Teaching Statistical and Thermal Physics Using Computer Simulations

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Why is Statistical and Thermal Physics Difficult to Teach?

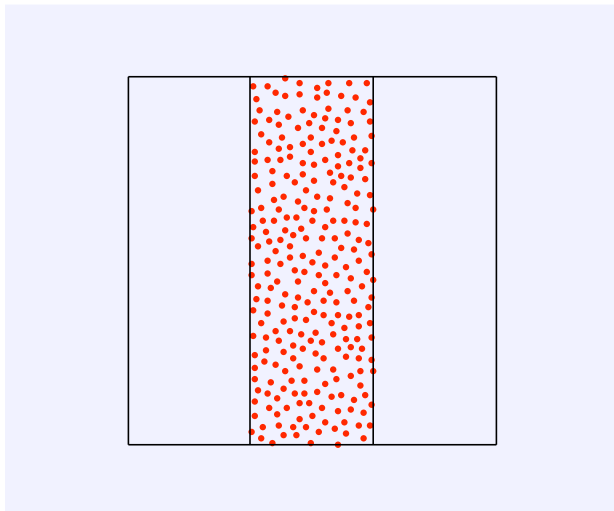
- No obvious organizing principle such as Newton's equations, Maxwell's equations, or the principle of least action. Statistical mechanics is frequently viewed as a collection of tricks. Baierlein has suggested:
  - Entropy and the second law.
  - The Boltzmann probability distribution.
  - The partition function.
  - The chemical potential.
- Students have many misconceptions about probability. The *central limit theorem* is the key to statistical mechanics, but its hardly mentioned in undergraduate texts.

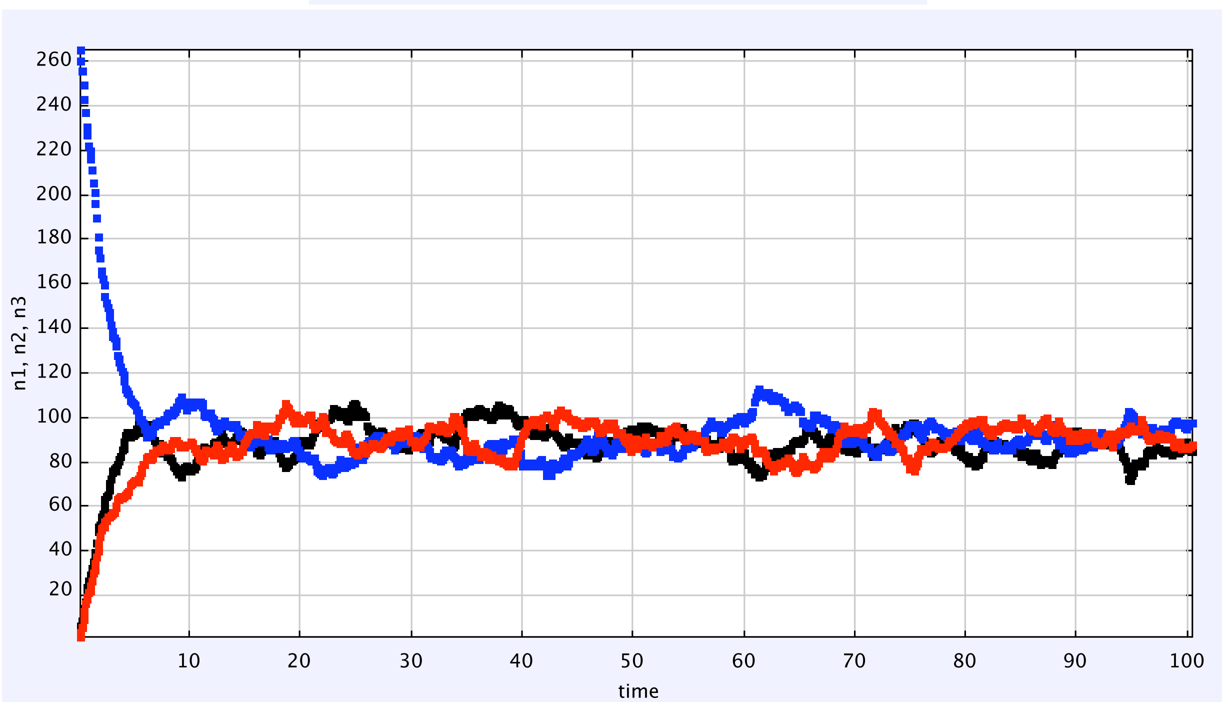
Why do Simulations?

- Qualitative observations:
  - Arrow of time.
  - Importance of fluctuations in equilibrium.
  - History independence.
  - Need for statistical approach.
- Talking about concrete models is more important than doing simulations. It is almost as effective to explain the model and algorithm, give students the data, and ask them to analyze it.
- A common student view of matter is similar to grains of sand bouncing off each other. Temperature is related to the "heat" given off when particles rub against each other.
- By discussing molecular dynamics (MD), we can discuss the forces between molecules.

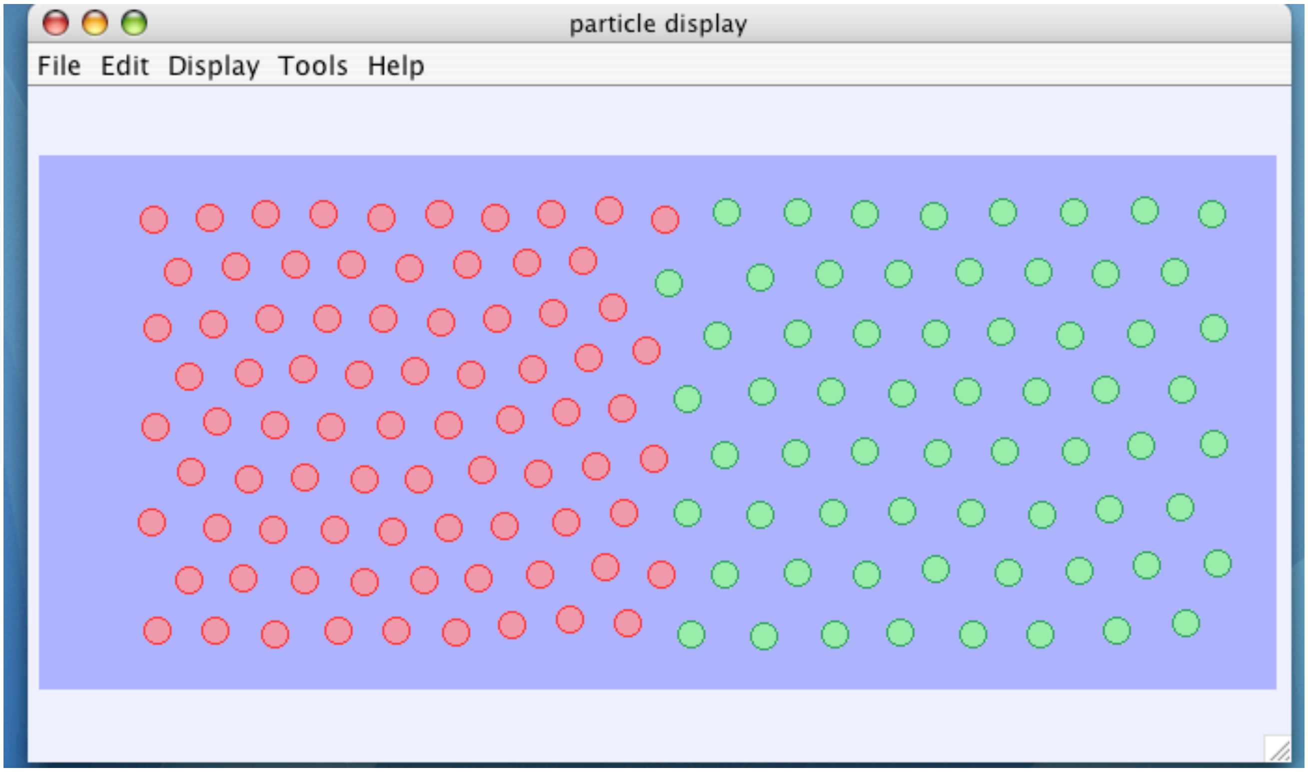
- Simulations can make concepts more concrete.
- Internal energy equals kinetic plus potential energy. First law becomes much easier to understand.
- Temperature proportional to KE for classical systems. Show by placing two systems in thermal contact.
- Pressure related to momentum transfer.
- Monte Carlo methods can make the different ensembles more concrete and illustrate ideas of probability.
- Can demonstrate the central limit theorem.
- Can compute integrals important in the context of the ideal Bose and Fermi gases.
- Can simulate interesting physical systems including a Lennard-Jones gas, liquid, and solid, random walks, diffusion, the Ising model, phase transitions, and the FPU problem.

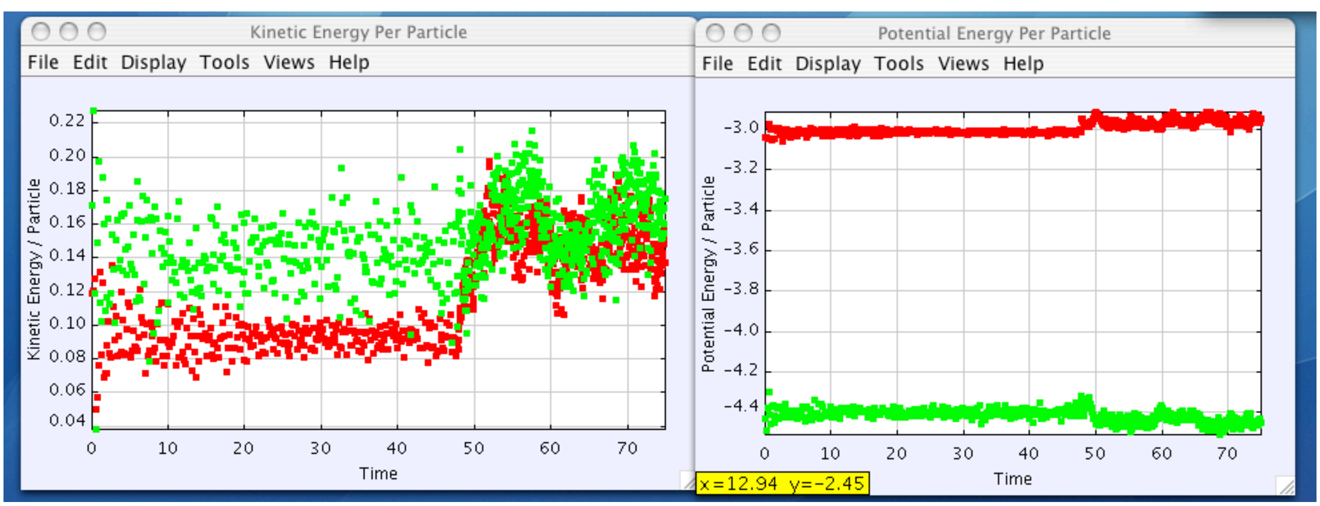
Approach to Equilibrium





Thermal Contact: What is the Temperature?





A Concrete Model of a Thermometer: The Demon Algorithm

- Demon has energy E_d and can exchange with a system. $E_d \geq 0$.

  1. Begin with system in initial configuration.

  2. Make random trial change in a degree of freedom in the system, for example, flip spin or move particle.

  3. If $\Delta E \leq 0$, accept change and give extra energy to demon.

  4. If $\Delta E > 0$ and demon has the energy, then demon gives the needed energy to system; otherwise, change is rejected.

  5. Repeat steps 3–5 many times and compute various averages.

The Demon as an Ideal Thermometer

- Demon algorithm simulates system in the microcanonical (constant energy) ensemble.

- What is the probability that demon has energy E_d? Example of a small system in equilibrium with a heat bath at temperature T.

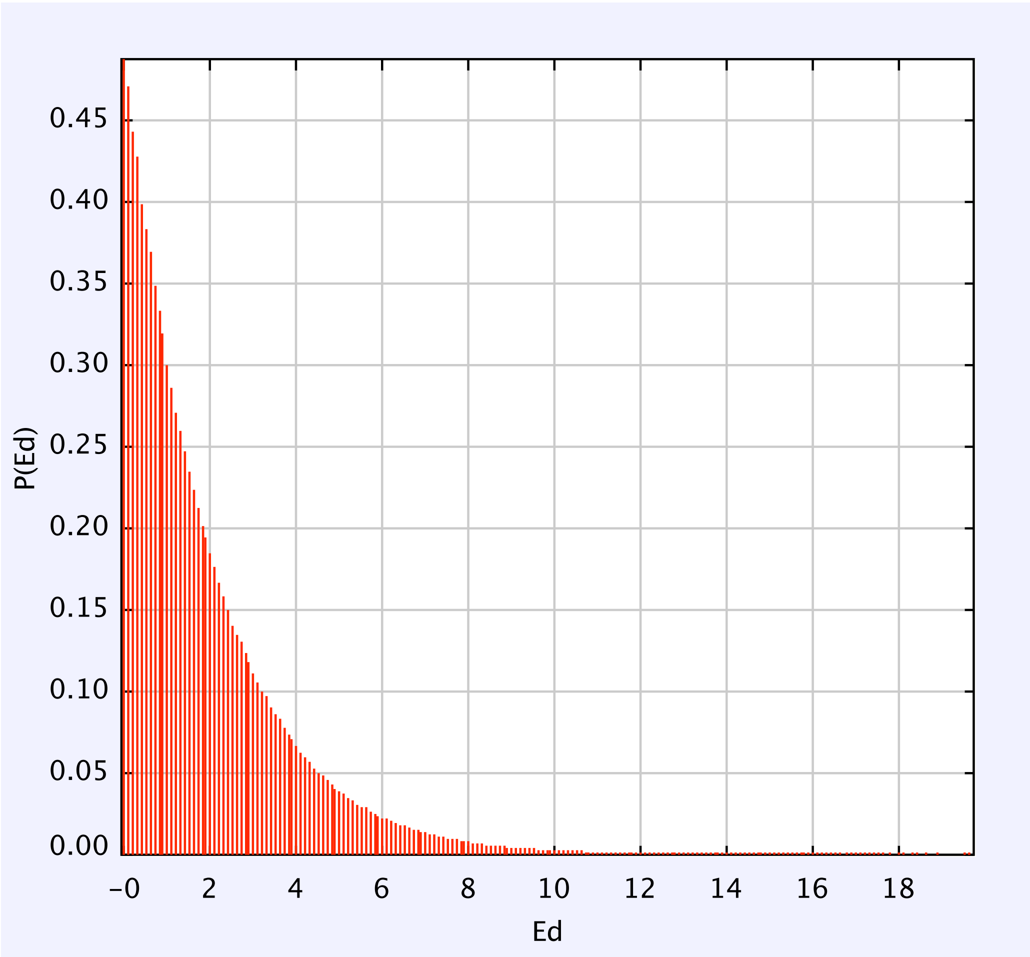
  $$P(E_d) \propto e^{-E_d/kT}.$$

  Temperature obtained from inverse slope of $\ln P(E_d)$ versus E_d.

- Demon interacts weakly with the system thermometer and attains the same temperature as the system, just like a real thermometer.

- Temperature is a measure of the ability of a system to transfer energy to another system. Temperature is not the same as energy.

Example Results



1D, $\epsilon \propto p^2$, $\overline{E}_d = 1.90$, $\overline{E}/N = 38.1/40 = 0.95 = kT/2$.
2D, $\epsilon \propto p^2$, $\overline{E}_d = 0.974$, $\overline{E}/N = 39.0/40 = 0.975 = kT$.

Other Simulations

1. Random walks.
2. Distribution of heads in a multiple coin toss.
3. Binomial distribution.
4. Central limit theorem.
5. Monte Carlo estimation. How does the error depend on the number of trials?
6. Einstein solid.
7. Molecular dynamics simulation of a Lennard-Jones fluid in two dimensions.
8. Simulation of hard disks and the mean free path.
9. Ising model.
10. Monte Carlo estimation of the density of states using the Wang-Landau algorithm.
11. Generalized demon algorithm that yields the chemical potential as well as the temperature.

Recent Text Books

<stp.clarku.edu/books/>

- Daniel Schroeder, *An Introduction to Thermal Physics*, Addison-Wesley (2000). Reviewed in AJP, December 1999, and Physics Today, August 2000.
- Ralph Baierlein, *Thermal Physics*, Cambridge Univ. Press (1999). Reviewed in AJP, December 1999, and Physics Today, August 2000.
- Craig F. Bohren and Bruce A. Albrecht, *Atmospheric Thermodynamics*, Oxford University Press (1998). Many practical applications. Reviewed in AJP, December 2000.

More Advanced Text Books

- Debashish Chowdhury and Dietrich Stauffer, *Principles of Equilibrium Statistical Mechanics*, Wiley-VCH (2000). Advanced undergraduate to graduate level. Comprehensive and excellent historical notes.
- Michel Le Bellac, Fabrice Mortessagne, and George Batrouni, *Equilibrium and Non-Equilibrium Statistical Thermodynamics*, Cambridge University Press (2004).
- Gene F. Mazenko, *Equilibrium Statistical Mechanics*, Wiley (2000). Reviewed in AJP, July 2003.
- James Sethna, Statistical Mechanics: Entropy, Order Parameters and Complexity, Oxford University Press (2006).
- Daniel C. Mattis, *Statistical Mechanics Made Simple*, World Scientific (2003). Reviewed in Physics Today, July 2004.
- Special theme issue of AJP, December, 1999.

Open Source Textbook

Freely available from `<stp.clarku.edu/notes>`.

H. Gould and J. Tobochnik, *Thermal and Statistical Physics*

1. From Microscopic to Macroscopic Behavior
2. Thermodynamic Concepts
3. Concepts of Probability
4. Statistical Mechanics
5. Magnetic Systems
6. Noninteracting Particle Systems
7. Thermodynamic Relations and Processes

Can the development of Linux and Apache be a model for the development of textbooks?