List of COS701 projects (2024)

1. Generate N randomly distributed points inside a three-dimensional cubic box of length L so that each point satisfies the following conditions simultaneously:

   a) The distance (r_{ij}) between any two points i and j is such that $r_{ij} \geq r_1$;

   b) None of the distances, r_{ij}, should lie between r_2 and r_3.

   Assume N = 10,000, L = 60, r_1 = 2.0, r_2 = 2.7 and r_3 = 3.0

2. Write a compute program to calculate the number of n-member irreducible rings that are present in the 3-dimensional random network listed in file 'xyz1000.txt'. Assume n = 3, 4, 5, and 6. A ring is called irreducible when it cannot be further subdivided into a smaller set of rings.

3. Write a computer program (in Fortran/C) to generate the permutation of k distinct integers without using recursion. Explain your algorithm in detail. Discuss the case of non-distinct integers. Assume k = 10 to 15.

4. Write a computer program that uses a linear combination of Gaussian functions to fit the data given in file 'dos.dat'. Discuss the quality of fit (with figures) for a varying number of Gaussian functions. Use of ready-made nonlinear fit routines/functions is permitted but not encouraged.

5. Generate N randomly distributed points inside a three-dimensional cubic box of length L so that the distance between any two points, r_{ij}, is greater than or equal to r_c = 2. Now construct a random matrix H_{ij} from this network as follows:

   a) $H_{ij} = 0$ $\quad$ for $\quad$ $i = j$

   b) $H_{ij} = h_0 \exp\left[-\frac{(r_{ij}-r_1)^2}{2\sigma^2}\right]$ $\quad$ for $\quad$ $i \neq j$,

   Assume $r_1 \in [r_c - 3\sigma, r_c + 3\sigma]$, $\sigma = 0.1r_c$, N = 50,000, L = 100 and h_0 = 1 to 5.

   Calculate the distribution of eigenvalues (ϵ_i) of H and their spacing, $\delta\epsilon = \epsilon_{i+1} - \epsilon_i$ for a few representative values of r_1, σ and h_0.