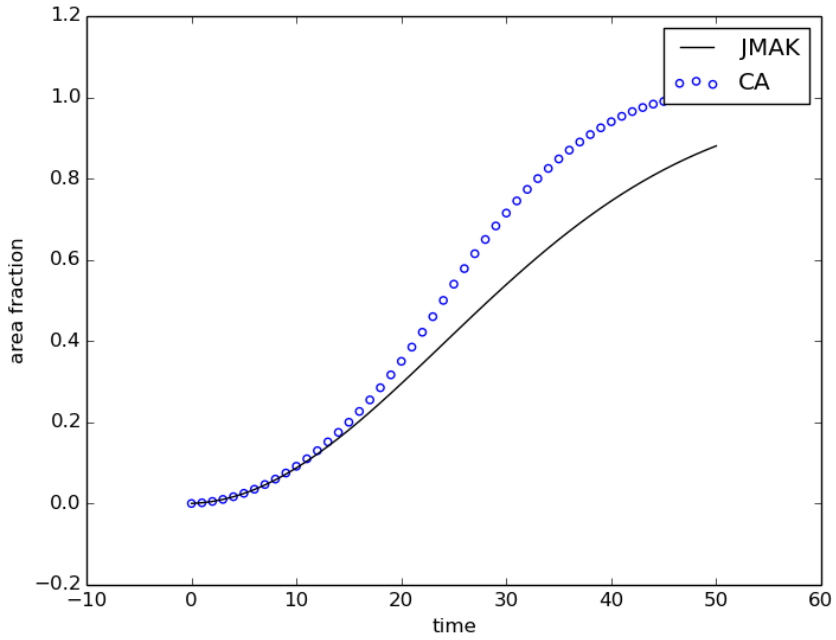
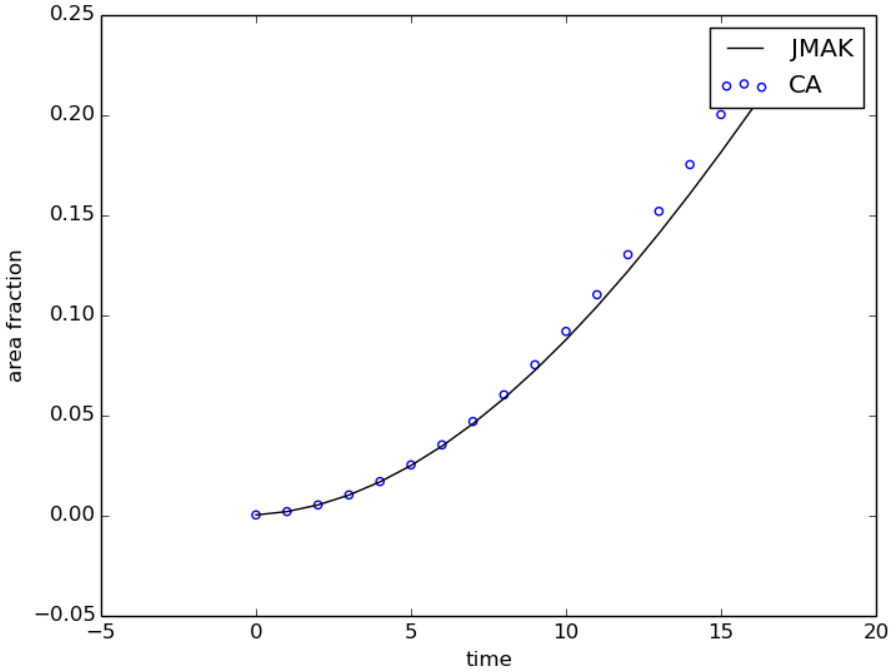
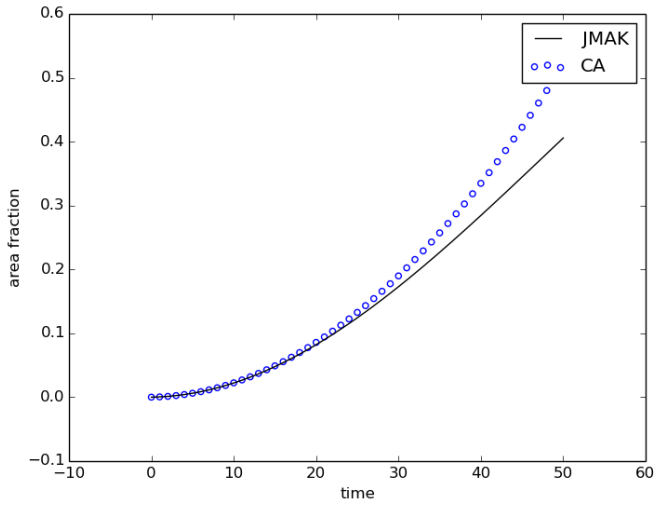
Laura (Kai Sze) Luk
27-734 HW 3

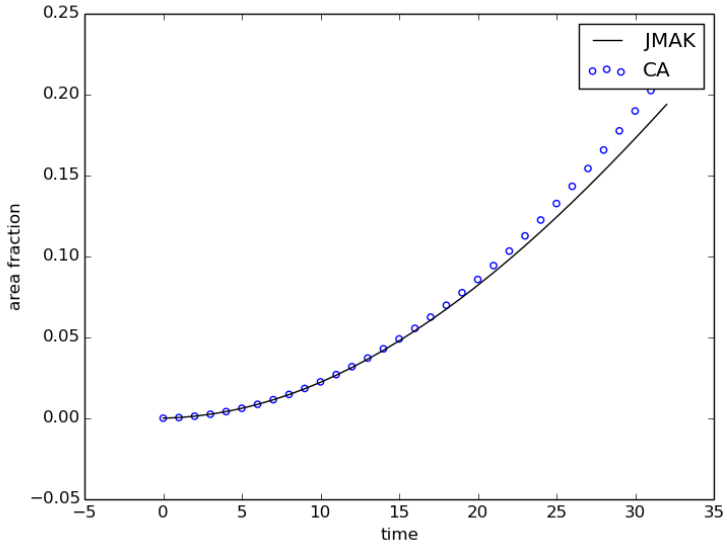
2a) Using input deck in single1.json, the estimated time over which the CA and JMAK models start to disagree from within 2% ($\Delta f > 0.02$) is at time = 16; so the time range over which the 2 models agree to within 2% would be from time = 0 to time = 15-16.
The plots are shown below (top– plotted over entire timespace, bottom– plotted up to time = 16):





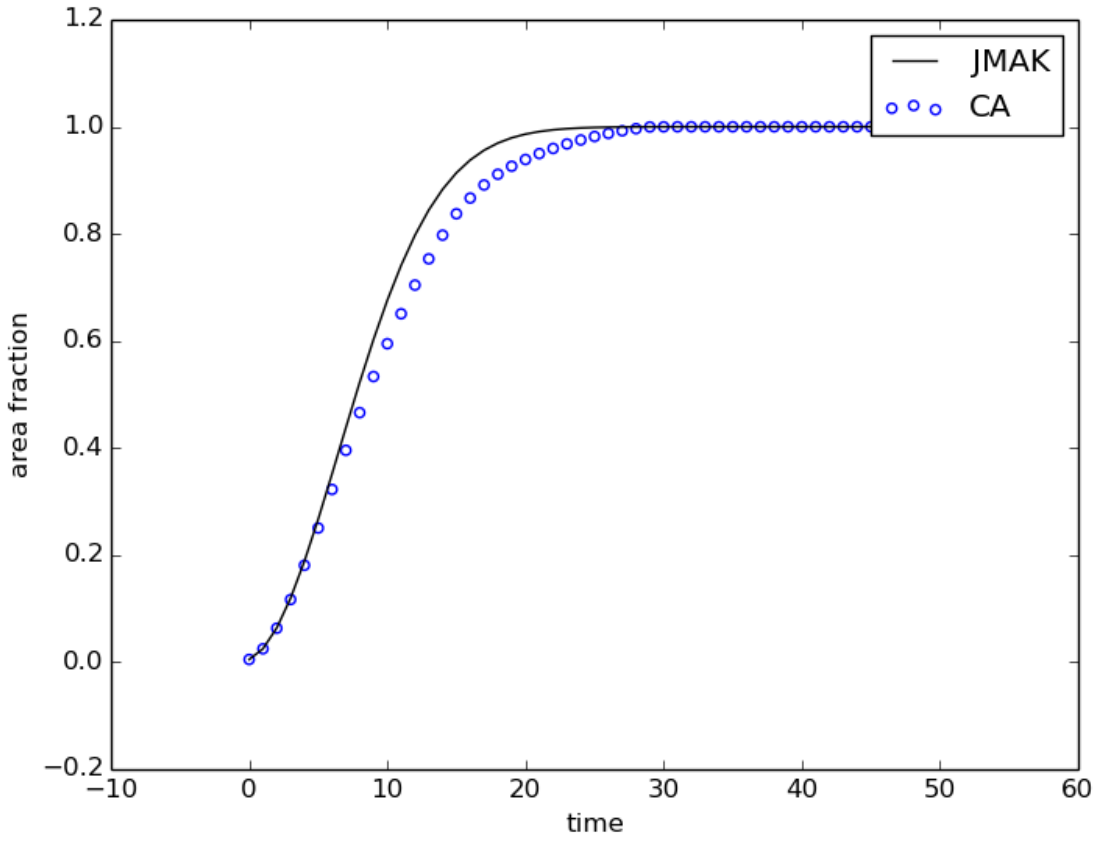
2b) Using input deck in single2.json, the estimated time over which the CA and JMAK models start to disagree from within 2% ($\Delta f > 0.02$) is at time = 32; so the time range over which the 2 models agree to within 2% would be from time = 0 to time = 31-32.
The plots are shown below (top– plotted over entire timespace, bottom– plotted up to time = 32):



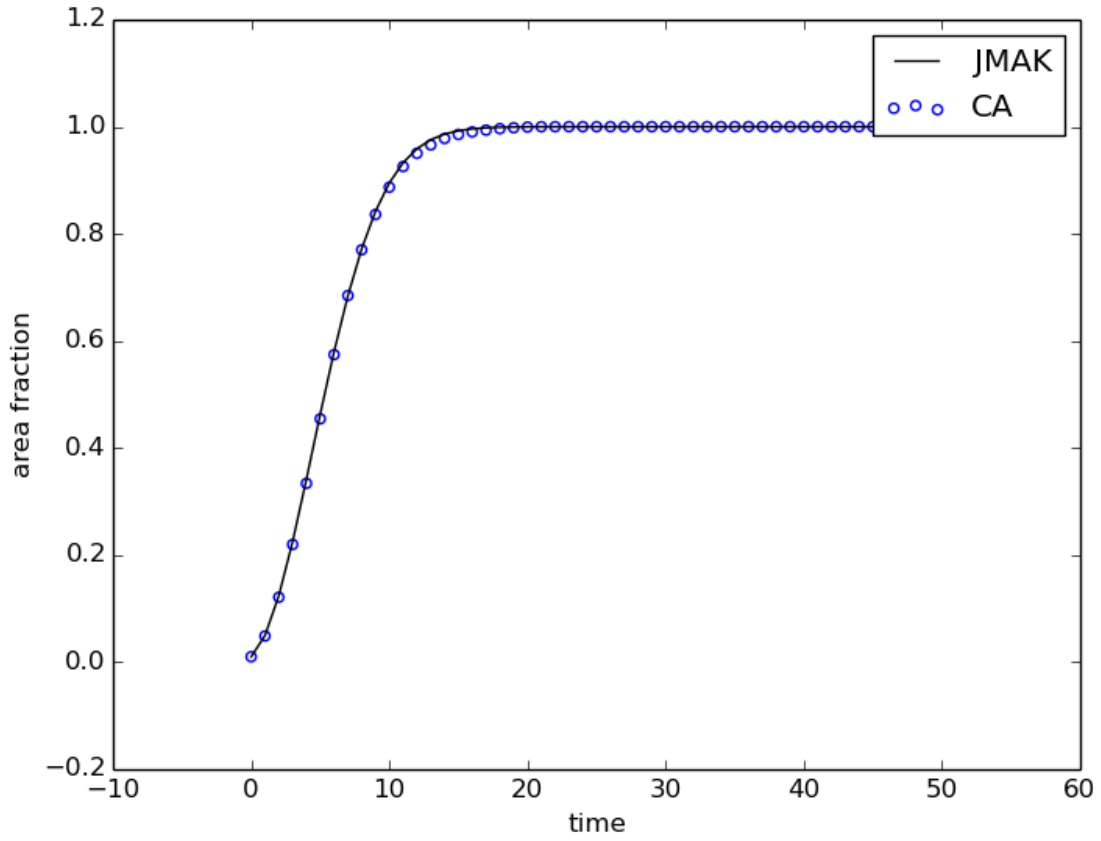


The only difference between the input decks in single1.json and single2.json is that single2.json has an input deck with double the size of that in single1.json (double the rows and columns). Both input decks start off with 1 nuclei, but because the total area is larger in single2.json, the effective area fractions (solid) is lower for both models. The JMAK equation for the area fraction (solidified) results in a smaller value (the value of exp(..) is larger, so 1 – exp(..) is smaller), and the fCA values are much lower due to how sparse the initial grid is. This allows the 2 models to agree over a longer time.

2c) Using the input deck in random1.json, we can see the disagreement occurs early (to middle) in the simulation. The maximum disagreement is 0.093135598525. The plot is shown below:

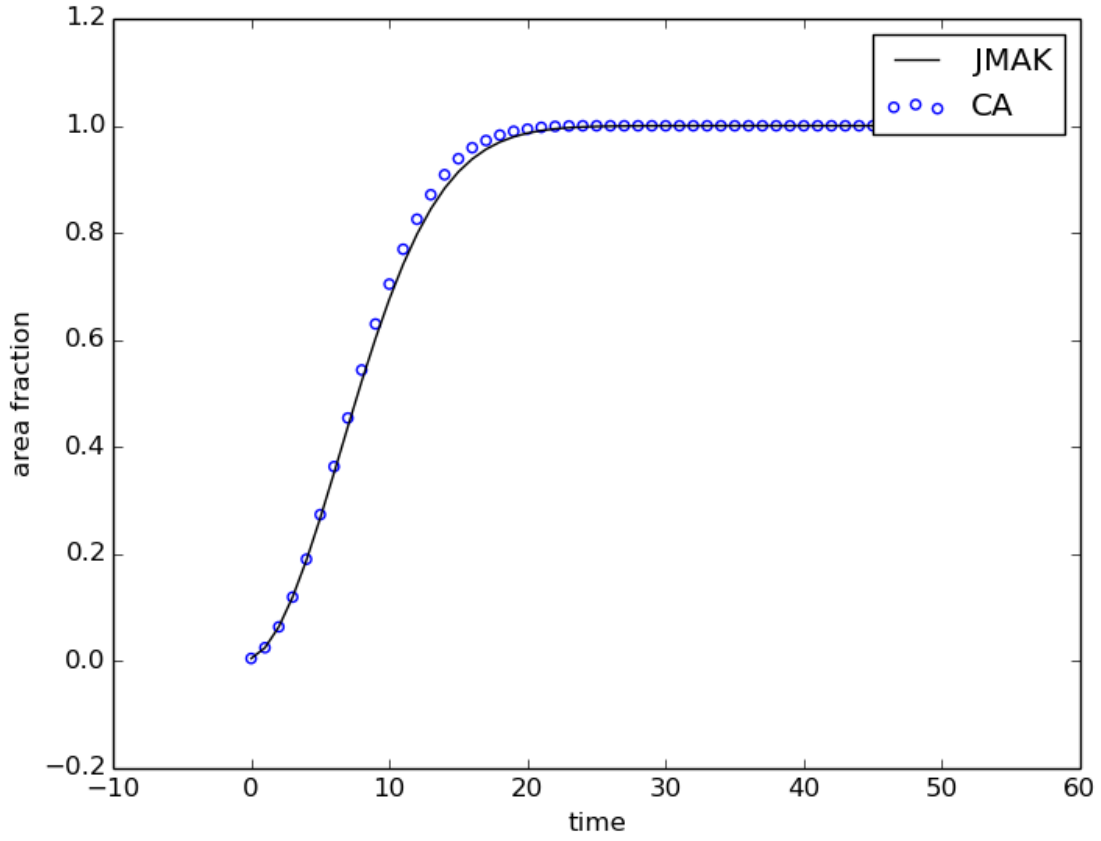


2d) Using the input deck from random2.json, we can see that the CA and JMAK models agree more closely. The maximum disagreement is 0.00973951864534. The plot is shown below:



The CA and JMAK models agree more closely because random2.json had 100 nuclei initially, but random1.json only had 50 nuclei initially. This aligns with our observation that the 2 models agree more closely because the JMAK model is intended for systems with multiple nuclei.

2e) Using the input deck from random3.json, we can see that the CA and JMAK models agree more closely than in part (c). The maximum disagreement is 0.028178470358. The plot is shown below:



When I displayed the initial list as an image, for both random1.json and random3.json, although they had the same number of initial nuclei, the initial nuclei in random1.json are more clustered and closer together, whereas the initial nuclei in random3.json are more spread out. This results in a closer agreement between the 2 models for random3.json because it's more representative of systems with multiple nuclei. If the initial nuclei are close to each other, they will solidify and combine, which is effectively less representative of a system with multiple nuclei.

2f) To model a polycrystalline metal solidifying from a melt, I would choose the CA model. The JMAK model is more idealized, and can only be validated if initial assumptions weren't violated. An important condition for the JMAK model is randomly dispersed nuclei, growing isotropically. Because the sample is polycrystalline, the CA model is better. The JMAK model is useful for providing "average" information; the CA model can give an evolution of grain morphology and solute concentration fields, along with macroscopic "average" information.

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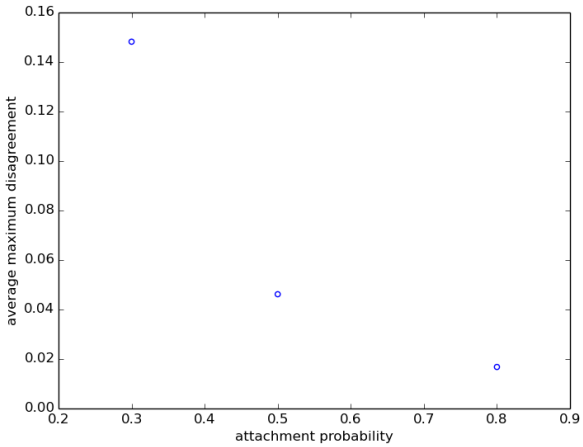
3a) For the system in single1.json (1 nuclei), and using timesteps = 20, prob = 0.5, the maximum disagreement is 0.047173470137.
If we run the program again, we get a different value; the maximum disagreement is 0.0355116625569. The answers vary slightly because it is a probabilistic CA model; the probability gives the slight variations in which nuclei are solidified, since they are not always going to combine with solid neighbors. The "right" answer can be obtained by running the simulation with the same parameters many times, and then taking the average of all the outputted maximum disagreements.

3b) For the system in random1.json, and using timesteps = 30, prob = 0.5, over 10 simulations, the average maximum disagreement is 0.0885287196645. Doing the same for the system in random2.json, but with timesteps = 25, the average maximum disagreement over 10 simulations is 0.0481381139924.
Yes, pCA follows the same trend observed in 2(d). The average maximum disagreement is smaller for the system in random2.json, and the trend observed in 2(d), graphically, was that the 2 models agreed more closely than that for the system in random1.json. Although the deterministic pCA in 2(d) had a much smaller maximum disagreement, the trend is similar.

3c) For the system in random2.json, and using timesteps = 30, prob = 0.3, over 10 simulations, the average maximum disagreement is 0.14899393780997178.
Doing the same for the system in random2.json, but using timesteps = 20, prob = 0.8, over 10 simulations, the average maximum disagreement is 0.01723664318222202.
The disagreements between the 2 models seem to vary with attachment probability, prob. The two values differ by a factor of 10. (When I ran it multiple times, I got very similar values.)
The trend seems to be, as the attachment probability increases, the maximum disagreement between the 2 models decreases. From 3(b) we can observe, when the probability = 0.5, the average maximum disagreement is in between the two values above (p = 0.3 and p = 0.8).
If we plot the disagreement with probability:



3d) I would choose probabilistic CA if I were to model solidification of a polycrystalline metal from melt. From the trend in 3(c), I inferred a higher attachment probability is correlated with a lower disagreement from the JMAK model. So, the highest attachment probability will result in the closest agreement with the JMAK model, and the highest probability possible is 1.0, i.e deterministic CA. Previously, I mentioned that a CA model would be a better choice than the JMAK model for solidification of a polycrystalline metal. So, even though it is a small discrepancy from the JMAK model, a probabilistic CA would be the better choice since the JMAK model is not the best for polycrystalline solidification. A probabilistic CA is a preferred model for seeing an evolution in physical morphology; the result looks more like nuclei, and there is a lesser effect from the underlying grid (lattice effects).