DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF TECHNOLOGY PALAKKAD

PH5018 Computational Physics **Assignment**

Last date for submission: 30/04/2022

Q 1. Consider the following matrix

$$\begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \\ 2 & 1 & 3 \end{pmatrix}$$

Write a code to output (a.) trace (b.) determinant and (c.) inverse of the matrix. **2**

Q 2. Take a polynomial function $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ and evaluate the integral between 0 and 0.8 using the multiple application of trapezoidal rule and Simpson's 1/3 rule. Reproduce the Fig 22.2 in the book (by Chapra and Canale). Play with the precision of the variable and look the changes and comment. **2**

Q 3. Using the Brent's method obtain the root of the following dataset. Illustrate the issue of slow convergence with bracketing method and divergence with open method. **2**

Q 4. Obtain the infinite frequency value, at small time (G_∞) and steady state value (large time) of the following stress-correlation function dataset. Use the fact that the derivative go to zero at these limits. Shear viscosity is given by the Green-Kubo formula,

$$\eta = \frac{V}{k_B T} \int_0^\infty \langle S_{xy}(t) S_{xy}(0) \rangle \, dt$$

Taking reduced temperature $T^* = 0.0525$ and $V^* = 1137.7$, obtain the viscosity from the stress-correlation function data. Obtain the stress relaxation time using the Maxwell's formula given by $\tau_S = \eta / G_\infty$, **3**

Q 5. Consider the following ODE

$$\frac{dy}{dt} = -1000y + 3000 - 2000exp(-t)$$

with y(0) = 0. Compare the explicit multistep method with the implicit single step method. See Fig 26.2 in the book (by Chapra and Canale). Obtain similar plot for comparison.

Q 6. Consider the following function $f(x, y) = ((x - 0.1)^4 + (y - 0.1)^4) - 10 * (x^2 + y^2)$. Obtain the minima in the positive y-quadrant. **6**

Q 7. Compute the radial distribution function g(r) from the following equilibrium dataset. Note that the file contains 1000 configurations and the g(r) has to be averaged over all these configurations. **6**

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