle$) of a large number of pollen grains.

2.5

Q2c. Imagine a pollen grain is swimming through honey instead of water. What will happen to the mean squared displacement of the grain? Explain.

1

Q2d. Design an experiment using a microscope and camera to track a pollen grain. How would you use image analysis to estimate the diffusion coefficient D? No derivation required. Provide qualitative idea.

1.5

Q3a. $$\frac{dx}{dt} = x - y^2; \ \frac{dy}{dt} = x + y\ ;$$

Find out the fixed points. Check if the fixed points are stable or not. Also, find out the eigenvectors.

1+1.5+1.5=4

(You have to calculate the Jacobian matrix and try to find the eigenvalues and eigenvectors of the Jacobian at the fixed points. No need to proof of the construction of Jacobian).

Q3b. Give an algorithm to numerically solve the above coupled differential equations. **2**

Q4a.

$$S_1 + S_2 \rightarrow S_3 \quad \textit{(rate constants: } C_1\textit{)}$$
$$S_3 \rightarrow S_1 + S_2 \quad \textit{(rate constants: } C_2\textit{)}$$
$$S_3 \rightarrow S_4 + S_2 \quad \textit{(rate constants: } C_3\textit{)}$$

Here S_1 is substrate. S_2 is an enzyme. S_3 is a complex and S_4 is product.

Write the master equations. Explain the terms.

Q4b. Write down the associated mean-field equations (coupled ODE model).

2+2=4

Q5. In a Gillespie stochastic simulation algorithm, how is the time until the next reaction determined? Explain the underlying principle and mathematical formulation. **2**

Q6a: Using the principle of conservation of energy, derive the one-dimensional heat equation that describes the temperature distribution along a thin, insulated rod. Clearly state all assumptions made during the derivation. **4**

Q6b. Prove that $f''(x_i) = \frac{f_{i+1}+f_{i-1}-2\,f_i}{\Delta x^2}$ (Using central difference method). If the heat conduction equation is $\alpha\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t},$ show that $T_i^{j+1} = T_i^j + (T_{i+1}^j + T_{i-1}^j - 2\,T_i^j\ )\alpha\frac{\Delta t}{\Delta x^2}$.

Assume i, j are grid points. **1+2=3**

2 **Q6c.** What physical meaning does the thermal diffusivity α carry in the context of your final equation, and how would increasing it affect the temperature distribution over time? **1**

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