Homework 35:

8.GH1 A number of MATLAB files have been provided on the homepage. The three files ising.m, energy.m, and bringIntoCell.m give you the ability to do Monte Carlo simulations of a two-dimensional Ising model, as discussed on pages 346–353. To use them, put them all in the same directory and run the main script, ising.m. (The other two files are function m-files used by the main script.) Read through the code and figure out where the parameters are defined that you will want to play with: simulation size, number of spin flips, $kT$, etc. Get a general feeling for how the code works. Experiment with the code and answer the following questions:

(a) Start by running the script using a starting $kT$ of 5 and an ending $kT$ of 0.5. Describe what happens in the magnet. At high temperatures, the spins should be randomly aligned so you should get $E = 0$ on average. Do you? Explain.

(b) According to the reading, what is the critical transition temperature? What do you observe in the simulations?

(c) Run the simulation at a constant temperature (set $kT_i$ and $kT_f$ to almost the same value). Try 3 values above the transition temperature: $kT = 10, 5, 2.4$, In all three cases the magnetization per spin is (close to) zero (on average). But there are qualitative differences in the behavior. What are they? (At the very least, consider the energy and the average size of clusters at each temperature.) If your data seems too noisy, try taking averages over more attempted flips by increasing nsweeps (and decreasing $kTsteps$ to speed things up).

(d) Reread problems 6.17 and 6.18. Now answer the preceding question again. (How am I calculating the specific heat?)

(e) As accurately as you have patience for, find the critical temperature for a $10 \times 10$ lattice and a $20 \times 20$ lattice. (You can speed things up by skipping many frames in the animations. Change line 103 to if mod(il,Nits)==0.) Are they the same? Use a small range of $kT$, between about 2.25 and 2.4.

There are lots of other things to try if you are interested. See pages 352–356 in your text.
The Ising model is applicable to many kinds of physical systems. In this problem, we will simulate a mixture of atoms. Go back and re-read the relevant parts of Sec. 5.4 in the book. (No really, go back now. Continue on after you re-read.) In the (binary) Ising model, each site has a ‘spin’ $s_i = \pm 1$ where the two different dipole directions are indicated by the $\pm 1$. In using the Ising model to simulate a mixture (we could call it an alloy), the $\pm 1$ instead represents A and B atoms. But we can’t just change a $+1$ to a $-1$ like we do in the magnetic version of the model, that would be something akin to a copper atom transmogrifying into a gold atom—those kinds of reactions aren’t typical. Instead, to model what happens in a mixture, we will exchange two ‘spins’. This represents two atoms changing places.

The next set of files, alloy.m and alloyEnergy.m (you still need bringIntoCell.m), are similar to the files you used in the last problem, only a couple of changes have been made. The biggest differences are that two unlike atoms are exchanged instead of the spin on one site flipping and that the interaction between like atoms can be either repulsive or attractive.

(a) If the variable epsilon is set to $+1$ in alloy.m, the Ising model mimics the physical problem you treated in prob. 5.58 and that was discussed on pg. 189. Start by running the script using a starting $kT$ of 5 and an ending $kT$ of 0.5. Describe what happens in the system.

(b) What is the critical temperature? Do you think it depends on the concentrations? Sketch a phase diagram for this system.

(c) Now change the interaction parameter epsilon to $-1$. With this setting, the Ising model mimics the physical problem where unlike atoms are attracted to each other. Why?

(d) Play with this case some. Answer the relevant questions you answered for the magnetic case and for the phase separating case.

(e) Sketch a phase diagram for this system.

(f) What other things did you try? Tell me what was interesting or what was confusing about these two problems. What questions came up?

Other things to try:

- Experiment with different starting concentrations. How could you use this information to build a phase diagram. How is the critical temperature affected?

- Extend the program to include second nearest neighbor interactions as well. The leads to much richer behavior in the model. You will see anti-phase boundaries and various ordered structures.
8.GH3 Where are the entropy and the free energy in all of this? Aren’t those the really important quantities in thermal physics and statistical mechanics?

8.GH4 What are the important concepts you learned in this class? What are the important examples that illustrate those principles? What things did you learn well? What things do you feel uncertain about still? Be as complete and detailed as you can in answering these questions.
Aux. 1& 2 Make up two problems that you think would be good final exam questions. Your problems should include ideas from Chapters 7 and 8, but don’t need to focus exclusively ther. Your problems could be of any type: multiple-choice, essay, short answer, computational, sketching, fill-in-the-blank, True-False, etc. Include with your problems a complete solution (explanations, not just answers). You may talk about your problems with others in the class and even distribute solutions if you wish. But if you do, make sure that your problems are unique (not the same as problems made by other students). The test will be closed-book but the formula sheet will be provided. (Are there things missing from the formula sheet? Let me know if you think so.)