MSE 515/APC 515/CHM 559: RANDOM HETEROGENEOUS MATERIALS

Prof. S. Torquato

HOMEWORK #8

Write a computer program to carry out a Monte Carlo simulation of the **particle exclusion probability** $E_P(r)$ in $\mathbb{R}^2$ for two different ensembles of disks. The simulation consists of the following 2 steps:

1. **Generation of Realizations**

   Place randomly and sequentially congruent disks of radius R into a square fundamental (unit) cell of side length L with periodic boundary conditions at some number density ρ. Consider two different types of particle additions:

   a) Spatially Uncorrelated (Fully Penetrable Disks) ($\lambda = 0$) Here disks of radius R are placed randomly and sequentially without regard to overlap.

   b) Spatially Correlated (Totally Impenetrable Disks) ($\lambda = 1$)
   Here an attempted particle addition is rejected if it overlaps an existing particle. An attempted particle addition is accepted when the overlap condition is not violated. This is the **random sequential addition** (RSA) process described in Chapter 3.

2. **Sampling**

   - For each of the ensembles given above, compute the **particle** exclusion probability function $E_P(r)$ as a function of r for $\phi_2 = 0.2$ and 0.5. Recall that for fully penetrable disks $\phi_1 = \exp(-\rho\pi R^2)$ and for totally impenetrable disks $\phi_1 = 1 - \rho\pi R^2$, where $\rho = N/A$ ($A = L^2$).
   - Compare your results for $\lambda = 0$ and $\lambda = 1$ for each volume fraction by plotting your calculations (using graphics software) for $E_P(r)$. Include in each of these two plots the corresponding analytical expressions for $E_P(r)$ for fully penetrable disks and **equilibrium** hard disks given in Chapter 5. **Discuss possible errors that may arise in your simulations**.
   - Finally, numerically differentiate your results for $E_P(r)$ for all cases to get corresponding estimates of $H_P(r)$ using the appropriate relationship. Plot your results and again compare them to corresponding analytical expressions for $H_P(r)$ for fully penetrable disks and **equilibrium** hard disks given in Chapter 5.

Remarks:

• You must employ a sufficient number of particles N (at least 1000) to obtain results that apply in the thermodynamic limit.

• To generate smooth curves, you must also average your results over a sufficient number of configurations.

• Consult Chapter 12 for helpful details (e.g., periodic boundary conditions) and references.