Welcome to (the second half of) Chemistry 348 - Physical Chemistry for ISP! We have five weeks to rush through topics in statistical mechanics and kinetics. The emphasis throughout will be on connecting behavior at macroscopic length scales, where most observations take place, and microscopic length scales, where material properties originate. Students should come away with a visceral understanding of: microscopic origins of entropy and free energies, the relationships between statistical mechanics and thermodynamics, phase transitions, and elementary kinetics. The topics are intrinsically technical and rely on some mathematical tools that may be unfamiliar, but effort will be made to keep things as simple as possible (and no simpler). To aid with the intuitive understanding, we will make use of computational techniques for simulating and visualizing these concepts, which will require that students have (or develop) some familiarity with basic computer programming.

Instructor: Prof. Todd Gingrich, Ryan 4018, todd.gingrich@northwestern.edu
Office Hours: Thursday 1 pm, Tech L221 (or by appointment in Ryan 4018)
Lecture: Monday/Tuesday/Wednesday/Friday, 1:00 - 1:50 pm, Tech L221
Course Website: http://gingrich.chem.northwestern.edu/teaching/348/348.html
TA: Ricky Jodts, jodts@u.northwestern.edu, Office Hours: Thursday 5 pm

Textbook: The lectures will not explicitly follow a textbook, but I will direct you to readings from Statistical Physics: An Entropic Approach by Ian Ford.

Notes I will post my lecture notes on the course website after each class.

Evaluation: There will be weekly problem sets as well as two exams. The first exam will be during the ordinary class time on Friday, May 24. The second exam will be during the final exam slot, Monday, June 10 at 9 am. I expect the first exam to cover statistical mechanics and the second to cover kinetics, but I will provide more information as we get closer to those dates.

Final grades (for my portion of the course) will be determined by weighting the homeworks and exams:

- Homeworks: 50%
- Exam 1: 30%
- Exam 2: 20%

Collaboration: I am attempting to create assignments that will improve your understanding. This is best achieved by collaborating early and often, with your classmates and with me. Figure out how to solve the problems with others. Write the solutions/code for yourself to confirm that you actually get it.

Programming Assignments: Relatively simple computer simulations can help illuminate several phenmomena we will discuss, so some assignments will include a computational component. **I do not expect you to be an expert programmer.** I am not picky about what programming language you use to complete these assignments. To make things as easy as possible for beginners, I will support a single programming environment—Mathematica—and will provide a basic framework to build off of. If you do not already have Mathematica, you can install it on a personal computer for free through Northwestern's site license.

Course Outline (subject to change):

1. Week 1–Preliminaries–**Recommended Reading: Chapter 1, Section 2.17, Chapter 4**
   (a) Dynamical systems
   (b) Elementary probability recap
   (c) Principle of equal a priori weights
   (d) Microstates versus macrostates
   (e) Coin flips
   (f) The Central Limit Theorem and large deviations
2. Week 2–Basics of statistical mechanics–**Recommended Reading: Chapters 5-9**
   (a) Hamiltonian dynamics and the Microcanonical Ensemble
   (b) Open systems and the Canonical Ensemble
   (c) The Boltzmann distribution
   (d) Partition Functions
   (e) Energy fluctuations and heat capacity
   (f) Legendre transforms–Statistical view versus thermodynamic view
   (g) Statistical independence and the ideal gas law
3. Week 3–Not-so-basics of statistical mechanics–**Recommended Reading: Chapters 15-17**
   (a) Work, heat, reversible work, and free energy
   (b) Nonequilibrium work relations–Crooks and Jarzynski
   (c) Phase transitions and the Ising model
   (d) Markov Chain Monte Carlo
4. Week 4–Introductory kinetics
   (a) First order, second order, etc.
   (b) Steady state approximations
   (c) Michaelis-Menton kinetics
   (d) Mass action
5. Week 5–Less-introductory kinetics
   (a) Diffusion controlled rates
   (b) Transition state theory
   (c) Marcus theory