

# Computer simulations as concrete models for student reasoning

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In many thermal physics courses, students become preoccupied with the manipulations of differentials and partial derivatives in thermodynamics and integrals and sums in statistical mechanics. One problem is the lack of concrete models that will help provide physical insight into the mathematics. For example, the internal energy  $U$  has little meaning to most students. We have used discussions of computer simulations to provide concrete models for students as well as applications of abstract ideas such as thermal averages, entropy, probability distributions, and density of states. I will discuss how to use discussions of molecular dynamics, Monte Carlo, and histogram simulations in thermal physics courses.

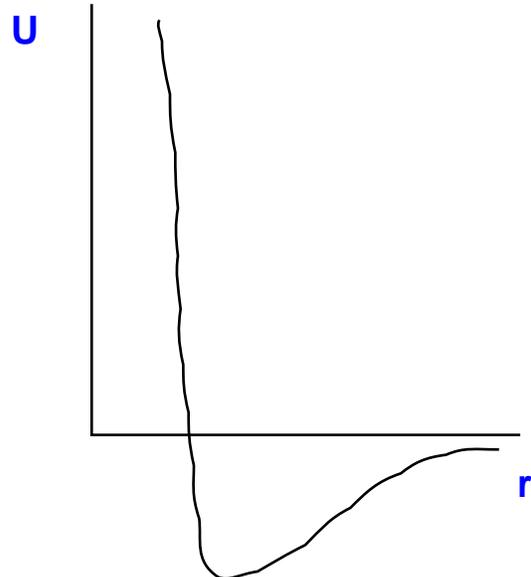
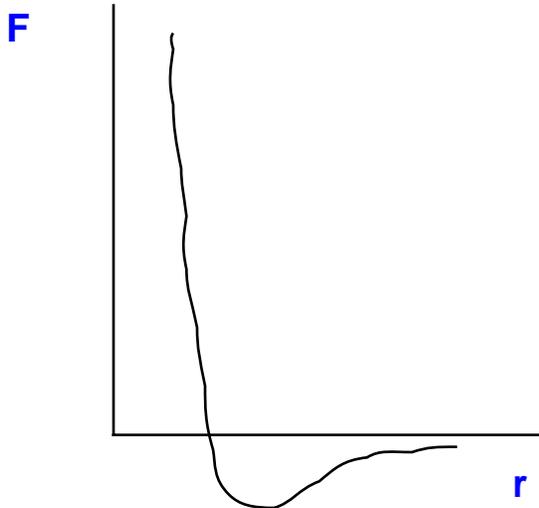
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## Molecular Dynamics: Providing students a microscopic model of matter

- Student's vision of matter is that of grains of sand bouncing into each other.
- Temperature is related to "heat" given off when particles rub against each other.
- Energy is a combination of kinetic and gravitational potential energy.
- Pressure is how close particles are to each other.

### By discussing molecular dynamics we can discuss forces between molecules:

- Repulsive force: must exist because matter doesn't collapse to a point.
- Attractive force: because liquids form.
- Forces lead to potential energy.



**Discussing numerical integration of Newton's laws makes these ideas more concrete and shows that molecular motion is random, but macroscopic quantities vary smoothly.**

- **Temperature related to kinetic energy - discuss putting two systems next to each other, collisions, energy transfer.**
- **Pressure related to momentum transfer with walls - depends on mass of particles, how often they hit walls, and their velocity.**
- **Energy is kinetic and intermolecular potential energy.**

## Demon Algorithm: A concrete model of a thermometer

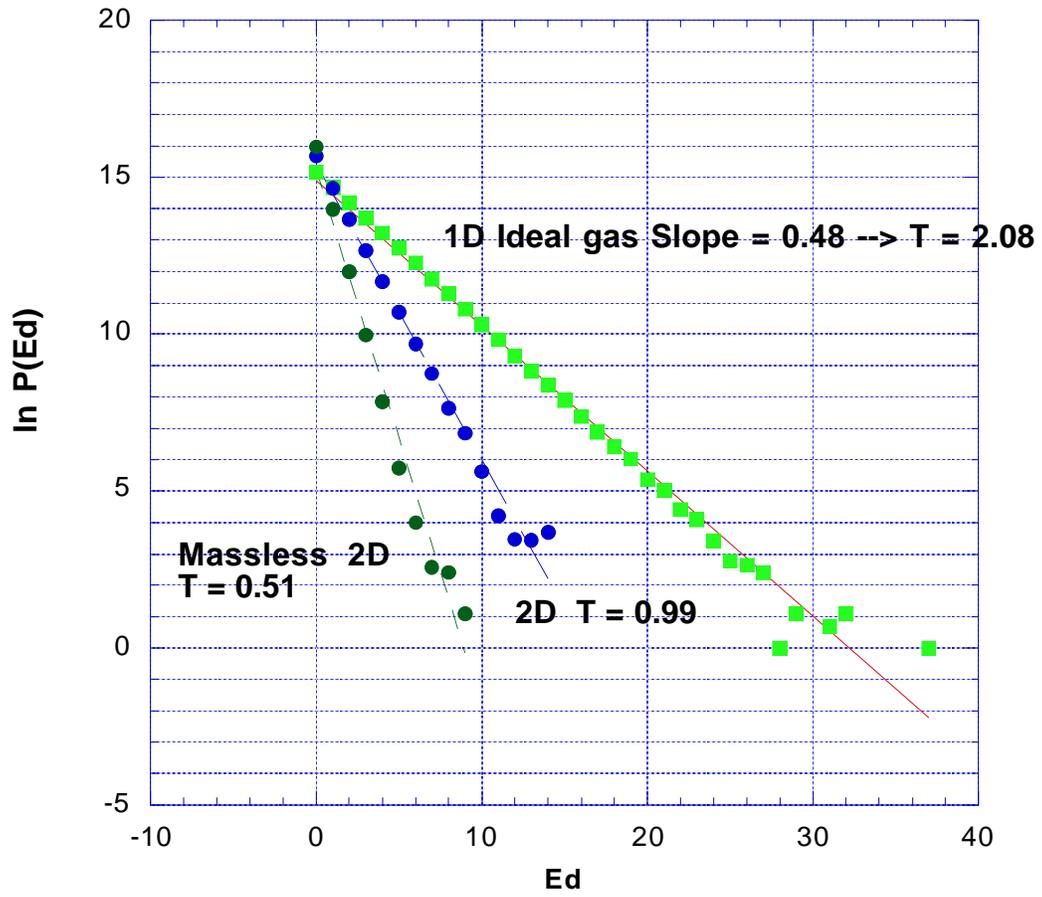
**Demon algorithm used to simulate systems in the microcanonical (constate energy) ensemble:**

1. Begin with system in some initial configuration.
2. A “demon” has energy which it can give to or take from the system.
3. A degree of freedom in the system is potentially changed, e.g., particle moves, spin flipped.
4. If energy of system is decreased, then change is made and change in energy given to demon.
5. If energy is increased and demon has the energy, then demon gives the needed energy to system; otherwise, change is rejected.
6. Repeat steps 3-5 many times.

## **Demon acts as a thermometer (example of a system in equilibrium with a thermal bath):**

- Temperature obtained from the slope of  $\ln (P(E))$  versus  $E$  of demon,  $P(E) \sim \exp(-E/kT)$ .
- Algorithm can be used for its own sake or just as a measuring device to measure temperature using some other algorithm (e.g., MD) to simulate system.
- Demon interacts weakly with system just as a real thermometer should.
- Demon comes to same temperature as system, just like a real thermometer.
- Temperature is not the same thing as kinetic energy by considering relativistic systems or photon gas.
- Can discuss how demon will work at high and low temperatures to obtain a concrete microscopic picture of what temperature means.

# Ideal gas results $E/N = 1.0$



# The Flat Histogram Method: Understanding the density of states

## Two key ideas in Statistical mechanics:

**Boltzmann distribution:**  $P(E)$  is probability density of a state of energy  $E$  occurring. Depends on  $T$ . Same for all matter.

**Density of States:**  $g(E)$ : number of states with energy  $E$  per unit energy interval. Does not depend on temperature. Different for each kind of material.

## Numerical method of estimating $g(E)$ (Wang and Landau):

1. Assign all energies  $g(E) = 1$ , and begin with an initial configuration, and an arbitrary parameter  $f > 1$ .
2. A degree of freedom in the system is potentially changed (e.g., particle moved, spin flipped). Energy would go from  $E_1$  to  $E_2$ .
3. If  $g(E_1) > g(E_2)$ , accept move and set  $g(E_2) = fg(E_2)$ .
4. If  $g(E_1) < g(E_2)$ , accept (and set  $g(E_2) = fg(E_2)$ ) if  $g(E_1)/g(E_2) > r = \text{random number on } [0,1]$ . Otherwise, reject and set  $g(E_1) = fg(E_1)$ .
5. Repeat steps 2-4 many times.
6. Let  $f$  go to  $f^{1/2}$  so that  $f$  moves towards unity. Repeat 5.

This algorithm produces a flat histogram of states  $H(E)$  because we are favoring energies with low  $g(E)$ , but there are more ways of getting to energies with high  $g(E)$ .

In class you can discuss how different systems would have different  $g(E)$ 's using this algorithm.

# Density of states for a particle in a Lennard-Jones potential

