Lab 11: Shape, Symmetry, 'Spectations, Surprise! Due 12:00 (noon) SUNDAY 7 May 2017

During today's lab explorations, you should come to understand why scientists say, "Interpolation is easy; extrapolation is hard." You may work in pairs but the work that you report must be your own. As a pledged activity, you must record your specific expectations at each stage for what you think will happen next, and then compare in detail your expectations to your observations. This is a "guided inquiry" exploration, with driving and directing questions to help you think more deeply about states of matter and how we are using nanotechnology to create new materials and new industries.

NOTE: This is BETA release software, so between each numbered exercise, you may want to (in some cases need to!) "reload" the application to reset some of the internal constants.

http://www.shodor.org/~aweeden/simsurfaceJS/

I. How Perfect is a Perfect Square?

Each of these next explorations should be repeated multiple times (reset annealing, THEN randomize the charges) to see what might be the range of observations. Use the measuring tools to quantify your observations. Remember to record your specific expectation (pledged).

1. Set the number of charges to 1, all 4 wall charges should be 10. What do you expect the ground state to look like? Do it. Where is the charge compared to where you expected it to be? How do you explain that?

2. Set the number of charges to 4, all 4 wall charges should be 10. What do you expect the ground state to look like? If you expect a specific shape, how would you prove that the ground state has the properties of that shape? How symmetric is your ground state? Randomize and anneal the system several times. Use the measuring tools to quantify your observations.

3. Set the number of charges to 9, all 4 wall charges should be 10. What do you expect the ground state to look like? If you expect a specific shape, how would you prove that the ground state has the properties of that shape? How symmetric is your ground state? Randomize and anneal the system several times. Use the measuring tools to quantify your observations.

4. Set the number of charges to 16, all 4 wall charges should be 10. What do you expect the ground state to look like? If you expect a specific shape, how would you prove that the ground state has the properties of that shape? How symmetric is your ground state? Randomize and anneal the system several times. Use the measuring tools to quantify your observations.

5. Set the number of charges to 25, all 4 wall charges should be 10. What do you expect the ground state to look like? If you expect a specific shape, how would you prove that the ground state has the properties of that shape? How symmetric is your ground state? Randomize and anneal the system several times. Use the measuring tools to quantify your observations.

II. Explorations of Isomers and Extrapolation

Each of the next several explorations uses 7 charges and different wall charge values. You are asked to measure, then predict the next measurement, then observe the actual measurements. You must record and report your expectations in your report (pledged).

1. Set the number of charges to 7. Set all 4 wall charges to 80. Before you anneal, what do you expect the ground state configuration to look like? Anneal the system multiple times, resetting the annealing, and then randomizing the charges. How does your observed ground state compare to your expectation? What is the degeneracy number? Measure all angles and distances, recording the values in such a way that you can identify which charges are involved.

2. Now set all 4 wall charges to 40. Before you anneal, what do you expect the ground state configuration to look like (qualitatively and quantitatively)? Anneal the system multiple times, resetting the annealing, and then randomizing the charges. How does your observed ground state compare to your expectation? What is the degeneracy number? Measure all angles and distances, recording the values in such a way that you can identify which charges are involved.

3. Now set all 4 wall charges to 20. Before you anneal, what do you expect the ground state configuration to look like (qualitatively and quantitatively)? Since you have 2 measurements, can you use them to estimate the new values? Anneal the system multiple times, resetting the annealing, and then randomizing the charges. How does your observed ground state compare to your expectation? What is the degeneracy number? Measure all angles and distances, recording the values in such a way that you can identify which charges are involved.

4. Now set all 4 wall charges to 10. Before you anneal, what do you expect the ground state configuration to look like (qualitatively and quantitatively)? Since you have 3 measurements, can you use them to estimate the new values? Anneal the system multiple times, resetting the annealing, and then randomizing the charges. How does

your observed ground state compare to your expectation? What is the degeneracy number? Measure all angles and distances, recording the values in such a way that you can identify which charges are involved.

5. What have you learned?

III. Explorations of Isomers and Nanomanipulation

In this last set of explorations, you will use your powers of observation and your imagination to explore isomers and new material designs, while testing how stable the new materials would be under small displacements. For comparisons, use 16 charges, and all 4 wall charges should be 10. Once you finish these, you can choose to try other combinations.

1. Randomize and anneal several times, and as the system liquefies and approaches the solid state, watch for "almost" arrangements of the charges that may appear. Do you always get the same final state? What are the energies?

2. When the system 'freezes', move individual charges to try to reconstruct some of these intermediate stages.* What are the energies?
   a. After you move the charges, start the annealing without resetting, and observe what happens.
   b. Set the temperature to .05 and the step size to .05 and start, observing what happens. Do this reset several times for each exploration.
   c. Set the temperature to .1 and the step size to .1 and start, observing what happens. Do this reset several times for each exploration.
   d. Reset annealing, randomize, rebuild several times to get an idea of reproducibility.

   *One shape to try: take the 4 "central" charges and arrange them as a diamond instead of a square. What is the energy? Start the annealing without resetting. The set the temperature to .05 or .1 and the step size to .05 or .1 and start, observing what happens.

   Another shape to try: take the 4 "central" charges and put one in the middle of each of the corner "triangles". What is the energy? Start the annealing without resetting. The set the temperature to .05 or .1 and the step size to .05 or .1 and start, observing what happens.

   For all of these, you should also look at the potential and then the field.

3. Use your imagination to try to construct alternative ground states that will be stable under small (0.05 or 0.1) disturbances. What do you see are the characteristics of stable states?

In your report, your introduction should include your own research into what annealing and simulated annealing are, and something about nanomaterials and how they are being developed. You should present captured observations sufficient to form the basis for your analyses, reflections, and conclusions.