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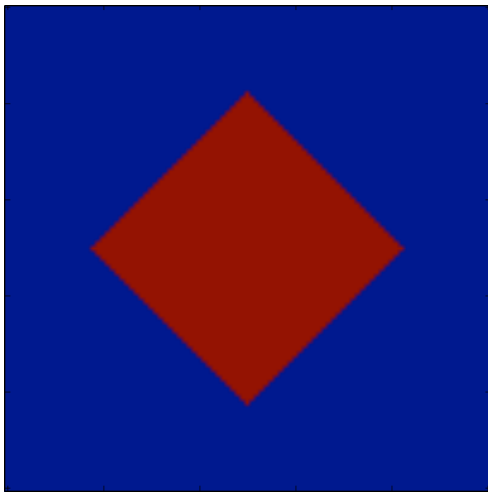
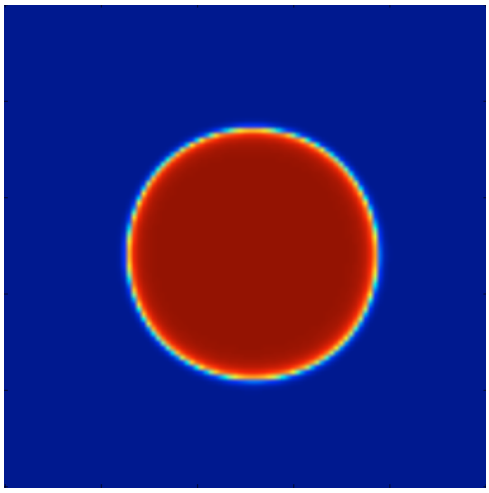
2a) Using input deck from single3.json, a single nucleus in the center grows until ⅓ of area.

Snapshot of CA model:



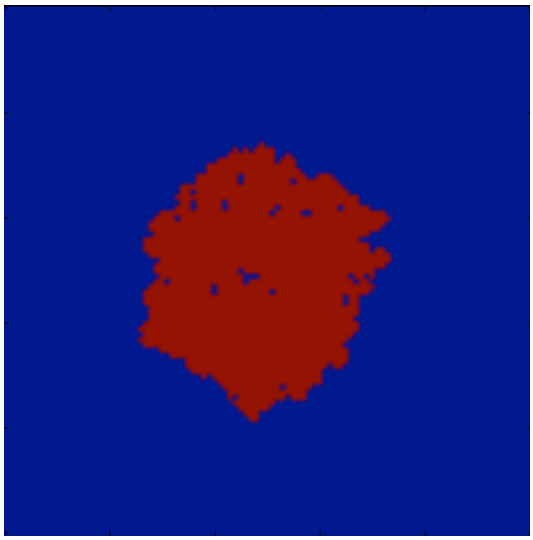
The shape of the growing nucleus is a diamond. There are very obvious lattice effects on the shape of the growing nucleus, since the CA model simulation was done on sq(1) lattice. Consequently, the interface character is sharp and is not “fuzzy”; there are pointy corners.

Snapshot of PFM:



The shape of the growing nucleus is a circle. Since the PFM is a continuum model, there is a gradient, and so the material changes state gradually. Thus, the interface character is fuzzy. The diffuse interface results from it spreading out in space; it is wide enough to see on the image.

Snapshot of MCPM:



The shape of the growing nucleus resembles a circular geometry.
The interface is not sharp; there are fuzzy curved interface edges/types.
The circular shape of the nuclei is similar to that of the PFM.
The interface is not as sharp/straight as that in the CA model, but also not as smooth as that in PFM, because the MC simulation is analyzing 2 sites next to each other, rather than a continuum model.

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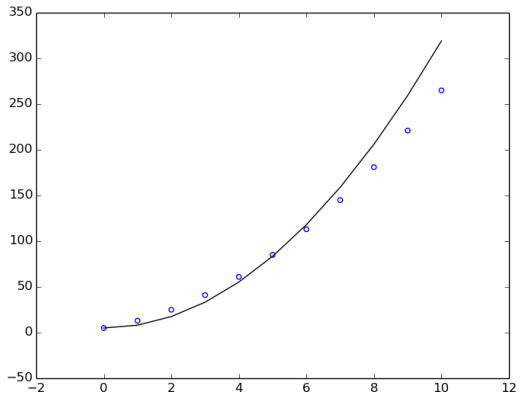
2b) For the CA model, timesteps = 10 results in the smallest absolute error (~54) between the area transformed in the simulation and the ideal growth equation.



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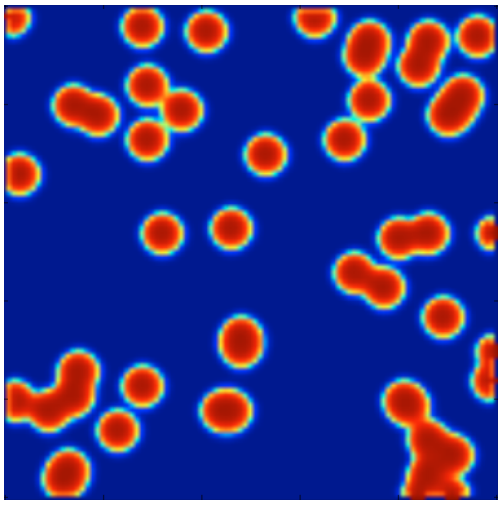
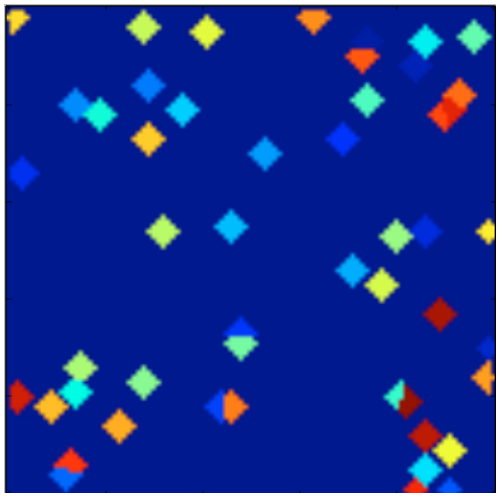
2c) Using input file random4.json, the CA, MCPM, and PFM simulations, for 20% and 100% solidified.

PFM at 20% solidified:



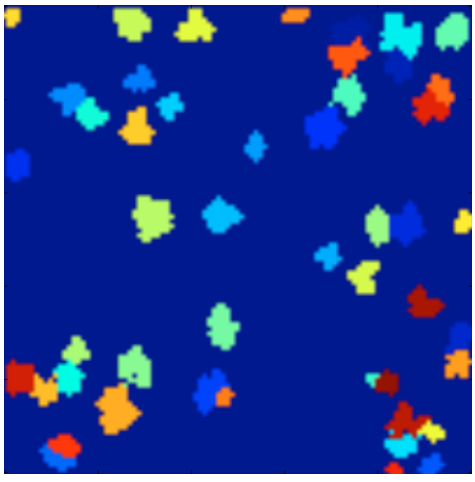
PFM at 100% solidified:

CA at 20% solidified:

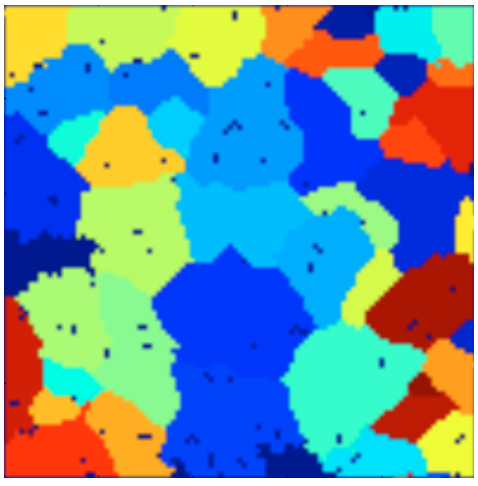


CA at 100% solidified:

MCPM at 20% solidified:



MCPM at 100% solidified:



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The intermediate structures of all 3 models are different.
The CA model has diamond shaped intermediate structures and sharp edges/pointy corners.
The PFM has circular/round nuclei and fuzzy, relatively wide interfaces.
The MCPM has nuclei that are relatively circular in shape, with fuzzy/curved interface edges.

The final structure of the CA model shows the different solid states, but due to lattice effects, still have sharp corner and interface edge types, but deviated from diamond/square shapes.
The final structure of the PFM shows a single solid, completely solidified. There is no depiction of differing solid states.
The final structure of the MCPM shows large grains that geometrically resemble microstructural grains.
The final structure for the CA model and PFM is completely solidified, while the final structure for the MCPM show parts of a grain of a specific state, with liquid points within the already solidified grain. I observed that when the time was increased past 65, the final structure of the grains melted again.

2d)

2e)

	Advantages	Disadvantages
CA	- easy to parallelize algorithm - easy to program/code	- strong lattice effects on interface type and the growing nuclei (sq(1)) - can lack rigorous thermodynamic basis
MC	- can be parallelizable - incorporates statistical mech + thermodynamic concepts/rules	- strong lattice effects, will cause sharp interfaces - at high temp, could risk melting system
PFM	- incorporates thermodynamic concepts/rules - easy to add crystallographic anisotropy effects to F, the energy function	- hard to program - can be susceptible to metastability in algorithm
JMAK	- generally accurate algorithm - simple model/equation that describes kinetics of nucleation/growth	- validated for randomly dispersed nuclei that grow isotropically - valid for large numbers of particles; bad for low nuclei density

If I had to simulate a solidification process, I would choose the CA model. It is relatively accurate, and is the easiest and most computationally efficient out of the 4. It is good for bulk energy driven and short range diffusive processes. Solidification can also be modeled with a reasonable rule set.

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I would not choose the JMAK model, because of its idealizations and limitations (isotropy).
I would not choose the MC model because of its susceptibilities to lattice effects, creating sharp interfaces. It is also harder to program compared to the CA.
I would not choose the PFM because it is harder to program and can be affected by metastable states.