BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: MSc/IMSc **SEMESTER : IV/X**
BRANCH: Physics **SESSION : SP/2025**

SUBJECT: PH514 THEORETICAL & COMPUTATIONAL FLUID DYNAMICS

TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	Draw a flowchart to clarify the general algorithm for solving problems in fluid dynamics.	[5]	1	2
Q.1(b)	The interaction potential acting between two particles is of the Lennard-Jones form, with $a \neq b$: $$U(r) = U_0 \left[\left(\frac{a}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6} \right]$$ Find the interaction force $F(r) = -\partial U(r)/\partial r$ acting between the particles. Show that this force vanishes at the equilibrium distance of $r = 2^{1/6}\,(a^2/b)$.	[5]	1	3
Q.2(a)	Briefly explain the meanings of microcanonical, canonical and grand canonical ensembles. What do you mean by ergodicity of a system (just the statement)?	[5]	2	2
Q.2(b)	Show that the ratio of standard deviation of energy and the mean energy of a system in a canonical ensemble goes to zero in the thermodynamic limit (i.e., number of particles →infinity), thereby establishing its equivalence with the microcanonical ensemble. You can use: $\sigma_E^2 = k_B T^2 C_V$, where the symbols have their usual meanings.	[5]	2	3
Q.3(a)	Describe the Verlet algorithm.	[5]	3	2
Q.3(b)	Given two quaternions a=(a_0,a_1,a_2,a_3) and b=(b_0,b_1,b_2,b_3), show that the quaternion product is given by (a_0b_0 - a.b, a_0b + b_0a + a x b). You can use the properties: $i^2 = j^2 = k^2$ = ijk = -1, ij = -ji = k, jk = -kj = i, ki = -ik = j.	[5]	3	3
Q.4(a)	Explain how you can find the value of π by using Monte Carlo simulations on a plane.	[5]	3	3
Q.4(b)	In a dichotomous Markov process, a particle goes from state x_1 to x_2 with rate 'a', and vice versa with rate 'b'. Write down the master equation and the W-matrix. Show that the sum of the elements in each column of this matrix equals zero.	[5]	3	3
Q.5(a)	Provide an algorithm to calculate autocorrelation functions using the direct method.	[5]	4	1
Q.5(b)	Write a short note on the Fast Fourier Transform method.	[5]	4	2

::::::25/04/2025::::::E