Generalize the Monte Carlo simulation program we wrote in class to the case of hard spheres, with diameter d, in three dimensions. We will focus on a density of $\rho^* = 0.5$, where $\rho^* \equiv (N/V)d^3$ is the dimensionless number N of particles per unit volume $V = L^3$.

Note #1: The Monte Carlo sampling strategy we discussed in class requires an initial configuration that is free of overlapping particles. At $\rho^* = 0.5$, this constraint can be satisfied very simply, by placing particles on a cubic lattice. For example,

```
count=0;
for (i=1; i<=Nside; i++) {
  for (j=1; j<=Nside; j++) {
    for (k=1; k<=Nside; k++) {
      count++;
      x[count] = i*L/Nside;
      y[count] = j*L/Nside;
      z[count] = k*L/Nside;
    }
  }
}
```

where `Nside` $= N^{1/3}$. (With this approach you should limit attention to systems comprising a number of particles that is a perfect cube, e.g., $N = 64, 125, \ldots$)

Note #2: When applying periodic boundary conditions in three dimensions, be sure to subtract off the appropriate number of factors of L in each direction, e.g.,

```
deltax -= L*round(deltax/L);
deltay -= L*round(deltay/L);
deltaz -= L*round(deltaz/L);
```

before calculating the squared distance

```
deltar2 = deltax*deltax + deltay*deltay + deltaz*deltaz;
```

between each pair of particles.

Note #3: The magnitude of particle displacements is an important parameter to optimize in Monte Carlo simulations. As a rough guide, useful displacements should allow you to accept roughly one half of the trial moves you propose. By performing short simulations with a variety of displacement sizes (and computing the fraction of moves that are accepted), you should be able to quickly identify a useful value.

You are encouraged to discuss programming problems and strategies with your classmates, but each student should develop and maintain his/her own code. Each student should also of course generate his/her own data and make his/her own plots.

Do not turn in printouts of your code. Your answers to the questions below will be sufficient evidence that you have created a working simulation.

1. Perform a Monte Carlo simulation of $N = 1,000$ hard spheres, tracking the position of a particular particle (choose any one you like!) over $1,000$ sweeps. Turn in a plot of the x, y, and z coordinates of this particle as functions of the number of sweeps elapsed (i.e., "time").

2. This problem concerns the occupation statistics of a small spherical probe volume v in a fluid of hard spheres. We will take the diameter $D = 0.9d$ of the probe volume to be so small that at most one particle's center could lie within v. In other words, since $D < d$, the number N_v of hard spheres whose center lies inside the probe volume can only take values of $N_v = 0$ or $N_v = 1$.

   (i) Using a Monte Carlo simulation of $N = 1,000$ hard spheres at density $\rho^* = 0.5$, compute the probability $P(N_v = 0)$ that a probe volume with diameter $D = 0.9d$ is vacant.

   (ii) Note that for such a small probe volume, $P(N_v) = 0$ for all $N_v > 1$. Using this fact, write a simple relationship between the probabilities $P(N_v = 0)$ and $P(N_v = 1)$.

   (iii) Again exploiting the small size of the probe volume, write a simple relationship between the average number $\langle N_v \rangle$ of particles in v and the probability $P(N_v = 1)$ of single occupancy.

   (iv) Combining your results, together with the exact relation $\langle N_v \rangle = \bar{\rho} v$ derived in class, calculate $P(N_v = 0)$ in terms of the bulk density $\bar{\rho} \equiv N/V$ and probe volume v.

   (v) For the case $D = 0.9d$ and $\rho^* = 0.5$, numerically evaluate your expression for $P(N_v = 0)$. Compare your answer with the simulation result from part (i).

3. In this problem you will explore the occupation statistics of somewhat larger probe volumes, again using Monte Carlo simulations of $N = 1,000$ hard spheres at density $\rho^* = 0.5$. Perform each of the calculations described below for spherical probe volumes of diameter $D = 2d, 3d$, and $4d$.

   Note: By imposing periodic boundary conditions, we simulate a fluid that is spatially uniform on average. You should therefore obtain equivalent results regardless of where you place the probe volume. Take advantage of this fact by accumulating statistics from probes centered at a large number of locations, e.g.,

   ```
   for (i=1; i<=40; i++) {
     for (j=1; j<=40; j++) {
       for (k=1; k<=40; k++) {
         probex = i*L/Nside;
         probey = j*L/Nside;
         probez = k*L/Nside;

         /* calculate number Nv of particles whose centers lie
         within a distance D/2 of (probex,probey,probez) */

         hist[Nv]++;
       }
     }
   }
   ```

   With this trick, you should be able to generate respectable averages and histograms with roughly $10,000$ sweeps. (You will probably want to discard data from the first ~ 500 sweeps if your initial configuration was not already equilibrated.)

   (i) Compute the average number of hard spheres whose center lies inside the probe volume. Plot your results for $\langle N_v \rangle$ as a function of the probe size D, along with the expected result $\bar{\rho} v$.

(ii) Compute the variance of N_v, i.e., $\langle \delta N_v^2 \rangle = \langle N_v^2 \rangle - \langle N_v \rangle^2$. Plot $\langle \delta N_v^2 \rangle$ as a function of the probe size D.

(iii) Compute a normalized histogram $P(N_v)$ of the occupation number N_v. Plot $\ln P(N_v)$ as a function of N_v. (Values of N_v for which you have gathered fewer than 100 counts are not statistically well represented. Do not include them in your plots.) Compare your result with a Gaussian distribution

$$p_G(N_v) = \left(2\pi \langle \delta N_v^2 \rangle\right)^{-1} \exp\left[\frac{-(N_v - \langle N_v \rangle)^2}{2\langle \delta N_v^2 \rangle}\right] \tag{1}$$

with the same mean and variance as $P(N_v)$. Include plots of $\ln p_G(N_v)$ alongside your simulation results, and comment on the quality of agreement.

(In Eq. 1, we have normalized and parameterized $p_G(N_v)$ by treating N_v as a continuous variable ranging from $-\infty$ to ∞. You are welcome to take a more careful approach, accounting for the fact that N_v is discrete and non-negative, but it is not necessary for this assignment.)