INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Department of Physics

PH415: Simulation Techniques in Physical Systems
MC Integrations: Test-1

Problem: Packing of hard spheres of radius R randomly inside a cube of side L taking $L = 20 \times R$. Chose a random R between 1 and 2 calling a uniform RNG. Print tjhe value of R. The spheres should not overlap. The condition for no overlap is

$$r_{ij} = \left[(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2\right]^{1/2} \geq 2R$$

Make sure that any part of the sphere is not outside the cube. The number of spheres can be put in is very much less than the number of spheres N_{max} in a hexagonal close pack and it can be expressed as

$$N \ll N_{\max} = \text{Int}\left(\frac{L^3 \times v_h}{4\pi R^3/3}\right)$$

where $v_h = 0.74$ is the volume fraction for hexagonal close pack. Since N is not exactly known, take a stopping criteria for a particular realization as the number of consecutive failure is equal to $10 \times N_{\max}$.

Take $M = 10000$ realizations. Plot a 3-d configuration of one of the realizations. Evaluate the following for each evaluation: (i) note the number of spheres N_k placed inside the cube for the kth configuration, (ii) Calculate $r_{k,\text{mean}}$

$$r_{k,\text{mean}} = \frac{2}{N(N-1)} \sum_{i<j} r_{ij}, \quad \text{for} \quad r_{ij} \geq 2R$$

Store the values N_k and $r_{k,\text{mean}}$ in a file. Plot the distributions of N_k and $r_{k,\text{mean}}$. Obtain the mean and standard deviation of the distributions. Arrange $r_{k,\text{mean}}$ (along with N_k) in ascending order. Plot $r_{k,\text{mean}}$ versus N_k.

Note: Make a report consisting of your plan of work, short algorithm, code, results and discussion. Upload a single pdf file. RNG means random number generator.