MDI 505 **Homework 2** Spring 2019

Due February 19, 2019

In class, we wrote a code for a random walk on a 2D square lattice. Now, we want to expand this to consider a random walk through more realistic crystal structures. Repeat the analysis from class, but instead model the random walk for a simple cubic structure (3D structure with atoms on the corners of a cube – ie. 1 atom per unit cell) and face centered cubic (3D structure with atoms on the corners of a cube and atoms in the center of each face – ie. 4 atoms per unit cell). Compare the mean square displacement and probability of displacement with what we calculated in the lecture. Assume that every lattice site contains the same type of atom / element, and that the lattice constant is equal to 1.