Computational Assignment 2: The Demon Algorithm

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In this computational exercise, you will learn to write an efficient Monte Carlo procedure for simulating systems at a given fixed energy E. Consider an isolated ideal gas of N particles of unit mass whose energy is given by

$$E = \sum_{i=0}^{N} \frac{1}{2} m v_i^2 \equiv \frac{1}{2} \sum_{i=0}^{N} v_i^2,$$

and imagine that we want to study the thermodynamic state of this system at equilibrium. One way to do this would be to find $\Omega(E)$ by brute force, but this is very inefficient and not practical even for small N.

An efficient method to do this is to slightly relax the energy conservation constraint. Let us assume that we add an extra degree of freedom to our gas. For historical reasons, this degree of freedom is called a *demon*. Since the demon is only one degree of freedom and a gas typically has $N \gg 1$, it can be thought of as a very small perturbation to the system. The role of the demon then is to act as a reservoir of energy as it attempts to change the state of the system. The total energy $E = E_s + E_d$ remains unchanged. The demon initially has $E_d = 0$. It then hops from particle to particle, and tries to change the particle's velocity. If its desired change lowers the energy of the system, the excess energy is given to the demon. If the desired change raises the energy of the system, the demon gives the required energy to the system, provided that it has enough energy to give. If not, it moves on and tries again with the next particle. The only constraint on this system is that the demon cannot have negative energy.

The algorithm is thus as follows:

- Choose a particle of the gas at random and make a trial change to its velocity. You can define a maximum velocity change $\Delta v_{\max}$ and choose values between $-\Delta v_{\max}$ and $+\Delta v_{\max}$.
- Compute ΔE, the change in the energy of the system due to this trial change.
- If $\Delta E \leq 0$, the trial configuration is always accepted and the energy is given to the demon, i.e.

$$E_d \longrightarrow E_d + |\Delta E|.$$

- On the other hand, if $\Delta E > 0$, the trial is only accepted if the demon can provide the energy needed for this change, i.e. if $E_d \geq \Delta E$. If the demon has enough energy to give, its energy is then changed to

$$E_d \longrightarrow E_d - |\Delta E|.$$

- This entire process is repeated N times. This constitutes one Monte-Carlo *sweep*.
- After a sufficient number of such sweeps, the demon and the system will agree on their respective average energies. Once this has happened, average over the stabilised values to get $\langle E_s \rangle$ and $\langle E_d \rangle$.

(a) In the code file provided, use the algorithm given above to complete the `oneMCS` function and thus simulate one Monte-Carlo sweep. [4]

(b) Let $N = 100$ and take $E_s = 15$ and $E_s = 25$, and give all particles the same initial velocity. Complete the `simulate` function which runs `n_mcsweeps` Monte-Carlo sweeps of the system and returns the system energy and the demon energy as a function of the sweep number. By plotting $\langle E_d \rangle$ or $\langle E_s \rangle$ as function of `n_mcsweeps`, estimate roughly by when equilibrium has been reached, and calculate both $\langle E_s \rangle$ and $\langle E_d \rangle$ once this happens for both $E_s = 15$ and 25. Obtain an approximate relation between the mean demon energy and the mean system energy *per particle*. [2]

(c) We will now explore why we can consider the demon to be an ideal thermometer. An ideal thermometer is one that does not affect the system of interest. Since the demon is a perturbation of order $1/N$, it satisfies this condition when $N \gg 1$. It exchanges energy with the system, but does not change its own energy very much.

As we are working with the microcanonical ensemble where all states with some energy E are equally likely, show that the probability that the demon has some energy E_d is given by

$$P(E_d) \propto \Omega_{\text{sys}}(E - E_d) \times \Omega_{\text{dem}}(E_d).$$

Since the demon is only one degree of freedom, it has only one state for each E_d, and so $\Omega_{\text{dem}}(E_d) = 1$.

Writing

$$\Omega(E - E_d) = e^{S(E-E_d)},$$

and using the definition of temperature you have seen in class as

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{V,N},$$

show that you can write

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

Find the constant of proportionality, and show that $\langle E_d \rangle = T$. [2]

(d) For the values of E_s in part (b), plot a histogram of the demon energy once equilibrium has been reached. Compare it to the analytical result in part (c). Use this in the approximate result you obtained in part (b) to obtain a relation between the average energy of the system and the temperature. How does your result compare with the relation given for a 1D gas in your thermodynamics course, $E_s = \frac{1}{2}NT$? Try to generalise your code to 2 and 3 dimensions. [2]