

HW 6

Due date: 15/3/18

In many biological processes random walk motion and/or directed transport are utilized as search strategies. During immune cell activation, for example, immune receptors (such as B or T lymphocyte receptors) are initially clustered by random diffusive motion but later utilize directed transport to reach locations of free energy minimum. The following problem is designed to study some aspects of receptor motion on a cell surface.

Use kinetic Monte Carlo method to simulate (one may use MATLAB or similar) the random walk diffusion of molecules (random walkers) on a two-dimensional integer lattice. Random walkers are allowed only four moves: to any of the four nearest neighbor sites. The variable r denotes the displacement from the initial position of random walkers.

Statistical data analysis: compute $\langle r \rangle$ (mean displacement) and $\langle r^2 \rangle$ (mean square displacement) from this simulation (average is computed over molecular trajectories). You may simulate the random walk diffusion starting with 100 randomly placed molecules on a 50×50 lattice (use reflective boundary).

Challenge question: Estimate the probability distribution $P(r)$ for a set of time of points (at least three).