A Novel Approach To Monte Carlo Sintering Simulation with Anisotropic Grain Growth

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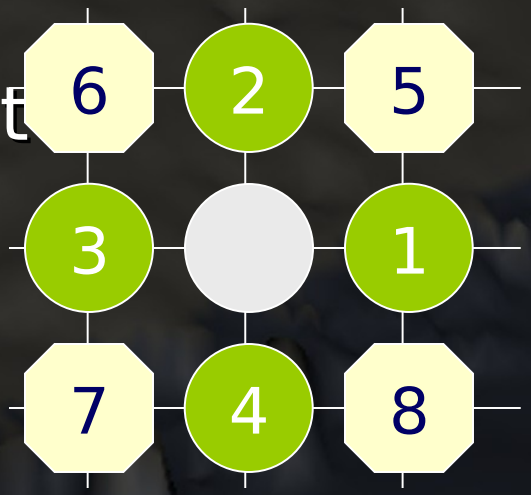
Introduction

- Monte Carlo (MC) Potts models are widely used by researchers to simulate grain growth and sintering, weather forecasting, ocean currents, etc.
- Grain Size is an important parameter for porous material properties.
- Most models assume isotropic materials to simplify the problem.
- Anisotropy has a significant effect on grain growth rates and other

The Potts Model

- Structure discretized on lattice of sites.
  - Energy associated with sit
  - Configurations have Boltzman Distribution
- Potts Model Features
  - Equilibrium
  - Kinetic



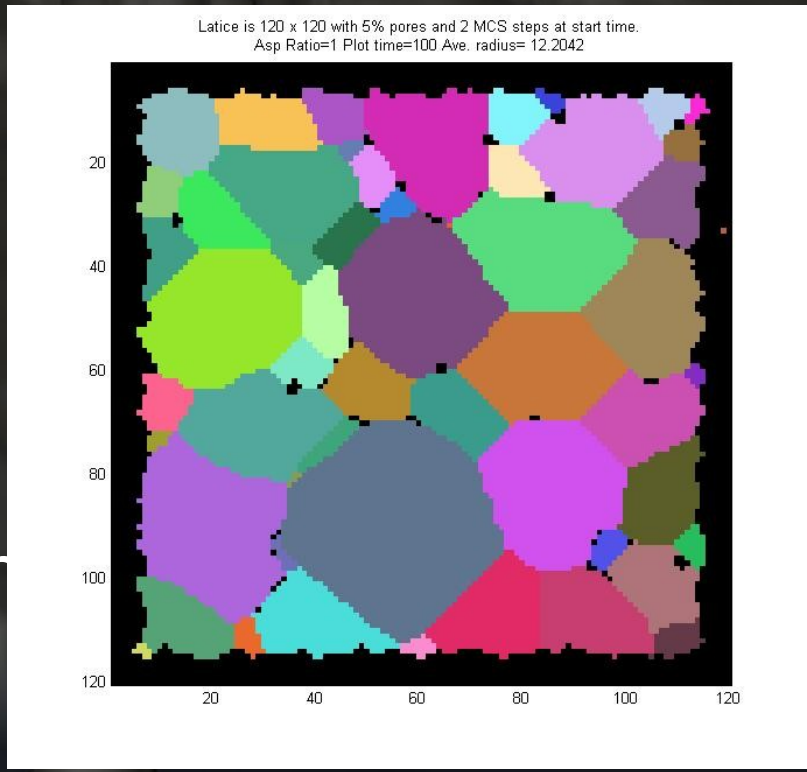
$$E(G) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{8} E_{ij}$$

1st Nearest Neighbors

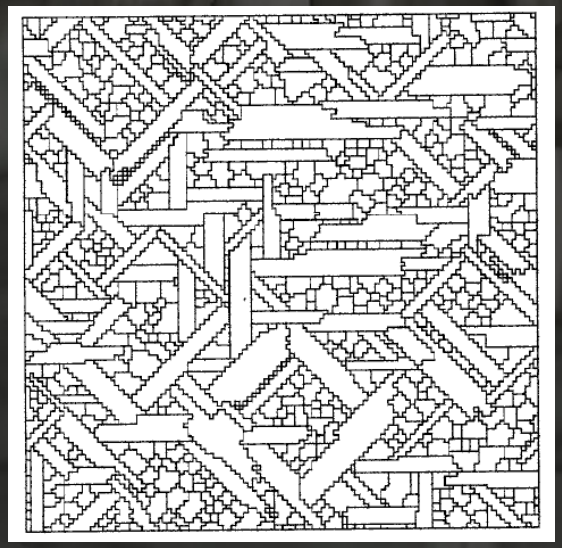
2nd Nearest Neighbors

Basic Potts Algorithm

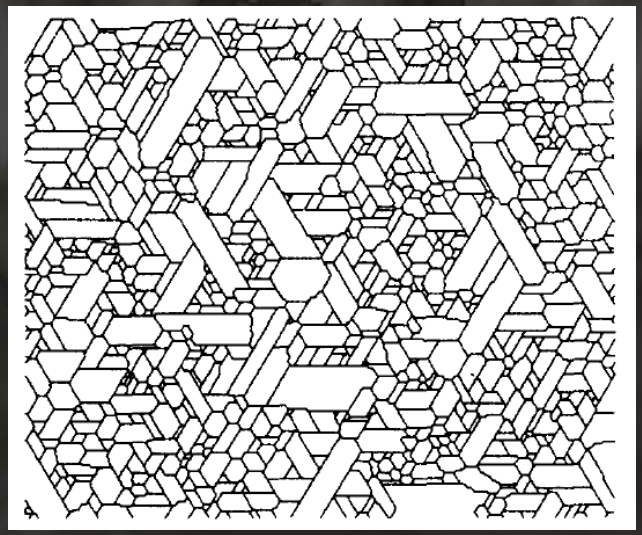
- Step 1: Initialize the Lattice
- Step 2: Grain Growth
  - Grain Site changing state
- Step 3: Pore Migration
  - Adjacent Grain/Pore Pair Transition
- Step 4: Vacancy Annihilation



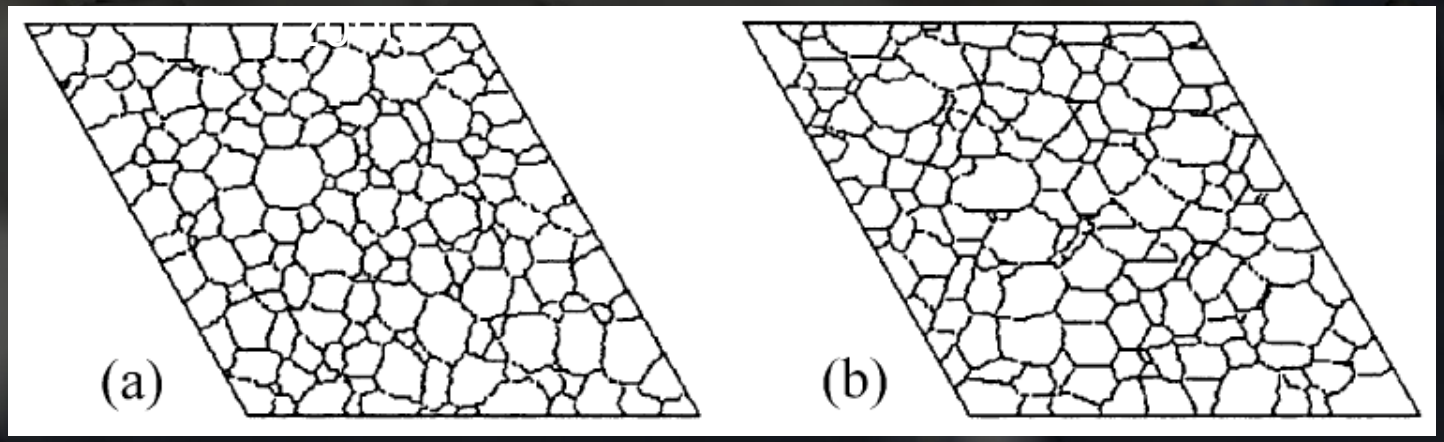
Introducing Anisotropy



Morhac & Morhacova



Yang et al. (1995)

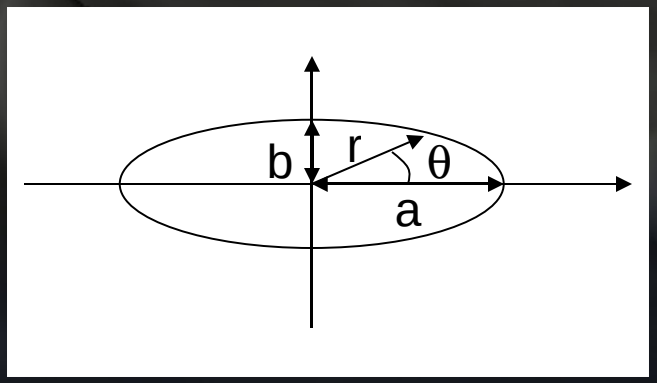


Misorientation Angle (0% & 60% of Max) Yu & Esche

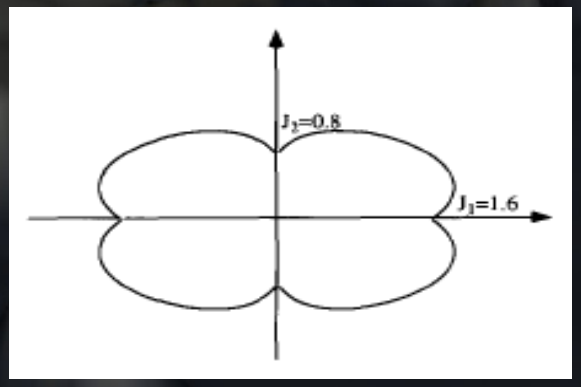
Introducing Anisotropy

- Energy Anisotropy is introduced in the Jacobian used to compute ΔE
  - Use Wulff Plot for surface energy

$$E_{ij} = \begin{cases} 0 & q_i = q_j \\ J_i + J_j - J_b & q_i \quad q_j \end{cases}$$



Ellipsoidal Wulff Plot



Two Cusp Wulff Plot

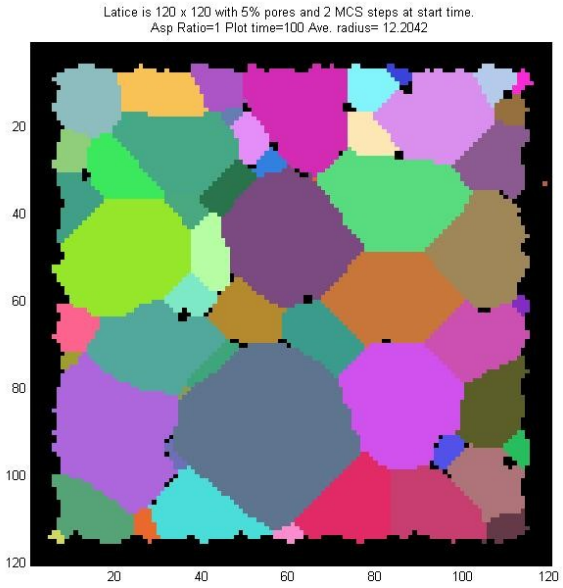
Introducing Anisotropy

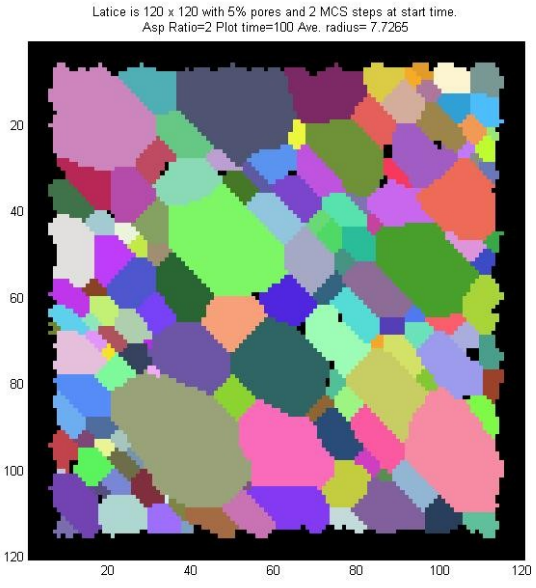
- A significant factor affecting anisotropy in the Binding Energy, J_b, is the misorientation between the two grains at the grain boundary.
  - This has not yet been implemented in the coded simulation.
  - Currently assumes constant J_b

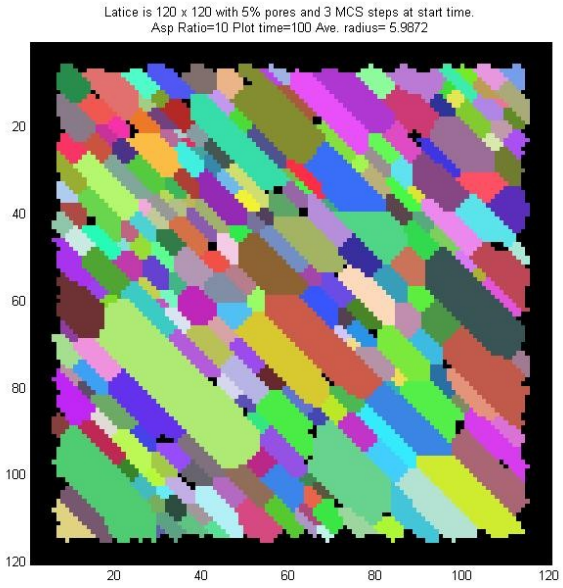
Anisotropic growth

Start with aligned grains to see effects (AR 1,2,10).

- Larger surface energy aspect ratios produce more anisotropy.
- Grain growth slows with anisotropy

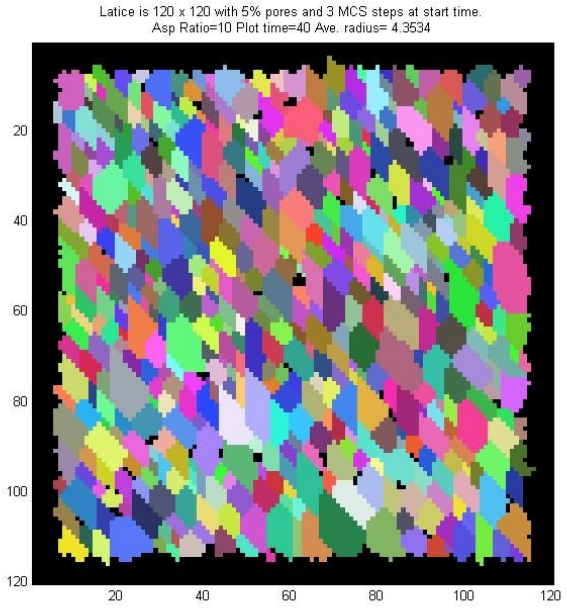


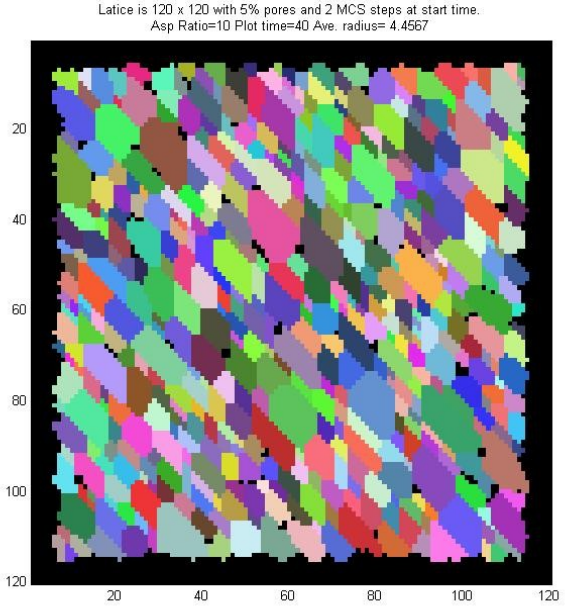


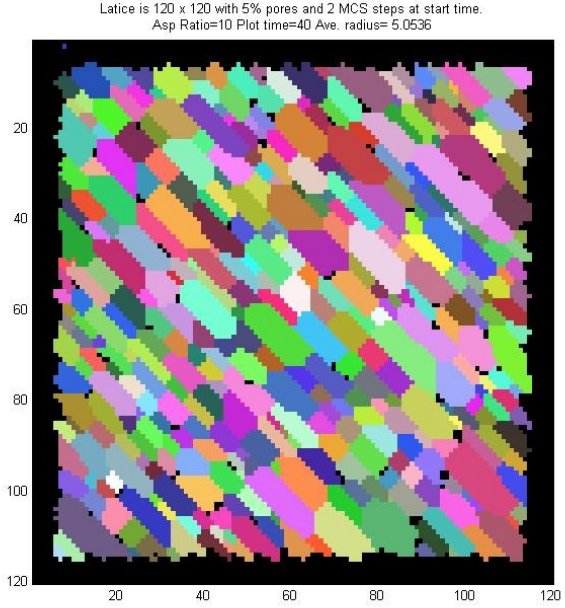


Anisotropic Observations

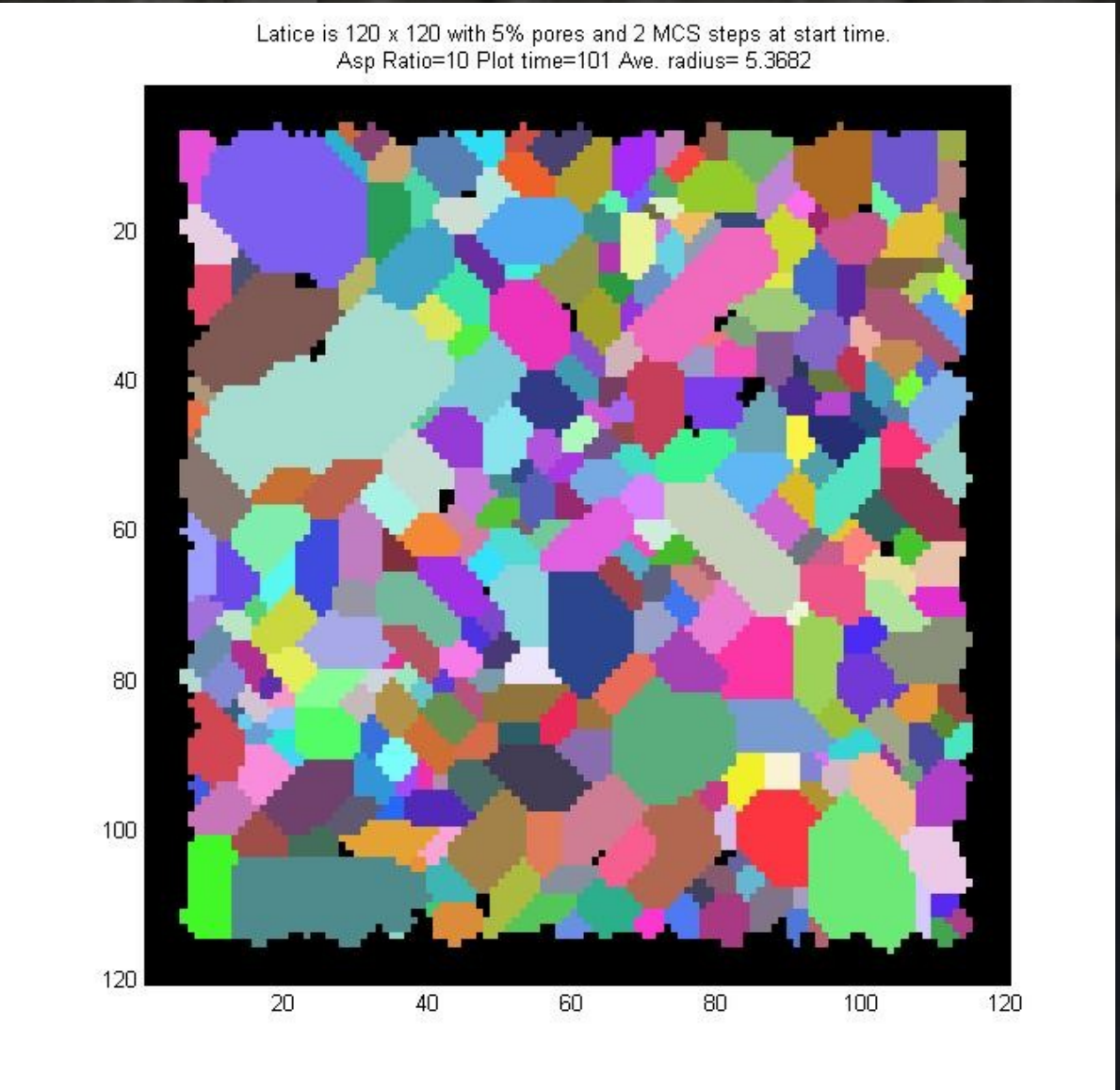
- Angles are correct (20, 30, & 40 deg.).
- Poor growth in non-neighbor directions.





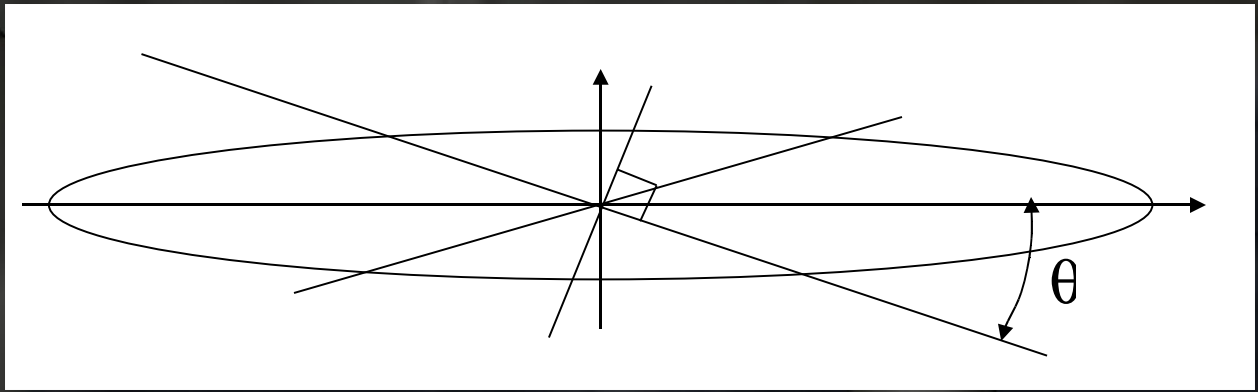


Random Orientation



Non-neighbor directions

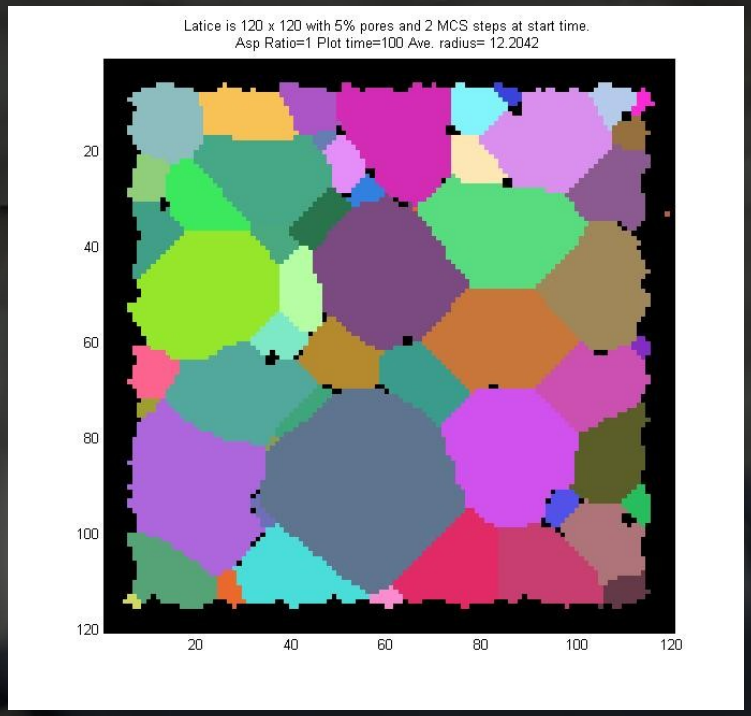
- The aspect ratio of the max energy to min energy reduces as orientation moves away from neighbor directions.

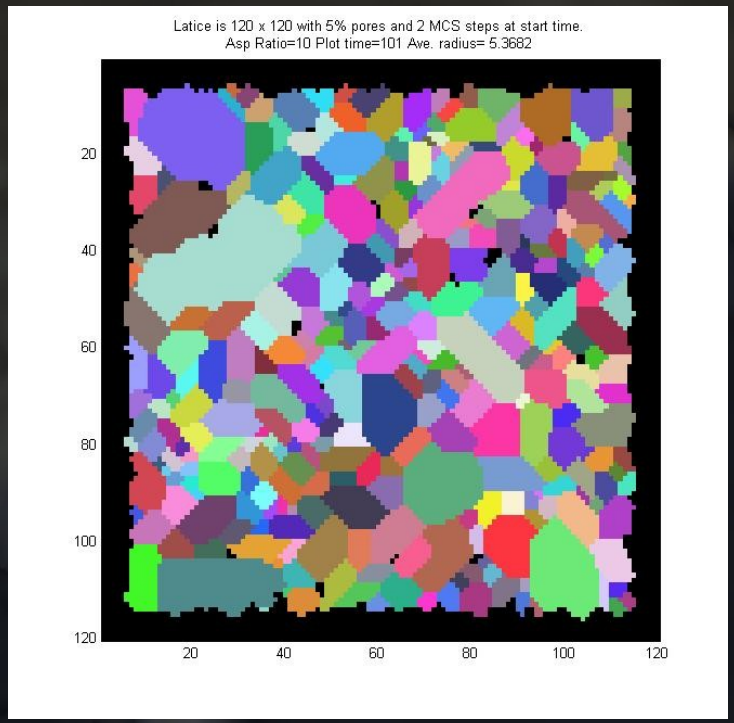


Aspect ratio gets smaller off neighbor directions

Anisotropy Discussion

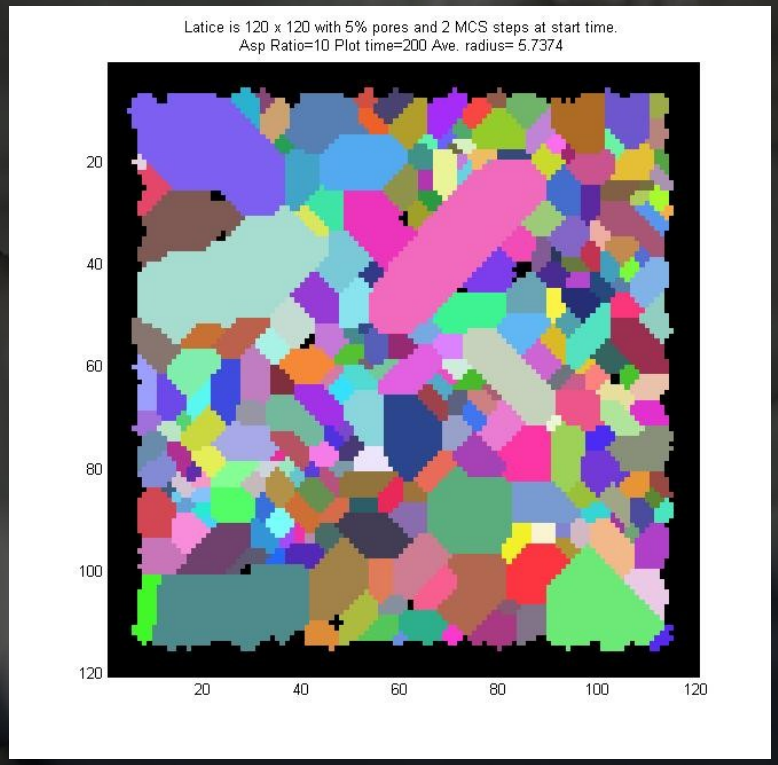
- Anisotropy is apparent
- Grain Growth is slower with

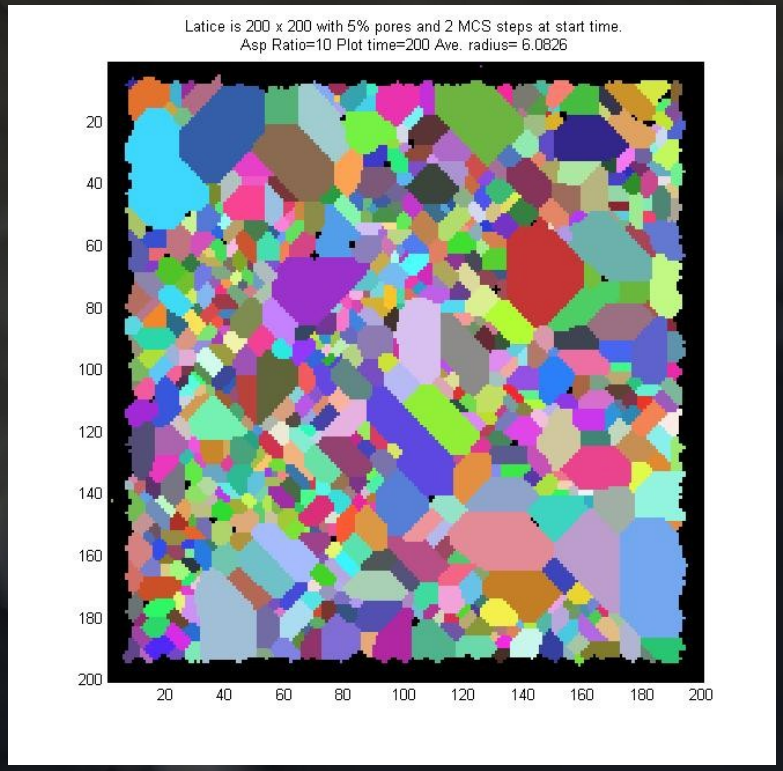




Anisotropy Discussion

- Growth is unaffected by lattice size.

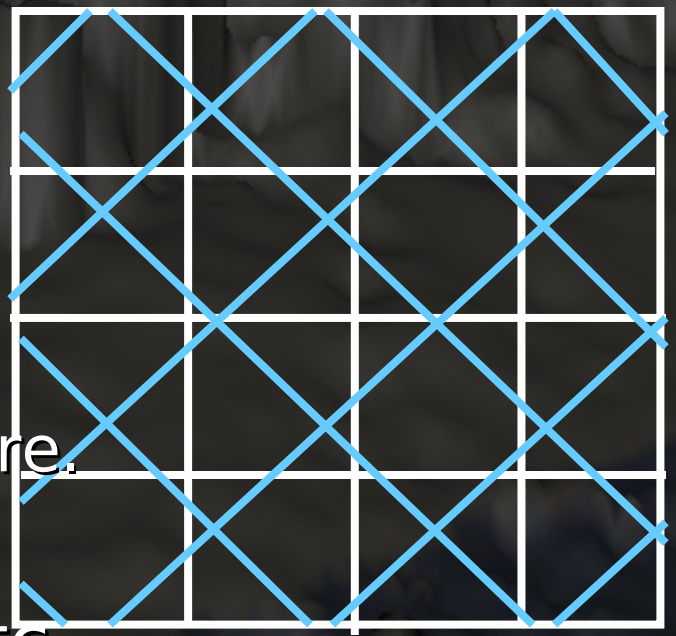




Anisotropy Discussion

- Growth is limited to lattice neighbor directions causing an artifact.
- Ideas to improve the artifact.
  - Periodically rotate compact through random U(0,π) angles within the borders, and rotate back before display.
    - Need to conserve mass, porosity, & grain size.

Rotation Issues



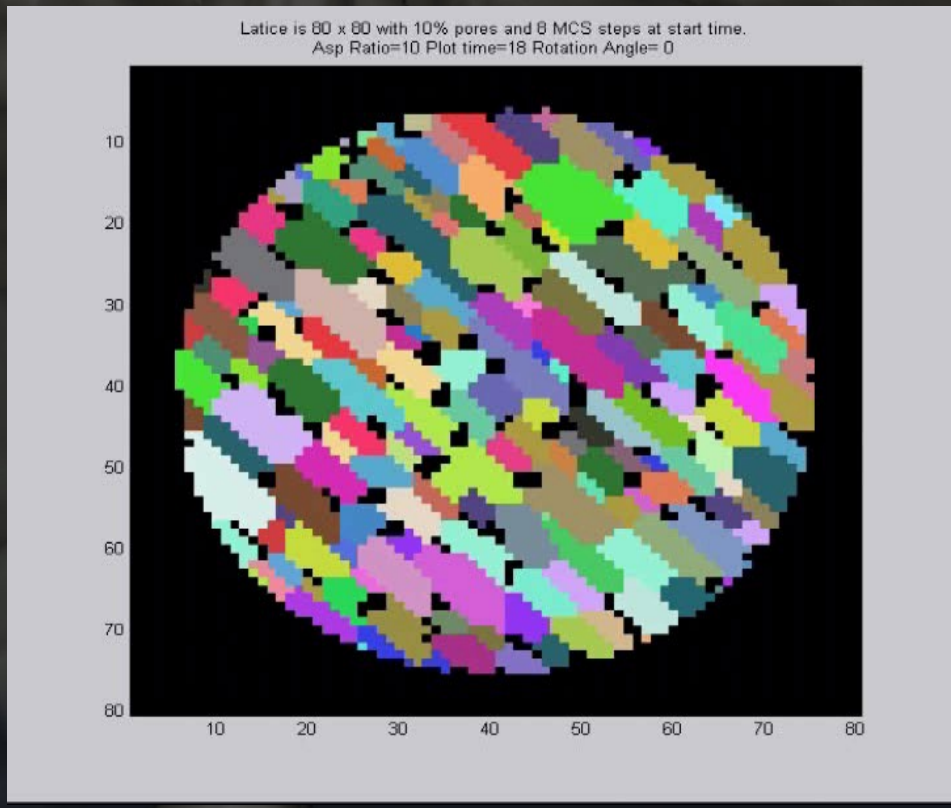
- Nearest site
  - Does not conserve mass.
- Interpolation
  - Loses meaning of grain/pore.
- Rotation by Shear, Rotation by Area Map, etc.
  - Many algorithms, a lot patented
  - None conserve mass, porosity, grain size, etc.

Rotation Concept

- Rotate in rings
  - Width of rings is adjustable parameter.
- Thicker rings
  - Less angular distortion
  - More radial distortion

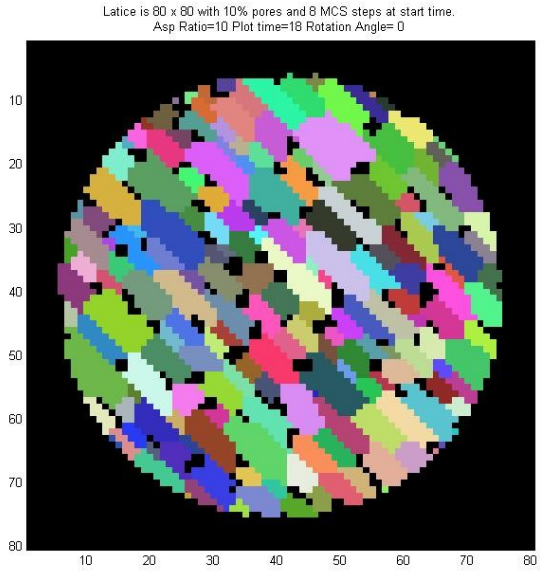
Circle Rotation

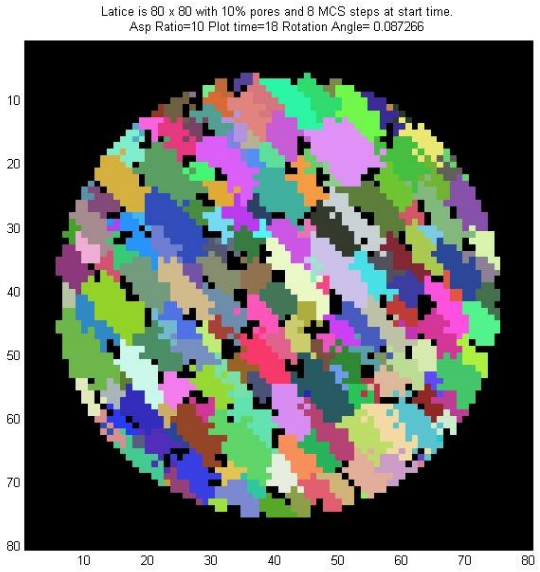
- To reduce distortion.
  - Use circular specimen on square lattice.
  - Use ring concept to maintain grain size, porosity, mass, etc. and minimize distortion.

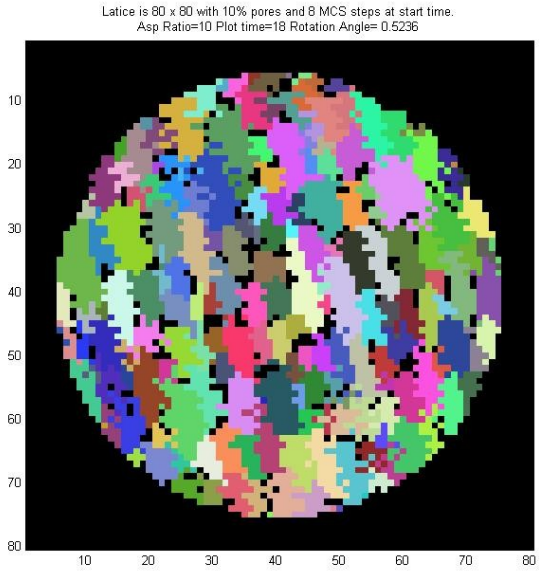


Circle Rotation

- To reduce distortion.
  - Use circular specimen on square lattice.
  - Use ring concept to maintain grain

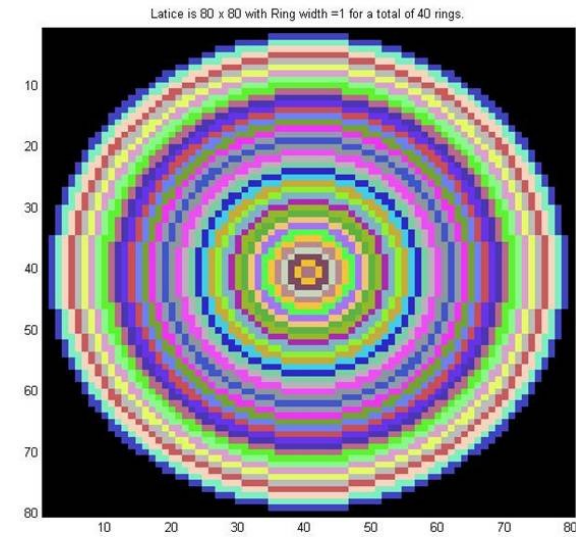


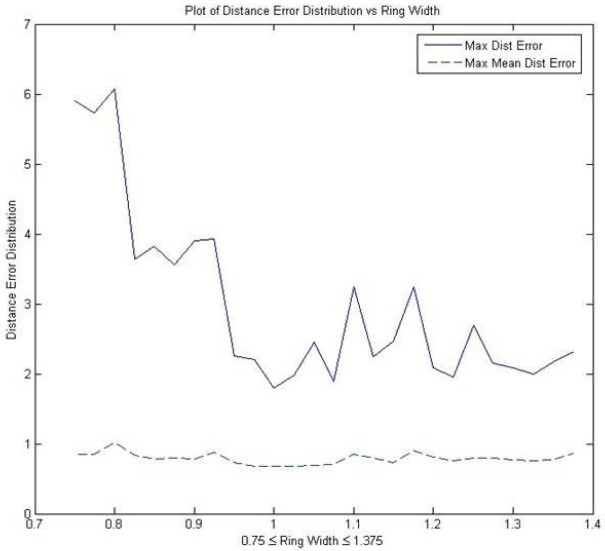


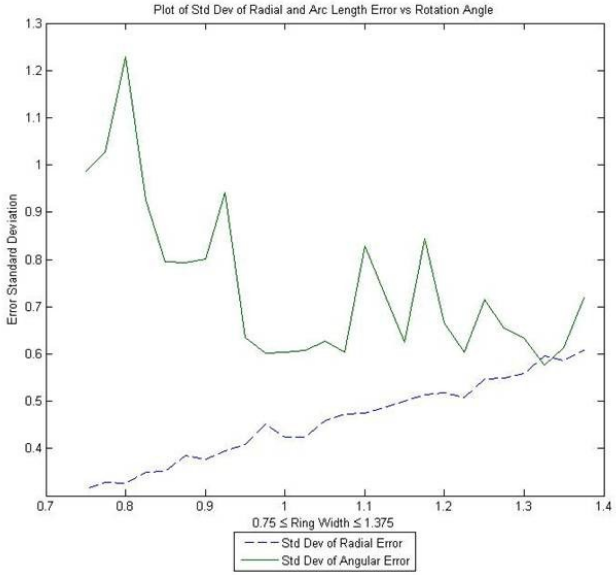


Algorithm Ring Analysis

- Ring Width is the main parameter.
  - Distortion: Angular, Radial.
  - Standard Deviation of Error.







Conclusions

- Potts model incorporating mechanisms of sintering with anisotropy achieved.
- Novel approach to solving lattice associated artifact problem.
- New Algorithm for implementing rotation concept.
- May provide better understanding of anisotropic affects for many models.

Further Work

- Incorporate anisotropic grain boundary binding energies based on misorientation angle.
- Quantitative analysis to confirm response consistent with other models and physical experiments.
- Analyze random oriented fine grains with aligned large grains for better understanding of Templated Grain Growth

Thank You!

Questions?

Analytical Approach

- Soap Froth Models
  - von Neumann (1952)

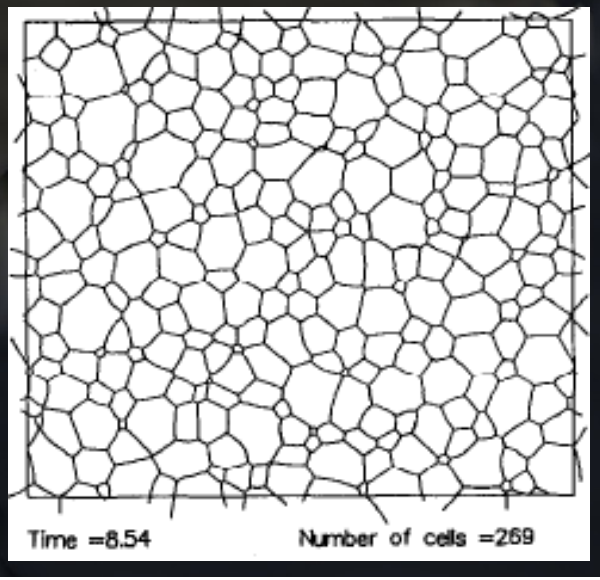
$$\frac{dA_n}{dt} = \frac{\pi \gamma m}{3}(n-6)$$

Von Neumann Mullins equation

- Mean Field Theories
  - Hillert (1965) “grains drifting”
  - Louat (1974) “grains diffusing”
- Overall:
  - Difficult to solve
  - Don’t capture local grain properties

Computer Simulation

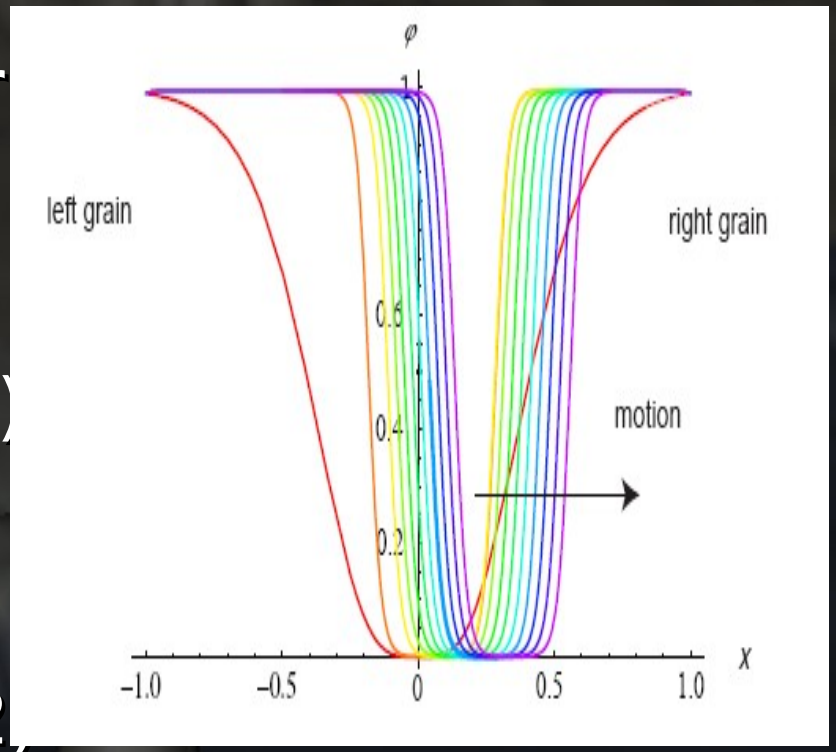
- Two categories
- Deterministic
  - Vornoi (Vertex) Methods
    - Fullman (1952)
    - Cocks & Gill (1996)



GILL and COCKS: GRAIN GROWTH—II

Computer Simulation:

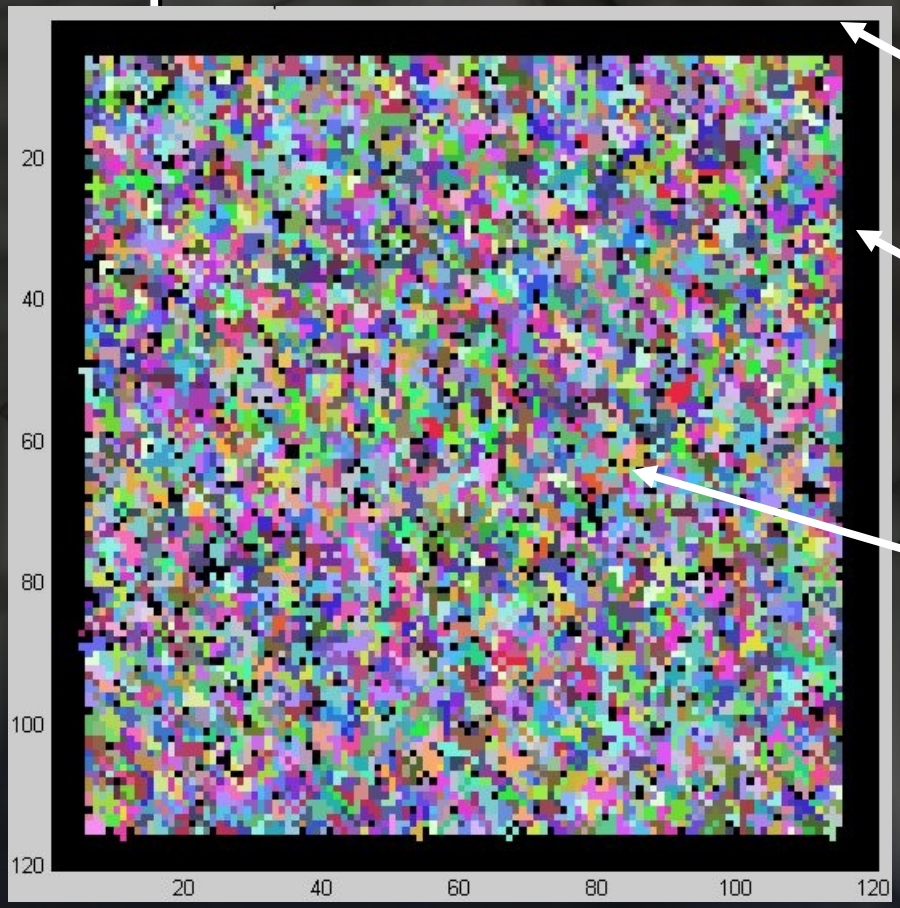
- Stochastic
  - Potts Monte Car
  - Phase Field
    - Lusk (1999)
    - Kazaryan (2001)
  - VMC
    - Cleri (2000)
    - Moldovan (2002)



Lusk: 1D order parameter motion

Basic Potts Algorithm

- Step 1: Initialize the Lattice



Inert Boundary

Active Border

Material Structure

Basic Potts Algorithm

- Step 2: Grain Growth
  - Select a site
  - Randomly select a new grain state (spin) from neighboring spins.
  - Calculate ΔE for changing the spin.
  - Generate random U(0,1) and $e^{-\Delta E / kT}$
  - If rand <= $e^{-\Delta E / kT}$ change to new spin

Basic Potts Algorithm

- Step 3: Pore Migration
  - Select a pore site with an adjacent grain
  - Randomly select a new grain state (spin) from neighboring spins.
  - Calculate ΔE for changing the grain site to a pore and the pore site to a grain with the new selected spin.
  - Generate random U(0,1) and $e^{-\Delta E/kT}$
  - If rand <= $e^{-\Delta E/kT}$ change to new

Basic Potts Algorithm

- Step 4: Vacancy Annihilation (1)
  - Theory from DeHoff (1989)
  - Compute Grain Boundary Length
  - Compute # attempts $t \quad \frac{L_{gb}}{L_0}^2$
  - Randomly select a pore site.
  - If it is a vacancy, annihilate it

Basic Potts Algorithm

- Step 4: Vacancy Annihilation (2)
  - Compute centroid of largest adjacent grain
  - Exchange farthest grain in compact a
  - **Vacancy** th become s grain
  - Grain become s pore