Homework 1

Due: Friday, 9/25/15

Objective: To learn how to program various lattice Monte Carlo techniques for simulating basic microstructure processes, including phase separation in multi-component alloys and grain growth.

Part A:

Write a simple Ising model code to simulate magnetic spin states on a lattice. Initialize the system to have a random 50/50 configuration of "up" and "down" spins on a 2D lattice of size 50×50 (or larger if you like). Without an external magnetic field, simulate the evolution of the magnetic spins for a spin-spin interaction of J = 0.4 at a temperature of kT = 1.5. Execute the system for 500 MC cycles. Next, decrease the temperature to kT = 0.8, 0.4, and 0.1. Describe your observations. Finally, impose an external magnetic field of M = 0.5, and describe the spin state for J = 0.4 and the above temperatures. Turn in plots of the lattice showing the spin states, your written descriptions, as well as your code.

Part B:

Modify your code to simulate an atomic A-B alloy system by enforcing global species conservation with a penalization term. Execute two simulations: one with an A-fraction of X_A = 0.3 and another with X_A = 0.5 using a temperature of kT = 0.1 and J = 0.4. Then, increase the temperature to kT = 1.5, and describe any observed differences. Next, change the interaction energy J = -0.4 for kT = 0.1 and 1.5, and describe what you observe. What does a negative J represent in terms of atomic bonding? Turn in plots of the lattice showing the atomic configurations, your written descriptions, as well as your code.

Part C:

Expand your code to conduct a Q-state Potts model simulation. Set Q = 10, and randomly assign an integer value between 1 and Q to each lattice node. Execute the simulation to observe grain growth, using a lattice size of at least 50×50. Show (at least) three snapshots from the simulation at different MC cycle numbers, illustrating the evolution of the grain structure. In your code, use a 2D square lattice and include both first-nearest and second-nearest neighbor nodes to calculate the lattice energy. Turn in plots of the lattice showing the grain configurations, your written descriptions, as well as your code.