Entropy and Information for an Automated Maxwell's Demon

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Abstract

In an attempt to create a Maxwell's demon that does not depend on information, we have developed a computational simulation of a demon that uses an automated, refrigerated trapdoor. We keep track of and compare the entropy reduction by the demon and the entropy cost of running the refrigerator.

Background and Rationale

Skordos and Zurek[1] have developed an ingenious type of Maxwell's demon, one that operates without any information on molecular positions or speeds. Their work is based on a suggestion made by Smoluchowski[2] in 1912 that a mechanical, perhaps spring-loaded trapdoor separating two chambers of ideal gas molecules might act as a one-way valve for faster molecules. Smoluchowski concluded that the Second Law would lead us to believe that thermal fluctuations would in fact prohibit such a mechanical demon from creating on average a net entropy reduction, although his work by no means proved this fact conclusively.

The idea of a mechanical demon is enticing, because of the conclusive work by Landauer, Bennett, and others in the physics of computation. Their work has shown that there is not necessarily any entropy increase associated with the gathering of information, but that in a reversible computation cycle there is an entropy increase associated with information erasure or the resetting of a memory. Their work has in a sense rendered obsolete the ideas of Szilard and Brillouin, not to mention the computational studies one of us (Rex) did in the 1980s.

But with a mechanical demon there should be no information to consider in the first place. The device developed by Skordos and Zurek consists of two gas chambers of equal area, with a hole between those chambers and a trapdoor that can just cover the hole (Figure 1). The door is free to slide back and forth on rails between two stops, one of them at the chamber interface and the other in the interior of one chamber. In this way an asymmetry is created, with molecules on one

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away from it when it approached the "closed" position. They discovered that this scheme could be used to create a density imbalance. Of course this does not in principle violate the Second Law, because there is some energy expense involved in slowing the door's motion.

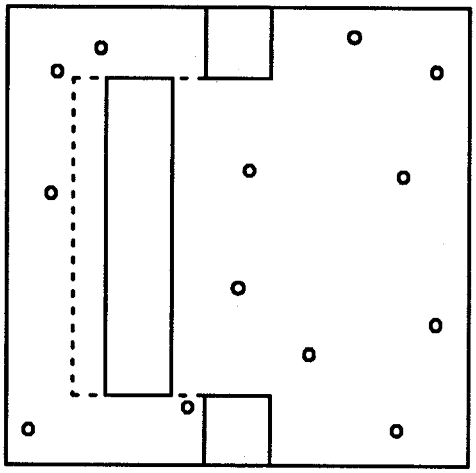

Figure 1. Schematic diagram of the mechanical demon system.

side tending to push the door open, but those on the other side tending to push it closed. A "run" consists of watching a computer-simulated evolution of the molecules as they collide elastically with the chamber walls, the trapdoor, and each other. Skordos and Zurek showed that their device could act as a "rectifier". That is, there is a natural tendency for molecules to flow one way through the trapdoor opening but a reluctance to flow in the other direction. Skordos and Zurek further showed that their device is not successful in defeating the Second Law, because it cannot be used to create a density difference between the two sides, due to the random thermal motion of the door itself, thus verifying what Smoluchowski had suspected 80 years ago. Following this logical line, they used a scheme for "refrigerating" their trapdoor, taking energy

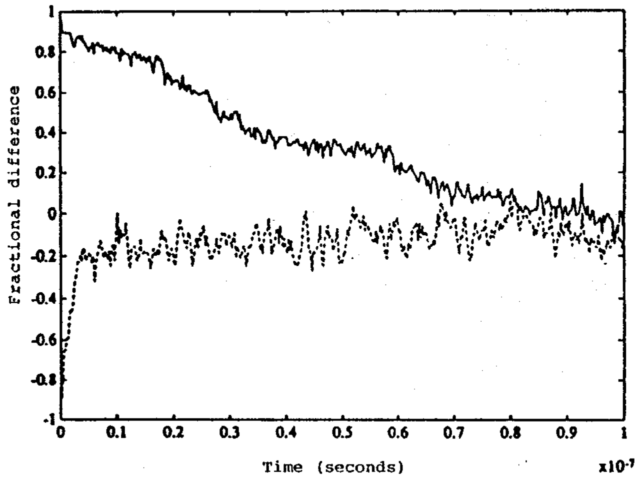

Figure 2. Rectifying behavior of the mechanical demon. When a run is started with all particles in the left chamber (top curve), the approach to equilibrium is slower then when the run is started with all on the right (bottom curve).

We have developed a simulation along the lines of the one made by Skordos and Zurek. We began by quickly verifying that our device could act as a rectifier (Figure 2). But instead of looking further at the qualitative behavior of the system, our work has focused on the measurement of entropy. If this refrigerated mechanical demon creates a density difference between the two sides of the container, it should be possible to compute the entropy reduction from fundamental relations. Specifically, Boltzmann's entropy equation S = k log w (where w is the number of microstates that will generate a particular macrostate) can be used to compute the entropy associated with various configurations of molecules. Actually the quantity w must be adjusted slightly by the fact that the door occupies a small fraction of the volume of one side of the container. The computation of the change in statistical entropy from one macrostate to another is then straightforward.

According to the Second Law, there must be an offsetting entropy increase, and in this case it is due to the energy dissipated in running the refrigerator. In the process of refrigeration we have extracted some energy from the door. In our model we refrigerate by letting the door (when it reaches the closed position) interact with a fairly low temperature heat bath. Then the entropy added to the heat bath is simply the energy lost by the door divided by the temperature of the bath, according to the well-known thermodynamic relation. We are then able to compare the thermodynamic entropy increase with the statistical entropy reduction mentioned above, or rather, compute their sum to find the net entropy change of the entire system.

Implementation

To implement our scheme, it is necessary to derive the collision and timing equation of the system. The collision equations give the new velocities of the colliding bodies in terms of their initial velocities. We assume perfectly rigid walls so that when a particle hits a wall, we simply reverse the component of its velocity that is perpendicular to the wall. This has the effect of treating the particles as light rays reflecting off of a mirror. In collisions between two particles, or between a particle and the trapdoor, the collision equations are derived using the conservation of energy, conservation of momentum, and the fact that the force of collision acts along the line connecting the particles' centers. This calculation is much easier if it is performed in the rest frame of one particle, so in our computer program we transform into the rest frame of one particle and calculate the new velocities before transforming back to the box's reference frame.

The timing equations tell us the amount of time until the next collision. For collisions involving a particle with a wall, another particle, or the trapdoor, these are straightforward to derive. Once the time to the next collision has been computed, the particles and trapdoor are moved along the straight line trajectories dictated by their velocities. The collision equations then change the velocities of the colliding bodies, and we calculate the time to the next collision.

Before we can run the program, it is necessary to initialize the positions and speeds of each particle. Since our program is supposed to model the real world, we choose to initialize the velocities so that the distribution of particle velocities closely approximates the two dimensional analog of the Maxwell-Boltzmann speed distribution. This is a straightforward procedure once the correct distribution is known. By modifying the arguments used in derivations of the Maxwell-Boltzmann distribution, it is straightforward to derive the two dimensional distribution:

$$F(v) = \frac{mv}{kT} \exp\left[-\frac{mv^2}{2kT}\right] \qquad (1)$$

This function, similar in shape to the well-known Maxwell-Boltzmann distribution, is known as the Rayleigh distribution.

The particles are assigned speeds according to the Rayleigh speed distribution F(v). Velocity is a function of speed and direction so once a particle has a speed, we assign it a direction using a random number generator. Having initialized the particle velocities, we now need to initialize their positions. We assign each particle to a random position on a predetermined side of the box. The number of particles to be placed in each side is varied from run to run. To initialize the door's motion, we give it a speed that we would expect it to have if it were at the same temperature, T, as the gas. We use the door's single degree of freedom and the equipartition theorem to compute the door's likeliest speed

$$v = \sqrt{kT/m} \qquad (2)$$

and give the door this speed initially.

The Door as a Pressure Demon

To test whether the trapdoor can create large pressure differences between the two sides, we record the fractional difference between the number of particles in each half as a function of time. The fractional difference is defined as the number of particles in the left half minus the number of particles in the right half, divided by the total number of particles. The system rapidly approaches an equilibrium about which it fluctuates. The equilibrium value of the fractional difference is nonzero because the trapdoor's finite width keeps some area from being occupied by the particles. Our simulations show that the fractional difference approaches exactly the value expected at equilibrium. This means that the trapdoor does not act as a pressure demon, and we are prompted to ask why this is the case. We have found that the door's speed increases over time, leaving the door open so often that a pressure difference cannot be maintained. This is consistent with the behavior Smoluchowski predicted for automated demons.

The above result suggests that the trapdoor cannot decrease the entropy of the system when left to itself, because the door's high speed lets particles pass through the opening. To test whether or not the speed of the door really affects the ability of the trapdoor to operate as a demon, we changed our program to remove energy from the door periodically, effectively cooling it. The energy removal scheme pulls energy out by slowing the door at the instant it collides with the center partition. This has the effect of keeping the door near the closed position longer than would otherwise occur. Our findings, which resemble Skordos and Zurek's, show that the cooled door can create large pressure differences between the two sides (Figure 3). Since we can create a measurable pressure difference, we need to find a way to see if the entropy change associated with cooling the door offsets the decrease associated with the pressure difference. We believe that this is the first time that actual measurement of the entropy change caused by the operation of an automated demon has been done, and we expect this to make our analysis of the demon's behavior less dependent on intuition than earlier analyses of automated demons. Below we outline a method of measuring the actual entropy change in our system, taking into account the energy removed from the system.

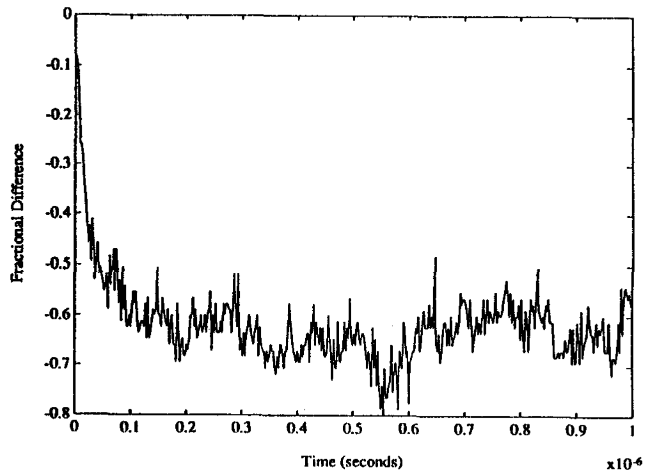

Figure 3. A pressure difference is created by the use of a refrigerated door.

Entropy in the Operation of the Heat Pump

To fully test the ability of the trapdoor to decrease the entropy of the box/heat bath system, we must first formulate a precise measure of the entropy of the system. It is straightforward to measure an entropy change due to a change in the number of particles on each side of the box. Less probable configurations correspond to a lower entropy than more probable configurations, a fact which is quantified using the Boltzmann distribution

$$S = k \log(w)$$

where w is the standard statistical weight used in statistical mechanics. The derivation of w is complicated by the fact that the two halves of the box are not of equal volume, due to volume excluded by the trapdoor. Let the left half of the box have volume V_L, the right volume V_R, and the box itself have volume V. The probability that L out of N particles will be on the left side in a random initial configuration is given by elementary probability theory as:

$$\frac{(V_L/V)^L \ (V_R/V)^{N-L} \ N!}{L! \ (N - L)!}$$

The number of macrostates is simply the total number of microstates times the probability of a single macrostate occurring. So, the number of microstates for the macrostate with L particles on the left is given by

$$w = \frac{2^N \ (V_L/V)^L \ (V_R/V)^{N-L} \ N!}{L! \ (N - L)!} \qquad (3)$$

The above w lets us define the entropy to be

$$S = k \log \frac{2^N \ (V_L)^L \ (V_R/V)^{N-L} \ N!}{L! \ (N - L)!} \qquad (4)$$

We shall henceforth call this value the statistical entropy. The change in statistical entropy is easily calculated since we compute S_0, the initial value of S, before we begin the time-evolution of our system.

We also need to measure the entropy change due to the energy removed from the system each time we slow the door. The change due to cooling the door will, for reasons that become clear below, be called the thermodynamic entropy. The magnitude of this entropy change depends on what method is used to cool the door. To keep the simulation physically reasonable, we assume that the trapdoor is momentarily put in contact with a heat bath at temperature T_b each time the door reaches its closed position. If the door had the same temperature as the heat bath, we would expect its speed to be:

$$v = \sqrt{kT_b/m} \qquad (5)$$

To cool the door, we try to bring its speed closer to the speed we expect the door to have if it is at the temperature of the bath. To do this we decrease the door's speed to an amount equal to the average of the door's initial speed and the expected speed every time the door has a collision with the center dividers; this removes energy from the door by an amount that increases as the temperature difference increases. The cooling process effectively takes a certain amount of energy, dQ, and dumps it into the heat bath. The well-known thermodynamic relation then gives us the entropy change associated with this process as:

$$dS = dQ/T_b \qquad (6)$$

Now that we have determined the form of both the thermodynamic and statistical entropy changes in our system, we can compute the total entropy change associated with each run. The change in the statistical entropy will often be negative, but we expect this to be offset by the entropy increase from the very cooling process that lets the door create the pressure difference. A bonus is that we make a direct connection between the entropy concept as it is defined in statistical mechanics and the entropy commonly used in thermodynamics. It is important to note that our statistical entropy is only defined to within an additive constant, as is the thermodynamic entropy. Since we are only interested in the change in entropy, there is no need to invoke the Third Law of Thermodynamics to determine the additive constant.

Entropy and Information in the Trapdoor System

Our simulations use 170 particles to keep computing time to a minimum. Larger particle numbers are not expected to change our results, but it is important to keep in mind that the trapdoor operates in a high vacuum. Studying the result of a representative simulation, that was started with approximately half of the particles on each side of the box, we find that there is a decrease of the net entropy (thermodynamic + statistical) of the system equal to -2.4×10^{-22} J/K (Figure 4). This data suggests that the trapdoor system does operate as a demon, easily violating the Second Law of Thermodynamics in virtually every run.

What will save the Second Law? It is the connection with information, the quantity we sought to avoid by using a mechanical demon. By starting a run in a maximum entropy configuration, we have in fact supposed that we have knowledge of the positions of all the particles. The maximum entropy state is indeed the most probable macrostate, but it is by no means the only likely one. Since we have restricted ourselves to a relatively small number of particles, the probabilities of other macrostates are not negligible. Therefore, the observed entropy decrease occurs because we start the system near its maximum entropy configuration. We need to store some information about the system to give the box this initial configuration, and this must be erased to complete a cycle. This erasure has a large entropy increase associated with it, according to Landauer's principle, that more than makes up for the decrease we see within the system.

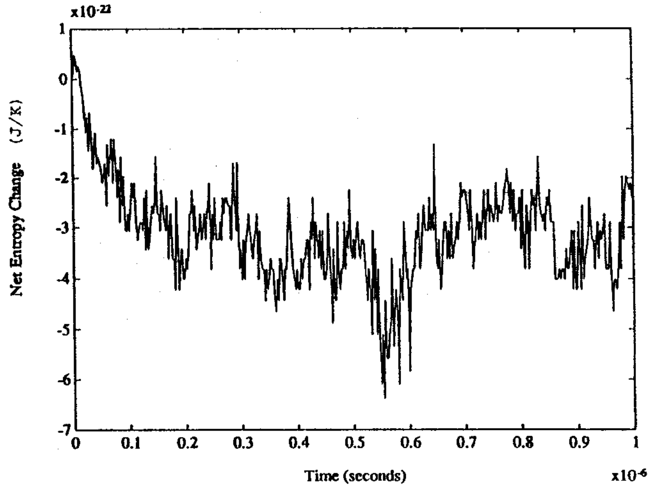

Figure 4. The demon creates a net entropy reduction when the run begins with equal numbers of particles on each side of the partition.

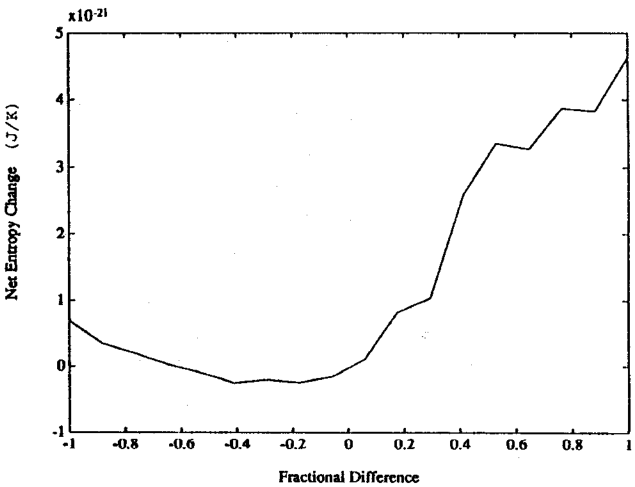

Figure 5. The net entropy change as a function of the initial fractional difference. Notice that there is a net entropy decrease for only a few special initial configurations, and for other initial configurations the entropy increase can be large.

Operation of the Demon in the Absence of Information

For the system to be truly automated, and to have a fully mechanical demon, we have to operate the demon without using any information about its initial state. To do this, the simulation must be run with initial conditions that range from all particles on the left to all particles on the right. Our procedure involves starting all of the particles on the left, then running the simulation. Then we place ten particles on the right and the rest on the left and run the simulation. We continue this process until we have run simulations with initial conditions ranging from all particles on the left to all particles on the right. Figure 5 shows the net change of entropy as a function of the initial fractional difference. Since each initial configuration is not equally likely, we compute the weighted average by multiplying the net change for a given fractional difference by the probability of this state occurring naturally. In our initialization procedure the particles are placed in equal volumes on each side of the box. Therefore, the probability of the various initial configurations follows the binomial distribution:

$$P(L) = \frac{N!}{2^N \; L! \; (N-L)!} \qquad (7)$$

It must be noted that our initialization scheme carries no information cost, since we can simply mask the forbidden regions before we toss the particles into the box. The weighted entropy curve (Figure 6) is simply the data from Figure 5 where each point has been multiplied by the appropriate weighting factor. By summing over this curve, we find the average entropy associated with each blind run of the door to be about 2.75 x 10^{-24} J/K. In the case shown, the entropy change associated with the operation of our totally mechanical demon is (barely) positive. We must note that the error bars on this data point are large enough to include the point $\Delta S = 0$. This data has been obtained after an exhaustive search for an optimal door configuration, which we believe we have reached, given the result $\Delta S \approx 0$.

Conclusion

We believe that the computational scheme and results presented in this paper provide some insight into the production of entropy by a Maxwell's demon. Further, we have presented a unique view of the connection between statistical entropy, thermodynamic entropy, and information.

Acknowledgement

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References

1. P.A. Skordos and W.H.Zurek, Am. J. Phys. 60, 876-882 (1992).

2. M. v. Smoluchowski, Physik. Z. 13, 1069-1080 (1912).

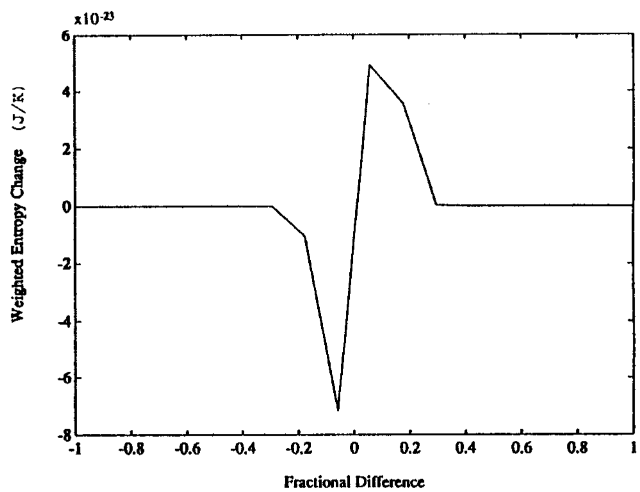

Figure 6. The net entropy change as a function of the initial configuration, weighted by the probability of the corresponding initial configuration occurring naturally. The sum of the weighted entropy changes over all possible configurations (basically the integral of this curve) is approximately zero.