HOMEWORK 4: MC AND PFM

Due electronically March 23 at midnight

As we've discussed in class, all of the mesoscale models we have worked with – cellular automaton, Monte Carlo, and phase field – can be adapted to simulate the same microstructural evolution phenomena. Thus, the choice of which model to use is up to you, the modeler.

In this homework, you will explore the Monte Carlo and phase field models for solidification, and you will compare them to each other and to the CA and JMAK models you examined last week. For this assignment, you will need:

- **mcpm.py**: python file where you will implement the Monte Carlo Potts model
- **pfm.py**: python file with a phase field model solidification code
- **single3.json, random4.json**: JSON files containing input decks for the mesoscale models. You will note that the solid nuclei in these files are not single cells. Both the MC and PFM models require larger critical nuclei to ensure growth.
- You will also use the cellular automaton code you developed in HW3.
- For general clarification questions, please ask publicly on Piazza. For private questions about the specifics of your code, please email your code to the TA's.

1. (8 pts) Implement the functions in mcpm.py. The instructions for each function are given in detail in its docstring.
   - Implement the functions in the order they appear in the file. This way you will gradually build up to the full Monte Carlo Potts Model.
   - For mcpm_slow(), use the metropolis0, delE, and mcpm_step functions in the implementation. This should be easier to implement, but slower.
   - For mcpm.efficient(), do not use these functions. The goal is to implement all steps in the model in a single function to improve the runtime efficiency.
     - You can use the other functions to help debug mcpm_efficient() while writing it. The random states are set up in a way that mcpm_slow() and mcpm_efficient() should produce the exact same outputs for the same given input.
   - Pay attention to the instructions regarding the seeding/use of random states. If implemented correctly the outputs should match the solutions exactly.

2. In class, we have asserted that CA, MC, PFM and JMAK models can simulate many of the same phenomena. Now it's time to provide some evidence. We have applied all of these models to the same nucleation and growth process, specifically solidification. Let's compare the outcomes.

(a) (4 pts) Using the CA, MCPM, and PFM models with input file **single3.json**, grow a single nucleus in the center of the system until it occupies about a third of the area of the system. Attach a snapshot of the final CA, kMC, and PFM nuclei. For each method, comment on the shape and interface character of the growing nucleus.

(b) (6 pts) Each of the methods has a different time scale, but all should be proportional to real time, and thus to each other. We will approximate the nuclei as growing circles, with the following ideal growth equation:

$$A_{nuc} = \pi t^2 + A_0$$

where t is the time and A_0 is the initial area of the nucleus at $t = 0$. For the CA and MC models, $A_0 = 5$, and for the PFM, $A_0 = 0$ due to the diffuse interface. Note that t will be proportional to, but not necessarily equal to, the number of simulation timesteps performed; that is, $t \sim \alpha$**timesteps* where α is a proportionality constant.

For each of the three methods, find and report the proportionality constant α that minimizes the absolute error between the ideal growth equation and the simulation. Plot the single nucleus growth curves (area transformed vs. scaled time) for all three methods on a single plot. Do the data collapse to a single curve (within reasonable error)?

(c) (4 pts) Now simulate site-saturated nucleation by using the CA, MCPM, and PFM models with input file **random4.json**. Attach snapshots of the CA, kMC, and PFM systems at about 20% and 100% solidified. How do the intermediate structures differ from each other? How do the final structures differ from each another?

(d) (6 pts) For the multiple nucleus simulations, the JMAK equation should be a good approximation of the growth behavior:

$$A_{JMAK} = A_{tot}\left[1 - \exp\left(-\frac{NA_{nuc}}{A_{tot}}\right)\right]$$

where N is the number of initial nuclei, A_{tot} is the total area, and A_{nuc} is the time-dependent area of a single nucleus in isolation (as given in part (b)).

Using the same time proportionality constants as in part (b), plot the area transformed vs. scaled time for all three methods and the JMAK on a single plot. Do the data collapse to a single curve (within reasonable error)?

(e) (4 pts) For all four models (CA, MC, PFM, JMAK), give two advantages and two disadvantages. If you were asked to simulate a solidification process, which would you choose?