Topics for Today

- What is Physics?
- Computational Thinking in Physics
- A Case Study in Thermal Physics

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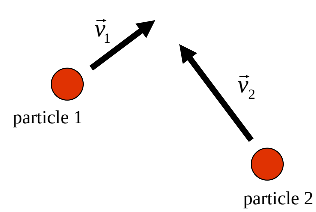
Physics

- discovers and applies fundamental principles to build models of physical systems that predict and explain more and more of what we observe in the Universe
- is built on foundations laid 300^{+} years ago
  - Newton's laws
  - Maxwell's laws
  - Einstein's relativity
  - Quantum mechanics

  ⋮



Present laws govern all types of matter and interactions in all situations!

Physics

- is constantly testing and refining its relatively small number of fundamental principles
  - to seek simplest possible explanations
  - to extend range and precision of its predictions
- increasingly relies on computation both to make predictions and to analyze data gathered to test our understanding

Computational Thinking in Physics

- modeling real physical systems beginning from fundamental principles involves layers of complexity
- computational thinking
  (exploiting layers of abstraction [Wing 2009])
  is makes it possible to manage such complexity
  - simulation to make predictions
  - data management and processing to test them

Thermal Physics

- treats emergent behaviors in macroscopic systems
  - macroscopic ≡ large number of interacting objects
    - Avogadro's number

$$N_A \approx 6 \times 10^{23} \text{ atoms / mole.}$$

- Case Studies: Thermal Equilibrium
  - distribution of energy among gas atoms or molecules
  - orientation of "spinning" atoms or molecules in a magnetic film

Modeling Thermal Systems

- in principle, track the motion of every particle and account for every interaction
  - molecular dynamics

Gas.py

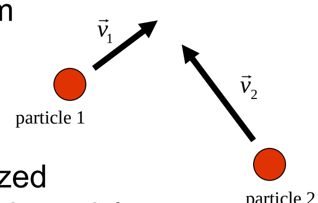
- in practice, dealing with macroscopic numbers of objects can be overwhelming
  - *N* particle trajectories
  - *N(N-1)* pairs of interactions
- essential to study behavior far from equilibrium, but …

Modeling Equilibrium Systems

- microscopic features of any thermal system are always changing
- macroscopic features of isolated thermal systems stop changing – systems settle into equilibrium
- a combination of physical and computational thinking leads to ways of efficiently predicting equilibrium properties of thermal systems!

An Ideal Gas in Equilibrium

- physical thinking
  - energy of an isolated system is conserved
  - microscopic interactions redistribute particle energies seemingly at random

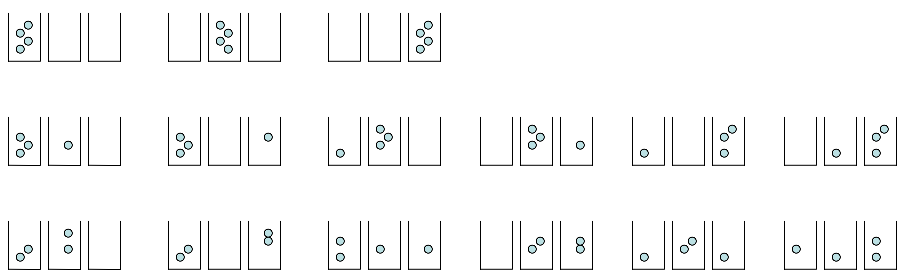


- emergent picture
  - system microstates characterized by particular velocities for each particle
  - interactions cause random microstate change

Fundamental Principle of Statistical Physics

- every microstate (microscopic distribution of energy) of a system corresponding to a given macrostate (total energy) of the system is equally probable
- This abstraction exhibits elements of both physical and computational thinking!
- Let's explore its consequences by considering all the microstates of a small system.
  - the system has just three constituents that can exchange discete amounts of energy.
    - we exploit the simple nature of a system of such "quantum" oscillators to make a general point.

The figure below depicts the microstates corresponding the macrostate of this system having 4 units of energy. Each unit of energy is represented by a blue dot. Each constituent is represented by a container.



Notice that there are more microstates with energy spread more evenly between the microscopic constituents. The probability of observing a microstate with one constituent having all of the energy is only 3/15 = 1/5.

- this tendency for energy to be spread evenly among system constituents becomes very pronounced in macroscopic systems.
  - the fundamental principle of statistical physics then implies that the equilibrium properties are determined by these highly probable microstates

- a computational approach of random sampling (Monte Carlo method), therefore, allows a very efficient way to generate these highly probable microstates so that they can be used to estimate systems' equilibrium properties.

We introduce a "demon" that interacts with the system to conserve energy!

The Demon Algorithm

Begin with the macroscopic system of interest and the demon in a state in which their total energy is equal to the energy of the desired macrostate of the system.

Let the demon "interact" with a random constituent of the system of interest, by trying to make a random change in the state of the constituent. We would, for example, try to make a random change in the velocity of an atom if the system of interest happened to be a gas.

If the trial change decreases the energy of the constituent, the change is made and the extra energy is transferred to the demon.

If the trial change increases the energy of the constituent, the change is made only if the demon has enough energy to transfer to the constituent.

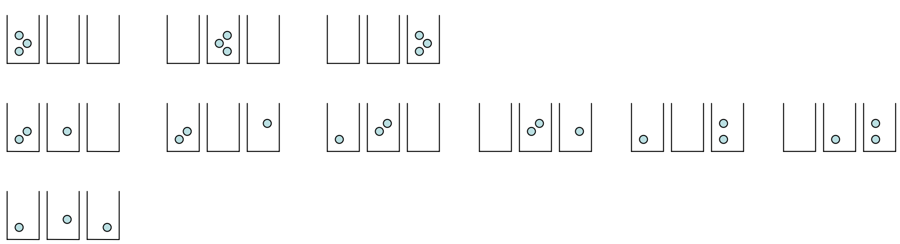
In this way, the energy of the system plus demon remains constant as new microstates of the system are generated.

Since the Fundamental Principle of Statistical Physics predicts that a system's energy will most likely be shared equally among the demon and constituents of the original system, the demon will barely change the average energy of a macroscopic system having an enormous number of microscopic constituents.

To illustrate how the demon algorithm works, lets add a demon to the tiny system of three microscopic constituents in a macrostate with 4 units of energy, the system we considered before.

The 15 microstates of that system that we listed earlier correspond to the microstates of the combined system-demon system with zero demon energy!

If we try to make a change in one of those micro states that decreases the energy of a system constituent by one unit, we can do so by giving that unit to the demon. The original system would now be in one of these 10 microstates corresponding to a macrostate with only 3 units of energy.



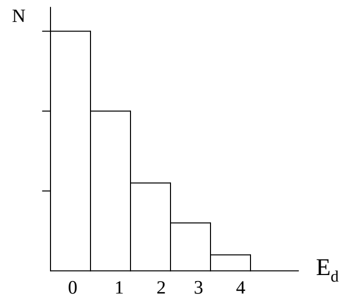
Since there are 10 of these microstates and 15 of the ones with zero demon energy, it follows that if we make a long series of random microstate changes, the relative probability of finding the demon with zero as opposed to one unit of energy would be 15/ 10 = 3/ 2.

While the demon perturbs this tiny system significantly, the system is still more likely to be found with the original macroscopic energy rather than any specific lower energy.

Check for yourself that if the demon has 2 units of energy, there are 6 microstates of the combined system-demon system.

If the demon has 3 units of energy, there are 3 such microstates. If it has all 4 units of the energy, there is only 1 microstate of the combined system.

Together our microstate counting results imply that if we use the demon algorithm to generate a large number of random microstates of our tiny system, the histogram below would represent the relative number of these microstates in which the demon has 0, 1, 2, 3 or 4 units of energy.



For a macroscopic system, the probability of generating microstates with demon energy E relative falls off exponentially relative to the probability of generating microstates with zero demon energy,

$$\frac{P(E_d = E)}{P(E_d = 0)} = e^{-E/kT},$$

where k is Boltzmann's constant and where T is the temperature of the macroscopic system.

This Boltzmann distribution governs the energy states of any microscopic constituent of a macroscopic thermal system in equilibrium.

Notice that by examining the distribution of demon energies when using the demon algorithm and the Monte Carlo method to predict the properties of a thermal system we can determine the temperature of the system as a function of its macroscopic energy.

In effect, we can use the demon as a thermometer!

Modeling an Ideal Gas using the Demon Algorithm

- Possible initial states
- Generating new microstates consistent with the gas’ macroscopic energy
- Accumulate the demon energy distribution
- Display the distribution of particle of velocity components in the equilibrium state

IdealDemon.py

Approximations and Idealizations

- Particle energy independent of particle position
- Can treat a 3-d ideal gas a 3 independent 1-d ideal gases!