Computational Modeling (Physics 2010)

Final Project

Due: Tuesday, April 18, 2023 at 6pm

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13 April 2023

Please submit the solutions as a single tar or zip file—including the Python codes and all written answers as a pdf—by email to sirker@physics.umanitoba.ca.

Crystal growth Models (100 points)

General remarks: The final project will be more open ended than a typical assignment, i.e., you have to figure out how to model the problem yourself. This is part of the project.

In the final project, we want to consider the growth of a crystal. We have a solution in which molecules perform Brownian motion (random walks). When a molecule gets close to an initial seed (an impurity which sits at a fixed position) then the molecule sticks, the crystal growths, and other molecules will get stuck at the enlarged crystal in the future. To simplify things, we will consider two-dimensional models. The task is to develop two models: (i) An agent-based model in which the particles (agents) move randomly in continuous space, i.e., the distance by which each particle moves at each time step is not fixed in length but rather follows some random distribution. (ii) A celular automaton, in which the particles perform two-dimensional random walks on a grid.

a) (20 pts) Describe how you will create the agent-based model and the cellular automaton, what the essential steps in each model are, and why you have chosen these implementations.

b) (30 pts) Write a code for the agent-based model.

c) (30 pts) Write a code for the cellular automaton.

d) (20 pts) Show at least one example for a crystal you have grown with the agent-based model and with the cellular automaton. Discuss if and why there are any differences between the results of the two models and how the results depend on the parameters of each model.