HOMEWORK 3: CA

Due electronically March 13 at midnight

Cellular automata (CA) is one of the two primary discrete mesoscale models (that is, computed on a grid). In this homework, you will explore the CA model for solidification. For this assignment, you will need:

- **twodsol.py**: python file where you will implement the CA model
- **single1.json, single2.json, random1.json, random2.json, random3.json**: JSON files containing input decks for the CA model

1. (8 pts) We will use a 2D cellular automaton to simulate the nucleation and growth of solid crystals in a liquid matrix, i.e. solidification. (Or, you may equivalently consider this to be nucleation and growth of new grains in a deformed matrix material, i.e. recrystallization.) Follow the prompt in the **twodsol.py** docstring to read in initial conditions given in a JSON input deck, construct the CA model, and output the results. Turn in your completed **twodsol.py** file with your solutions filled in (including the modifications made in questions 2 and 3); there is no need to turn in the input or output files you used.

2. For this problem, we will use the CA in its deterministic mode (where the probability of attachment $p = 1$). We are interested in comparing the results of the CA model to a mathematical model for nucleation and growth, the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. For site saturated nucleation (where the nuclei all exist at the start of the process), the JMAK equation for the fraction of material transformed f_{JMAK} is given by:

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

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 (i.e. without impingement). For the sq(1) lattice with deterministic CA growth rules, A_{nuc} is given by

$$A_{nuc} = 2t^2 + 2t + 1$$

where t is the time, measured in CA timesteps starting from $t = 0$. At a given time t, we can compute the disagreement Δf between the CA and JMAK model simply as

$$\Delta f = \left| f_{CA} - f_{JMAK} \right|$$

where f_{CA} is the fraction of material transformed in the CA simulation.

(a) (2 pts) Because it presumes that nuclei impinge, the JMAK model is accurate for a single, isolated nucleus only at early times. Using the input deck given in **single1.json**, estimate the time over which the CA and JMAK models agree to within 2% ($\Delta f \leq 0.02$). Show a plot supporting your conclusion.

(b) (2 pts) Repeat your analysis for the input deck given in **single2.json**. Why do the CA and JMAK models agree closely over a longer time in this case?

(c) (2 pts) The JMAK model is intended for systems with multiple nuclei. Perform CA solidification of the system given in input deck **random1.json**. Make sure to run the simulation to complete solidification. What is the maximum disagreement between the models? Does the disagreement occur early or late in the simulation? Show a plot supporting your conclusions.

(d) (2 pts) Repeat your analysis for the input deck given in **random2.json**. Why do the CA and JMAK models agree more closely in this case?

(e) (2 pts) Again, repeat your analysis for the input deck given in **random3.json**. Compared to the system in **random1.json**, why do the CA and JMAK models agree more closely in this case?

(f) (2 pts) If you were tasked to model solidification of a polycrystalline metal from a melt, which of these models (CA or JMAK) would you choose? Are there different conditions under which one model would be preferred over the other? Discuss.

3. Now, we will revise the model to make the nucleus shapes more realistic (i.e. round). We will use a probabilistic attachment rule to "roughen up" the nucleus interface by not always accepting every state change. Nuclei in the probabilistic CA (pCA) will grow more slowly than in the deterministic CA. Specifically, we expect that if the deterministic nucleus grows at a rate G, the probabilistic nucleus grows at a rate pG where p is the attachment probability. This means that the JMAK model for the probabilistic system predicts

$$f_{JMAK}^{*} = 1 - \exp\left(-\frac{NpA_{nuc}}{A_{tot}} \right)$$

where p is the attachment probability.

(a) (2 pts) Consider the system with a single nucleus, given in **single1.json**. For $p = 0.5$ and 20 timesteps, what is the maximum disagreement between the pCA and JMAK models? (Ignore the disagreement at $t = 0$ – it is an artifact of the fact that we can't have fractional nucleus sizes.) Now run the model again. Do you get a different answer? Why? How might you find the "right" answer?

(b) (2 pts) Perform 10 simulations for the system given in the **random1.json** input deck, again with $p = 0.5$. Estimate the maximum disagreement between the pCA and JMAK models, averaged over 10 runs. Now do the same for **random2.json**. Does pCA follow the same trend that you observed for the deterministic CA in 2(e)?

(c) (2 pts) Now perform 10 simulations of **random2.json** with $p = 0.3$ and $p = 0.8$. Does the disagreement between the pCA and the JMAK model vary with attachment probability p? If so, what is the trend?

(d) (2 pts) If you were tasked to model solidification of a polycrystalline metal from a melt, would you choose a deterministic or probabilistic CA model? Are there different conditions under which one model would be preferred over the other? Discuss.