Series 3

1. Problem 2.23 from the textbook (1d only)

2. Simulations of a single-species annihilation reaction on hypercubic lattices as a function of the lattice spatial dimension d.

Consider lattice dimensions $d \leq 3$, and choose a lattice size L large enough (such that the results do not depend on L). For $d = 2, 3$ hypercubic lattices. Apply periodic boundary conditions in all lattice directions. Introduce the lattice site occupation variable

$$\rho(x,t) = 1, \;\; if\ x\ is\ occupied\ \ 0, if\ \ x\ is\ empty$$

Assume $\rho(x, t = 0) = 1$, for all x.

<u>Simulation approach 1</u>

At each time step Δt

1. Choose one lattice site randomly
2. A) If the chosen lattice site is occupied by a particle ($\rho = 1$ on that site), that particle performs one random jump to one of the neighboring lattice sites with the probabilities

   $$p = \frac{1}{2}\ in\ d = 1\,, \qquad \frac{1}{4}\ in\ \ d = 2, \qquad \frac{1}{8}\ in\ \ d = 3$$

   If the new position is occupied, annihilate both particles (set $\rho = 0$ on the sites from where the particle started and ended). If the new position is empty, the particle stops at the new position. Go to item #3 below.
   B) If the chosen lattice site is empty, do nothing and go to item #3 below.
3. Update time $t_{n+1} \;= t_n + \Delta t$

Plot the average (over many simulations with different seeds for the random number generator) number density $\rho(t) = \frac{N\_occupied(t)}{L^d}$ as a function of time for $d = 1, 2, 3$. In this approach $\Delta t \propto \frac{1}{L^d}$.

<u>Simulation approach 2, “rejection free”</u>

A randomly chosen lattice site must be occupied. All the other steps are as above. For this you will need at each time a list of occupied lattice sites (keep in mind that the list is time-dependent).

In this approach the time step $\Delta t(t) \propto \frac{1}{\rho(t)}\frac{1}{L^d} = \frac{L^d}{N_{occupied}(t)}\frac{1}{L^d} = \frac{1}{N_{occupied}(t)}$.

Plot the average number density $\rho(t) = \frac{N\_occupied(t)}{L^d}$ as a function of time for $d = 1, 2, 3$.