

# Computational Implementation of Maxwell’s Knudsen-Gas Demon and Its Extension to a Two-Dimensional Soft-Disk Fluid

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**Abstract:** An interesting preprint by Puru Gujrati, “Maxwell’s Demon Must Remain Subservient to Clausius’ Statement” [of the Second Law of Thermodynamics], traces the development and application of Maxwell’s Demon. He argues against the Demon on thermodynamic grounds. Gujrati introduces and uses his own version of a generalized thermodynamics in his criticism of the Demon. The complexity of his paper and the lack of any accompanying numerical work piqued our curiosity. The internet provides well over two million “hits” on the subject of “Maxwell’s Demon”. There are also hundreds of images of the Demon, superimposed upon a container of gas or liquid. However, there is not so much along the lines of simulations of the Demonic process. Accordingly, we thought it useful to write and execute relatively simple FORTRAN programs designed to implement Maxwell’s low-density model and to develop its replacement with global Nosé-Hoover or local purely-Newtonian thermal controls. These simulations illustrate the entropy decreases associated with all three types of Demons.

**Key words:** Maxwell’s Knudsen-Gas Demon, entropy, Nosé-Hoover Demon, Dense-Fluid Demon

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## I. Introduction and Goal

Maxwell’s Demon is a familiar example of a dynamical system designed to violate the Second Law of Thermodynamics. By deciding whether or not to reflect particles nearing a movable barrier, open or shut based on kinetic energy or species, Maxwell’s Demon is able to generate a temperature or concentration difference without violating any mechanical laws. Gujrati [1] provides extensive references to the Demon problem in his arXiv preprint. Wikipedia is another useful source reference.

We have two goals here: first, we implement Maxwell’s original idea, quite suitable for informal laptop simulations. This implementation pointed out a need for extending Maxwell’s idea to dense fluids. That work, our second goal, is a surprisingly tall order. We achieve it here, first by introducing two Nosé-Hoover Demons, and next, a Soft-Disk Dense-Fluid Demon. We believe that such numerical demonstrations are superior to theoretical armchair

discussions and speculations. Our hope is that the reader will find our implementations interesting, perhaps motivating further improvements extending the reach of Maxwell’s Demon idea. We begin by modelling entropy reduction with a two-dimensional (collisionless) Knudsen gas. That approach fails for dense matter, as Gujrati stresses. We extend the scope of Demons by formulating new ones based on contemporary Nosé-Hoover dynamics as well as a Newtonian soft-disk dense-fluid Demon with a bit of memory.

## II. Entropy Decrease Model: a Two-Dimensional Knudsen Gas

For convenience we choose 200 particles in the square-lattice configuration shown in Fig. 1. The particles inhabit a  $20 \times 10$  container centered at the origin. The boundary conditions at the four walls are enforced, using cubic repulsive forces, by four lines of code:

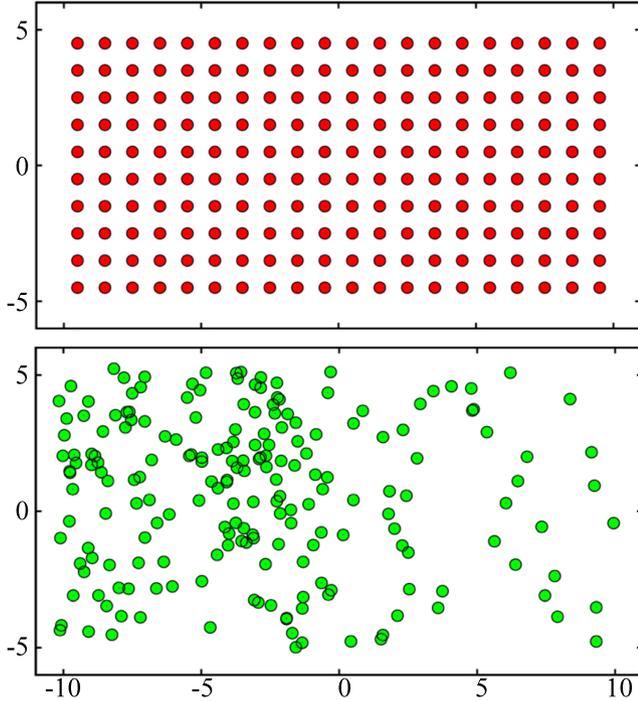


Fig. 1. Configuration of 200 particles at time = 0 (above) and at time = 10 000 (below). Here the parameter of borderline energy between reflection and penetration is  $1/10$  where  $E/N$  is unity. Energetic particles go “right” while the less-energetic particles are reflected to the “left”

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if (x(i).gt.+10) fx(i)=-800*(x(i)-10)^3
if (x(i).lt.-10) fx(i)=-800*(10+x(i))^3
if (y(i).gt.+5) fy(i)=-800*(y(i)-5)^3
if (y(i).lt.-5) fy(i)=-800*(5+y(i))^3

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The quartic boundary potential generating these forces was selected to resemble the short-ranged purely-repulsive soft-disk potential  $\phi(r < 1) = 100(1 - r^2)^4$ . That pair potential has been used to determine the number-dependence of the shear viscosity in relatively large two-dimensional simulations, with as many as  $N = 514 \times 514$  particles [2]. To begin we consider a confined dynamics without any particle-particle interaction, a “Knudsen gas”. Later we will take up the extension of Maxwell’s goal to the case where particles interact with the simple repulsive soft-disk pair potential. For an introduction to the Maxwell problem we consider dynamics solely subject to the four reflecting boundaries at  $x = \pm 10$  and  $y = \pm 5$ .

We choose our initial velocities  $\{p_x, p_y\}$  randomly in the interval  $\pm 0.5$ :  $\{r - 0.5\}$ . The FORTRAN routine `random_number(r)` is a convenient choice. Next, the particle velocities are scaled so as to give an initial kinetic energy per particle of unity. For a well-posed problem all we need do subsequently is to specify the workings of the Demon. He does not disturb mass or energy conservation. His only job is to break the thermal symmetry between the two halves of the system, creating a temperature difference across the

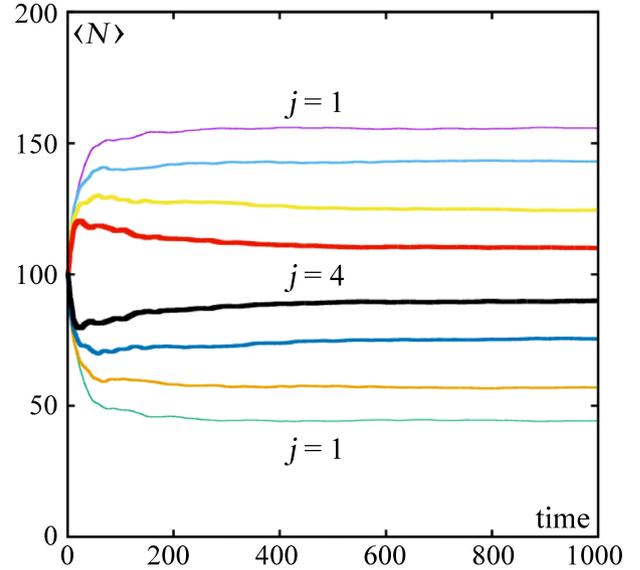


Fig. 2. Time averaged hot (below) and cold (above) populations  $\langle N \rangle$  with four mirror settings,  $(j/8)$  for  $j = 1, 2, 3,$  and  $4$ . The mean particle energy is unity. These four Knudsen gas simulations exclude interactions between pairs of particles. Instead all particles are confined by repulsive quartic potentials at  $x = \pm 10$  and  $y = \pm 5$ . Any particle crossing the center line  $x = 0$  is transmitted or reflected according to its total energy (same as its kinetic temperature within the  $20 \times 10$  rectangle) as explained in the text

midline  $x = 0$ . He can do this by implementing four lines of FORTRAN applied whenever the product of a current  $x_i(t)$  coordinate at time  $t$  and its previous value  $x_i(t - dt)$  at time  $t - dt$  is negative, indicating a crossing of the midline at  $x = 0$ :

$$\begin{aligned}
 (p_{x_i}^2 + p_{y_i}^2)/2 < (1/10)(E/N) &\rightarrow x_i = -\sqrt{x_i^2}; p_{x_i} = -\sqrt{p_{x_i}^2}; \\
 (p_{x_i}^2 + p_{y_i}^2)/2 > (1/10)(E/N) &\rightarrow x_i = +\sqrt{x_i^2}; p_{x_i} = +\sqrt{p_{x_i}^2}.
 \end{aligned}$$

Fig. 1 displays both the initial configuration and another much later, at a time of  $10^4$ , for the particular reflecting borderline choice  $\frac{E}{10N}$ . Notice that the reflection of left-to-right travel results in a higher density and lower temperature in the left half of the system. Fig. 2 shows the cumulative populations of the hot and cold regions for four equally-spaced values of the borderline reflection energies. If one is of order the mean particle energy of unity the differences in densities and temperatures are scarcely noticeable above the fluctuations, of order  $\sqrt{100}$ . This Knudsen gas problem is a good example of entropy loss using standard Newtonian mechanics. There is a clearcut successful energy separation between the hot and cold regions for this particular formulation of Maxwell’s Demon.

There is no doubt that the separation of hot particles from cold demonstrated here can be predicted by kinetic theory (balancing the different densities and temperatures so that the left-to-right and right-to-left mass fluxes sum to zero). The successful separation of the energy into hotter and

colder spatial regions has required nothing more than a pair of conditionals in the motion equations, which satisfy the conservation of energy as well as mass. Though no work is done momentum is not conserved due to the stationary positions of the walls at  $x = 0$  and  $\pm 10$  and  $y = \pm 5$ . A dense fluid provides a real challenge to the Demon in that heat conductivity works against the thermal separation he promotes.

### III. Failure of Maxwell's Demon for a Dense Fluid

Fig. 3 is taken from a simulation exactly similar to the Knudsen-gas model of Fig. 2 with the difference that the pair potential has been turned "on". Now the particle energies are partly pair potential and the dynamics is no longer that of an ideal gas. Exploration of such problems soon convinced us that the Demon was unable to defeat the stabilizing energy flow due to heat conductivity enabled by pair-potential interactions. We had not expected this problem though it is forecast by Gujarti in his thermodynamic exploration of Maxwell's Demon [1]. Once the Demon's failure became apparent in the dense-gas case we were at first unable to imagine and formulate a useful Demon operating on individual particles. Instead we came to visualize two nonlocal Demons. One of them operates solely left of center to lower the kinetic temperature there. The "hot" Demon operates at

the right, raising that temperature, establishing a "hot" chamber. The two-Demon idea can be implemented with Nosé-Hoover dynamics, a stable modification of Hamiltonian dynamics that makes it possible to specify a mean kinetic energy imposed by integral feedback [3–5]. Specifying two temperatures is a useful possibility. We explore that next.

### IV. Hot and Cold Temperatures with Two Thermostats

To address Maxwell's problem with Nosé-Hoover thermal control we introduce *two* new dynamical variables,  $\zeta_{\text{cold}}$  and  $\zeta_{\text{hot}}$ . The equations of motion are then modified for every particle at all times. This modification includes the influence of one or the other of the two thermostat variables:

$$x < 0 \longrightarrow \dot{p} = F - \zeta_{\text{cold}}p; \quad x > 0 \longrightarrow \dot{p} = F - \zeta_{\text{hot}}p.$$

The two friction coefficients obey feedback equations based on the two fluctuating kinetic energies  $K$  and their fixed target values  $T$ :

$$\begin{aligned} \dot{\zeta}_{\text{cold}} &= [(K/N)_{\text{cold}} - T_{\text{cold}}]/\tau^2; \\ \dot{\zeta}_{\text{hot}} &= [(K/N)_{\text{hot}} - T_{\text{hot}}]/\tau^2. \end{aligned}$$

The relaxation times  $\tau$  are free to choose. We set them equal to unity in the present work. The two integral control variables  $\zeta$  are the "Nosé-Hoover Demons".

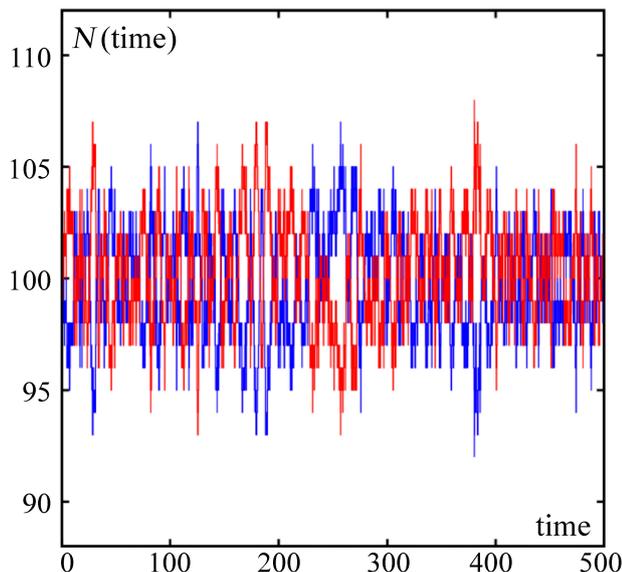


Fig. 3. Time-dependence of the hot (red and in the right chamber) and cold (blue and at the left) populations with a mirror kinetic energy of  $0.2(E/N)$ . Repulsive interactions between pairs of particles are included here, increasing the mechanisms for heat transfer. As a result Maxwell's Demon is relatively ineffective. The resulting systematic temperature difference between the "cold" and "hot" regions is rather small. Just as in Fig. 2 any particle crossing the center line  $x = 0$  is transmitted or reflected according to its kinetic temperature

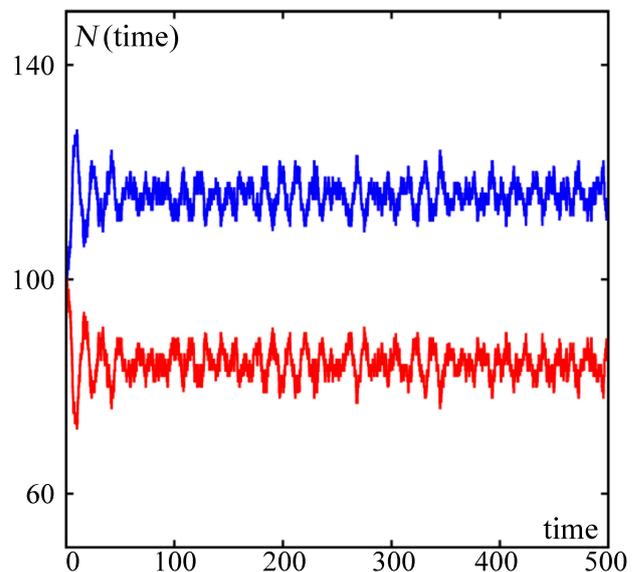


Fig. 4. Time-dependence of the hot and cold populations with target temperatures of 0.5 and 1.5 using Nosé-Hoover thermostat variables. Repulsive interactions between pairs of particles are included here, greatly increasing the heat conductivity. The Nosé-Hoover Demons affect all particles simultaneously and maintain, along with fluctuations, a systematic temperature difference between the "cold" and "hot" regions. Just as in Fig. 2 any particle crossing the center line  $x = 0$  is transmitted or reflected according to its kinetic temperature, relative to unity

Fig. 4 shows the straightforward approach of 200-particle dynamics with control of the two temperatures  $T_c = 0.5$  and  $T_h = 1.5$ . Here no reflecting mirror is used and all particles eventually sample the entire volume. Although the dynamics is no longer Newtonian it does accomplish the goal of reducing the entropy by extracting heat at the lower temperature and adding heat at the higher. The entropy production,

$$\dot{S} \equiv (\dot{Q}/T_{\text{cold}}) - (\dot{Q}/T_{\text{hot}}), \text{ with } \dot{Q} > 0,$$

is extracted from the system and obviously inexorably reduces the entropy, eventually to  $-\infty$ , and signals the formation of a fractal attractor within the 802-dimensional phase space, which includes the two friction coefficients. Though this modification of Newtonian mechanics lacks the purity of Maxwell's Demon, who works with purely Newtonian motion equations, it was our first attempt to extend the Demon idea to dense fluids. Within 24 hours, on New Year's Eve, 2021→2022, a better approach suggested itself. We describe it next.

### V. Maxwell's Demon for Soft-Disk Nonequilibrium Fluids

How to approach the dynamic purity of Maxwell's Knudsen-gas Demon in a dense fluid? First of all, one needs an initial state from which a stationary, or time-periodic, nonequilibrium system can result. Next, one needs a means, such as a Demon, for sustaining a distribution different to any of Gibbs' equilibria, a state of less than maximum entropy. Finally, one needs a means of understanding the re-

sults of such a computation in thermodynamic or hydrodynamic terms.

Pondering these needs led us to develop a dense-fluid molecular dynamics in which energy is closely conserved through a Newtonian dynamics, with or without the actions of a Demon. A simple task is reflecting particles at the system midline  $x = 0$ . Computations soon revealed that equilibrium excursions from the mean number, 100, in the numbers of "left" and "right" particles were of order five. This work all used the short-ranged soft-disk pair potential. By turning a diligent Demon "on" when the left and right chambers in a purely-equilibrium simulation had populations 105 and 95, a nonequilibrium dense-fluid soon develops. The two chambers do interact "across" the mid-line barrier which prevents their mixing. See the left side of Fig. 5 which shows the close correlation of the left and right chamber temperatures. The interacting chambers evidently generate very similar (no doubt identical) average temperatures despite their markedly different densities (ten percent) and pressures, sustained by the rigid midline wall. The Demon's dynamics for the situation shown in the figure is particularly simple. By remembering the values of  $x_i$  and  $p_{x_i}$  from the previous timestep the Demon can simply set the post-collision coordinate  $x(t+dt) = x(t)$  and momentum,  $p_x(t+dt) = -p_x(t)$ . The result conserves energy relatively well with  $dt = 0.002$ , ending up with an increase of 1/50 percent after five million timesteps. Such a simulation requires only about thirty minutes on a laptop computer.

Evidently it is feasible to construct and maintain a nonequilibrium two-chamber system so as to maintain thermal contact far from equilibrium by the diligent actions of a Demon stationed at the wall common to both chambers. The Demon can easily be given more complicated instruc-

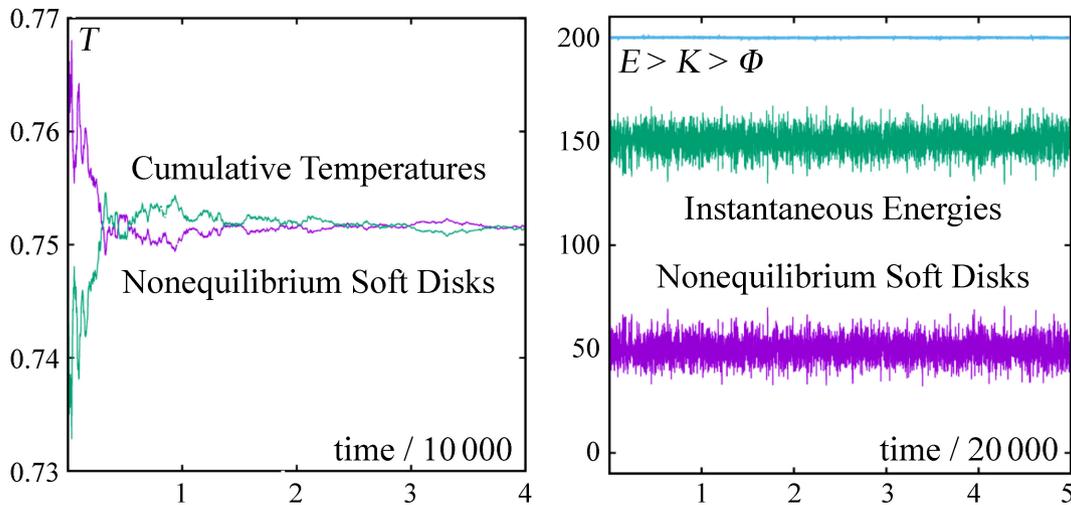


Fig. 5. Energy relationships for a two-chamber nonequilibrium soft-disk fluid with densities of 1.05 and 0.95. At the left we see that the time-averaged temperatures of the two chambers match. At the right we see that despite the density and pressure differences between the two chambers the nonequilibrium energy,  $E = N = 200$ , plotted at the top is a constant of the motion. The dense-fluid Demon in this case causes all particle collisions with the mid-line barrier at  $x = 0$  to be instantaneous and energy conserving

tions, periodic in the time for example, without the need for thermostats modifying Newton's laws of motion. We believe that this development sets the stage for the simulation and analysis of a dynamics every bit as paradoxical as Maxwell's Knudsen-gas idea. How this relates to the storage and erasure of information is still a mystery to us. Perhaps a kind-hearted soul will consider such a problem and provide an explanation which again saves the Second Law of Thermodynamics from Demons?

Fig. 5 shows the development of the instantaneous energies in a system with two equal-volume chambers containing 105 and 95 soft disks. At the left the mean (cumulative) kinetic temperatures in the two chambers are shown. It is noteworthy that the mean kinetic energy,  $K/200$  has relatively small fluctuations compared to those of the two chambers.

## VI. Summary

The implementation of Maxwell's Demon using constrained versions of molecular dynamics is straightforward. Any small energy errors due to a finite timestep (0.01 and 0.002 for the fourth-order Runge-Kutta integrator used here) can be offset by a rescaling of the particle velocities at the end of each timestep. With an exact interpolative treatment of the mid-line collisions, the fourth-order Runge-Kutta errors can be reduced 16-fold by simply halving the timestep.

Much has been written about the increase in entropy which must somehow compensate for the lost entropy observed in the dynamics of thermal separation, where the entropy is of order  $N_{\text{cold}} \ln T_{\text{cold}} + N_{\text{hot}} \ln T_{\text{hot}}$  and is obviously maximized for the case in which the numbers and temperatures in the two compartments are identical. Though our dense-fluid model with two interacting compartments does come to thermal equilibration the pressures and densities in the chambers necessarily differ from equilibrium states and so indicate an entropy loss.

The computational work involved in the models introduced here is hardly different for the equilibrium situation in which crossings of the midline are entirely ignored. A discussion of the Second Law for this model would likely note that a tremendous amount of mental and numerical work needs to be carried out for any simulation, at or away from equilibrium. Evidently the amount of this work has nothing to do with the mechanical work envisioned in the First Law of Thermodynamics or the reversible heat transfers visualized in the Second Law.

## Acknowledgment

We thank Professor Gujrati for sharing his work with us prior to its publication. Brad Holian kindly reminded us of his own seminal work on two-chamber problems using thermostats to impose nonequilibrium gradients [6, 7].

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**Bill and Carol Hoover** at the wedding of Carol's Brother Larry Griswold to Kim Moore in Colorado Springs, just before Christmas 2021. Bill and Carol moved to Ruby Valley Nevada from California in 2005, after decades of work together at the Lawrence Livermore National Laboratory. They have published four books since their move to the Silver State: *Time Reversibility, Computer Simulation, Algorithms, Chaos; Smooth Particle Applied Mechanics—The State of the Art; Simulation and Control of Chaotic Nonequilibrium Systems*, and *Microscopic and Macroscopic Simulation Techniques: Kharagpur Lectures*. They are currently working with Clint Sprott on *Elegant Simulations*, scheduled for completion in 2022.