

# Time-Reversible Thermodynamic Irreversibility: One-Dimensional Heat-Conducting Oscillators and Two-Dimensional Newtonian Shockwaves

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**Abstract:** We analyze the time-reversible mechanics of two irreversible simulation types. The first is a dissipative one-dimensional heat-conducting oscillator exposed to a temperature gradient in a three-dimensional phase space with coordinate  $q$ , momentum  $p$ , and thermostat control variable  $\zeta$ . The second type simulates a conservative two-dimensional  $N$ -body fluid with  $4N$  phase variables  $\{q, p\}$  undergoing shock compression. Despite the time-reversibility of each of the three oscillator equations and all of the  $4N$  manybody motion equations both types of simulation are irreversible, obeying the Second Law of Thermodynamics. But for different reasons. The irreversible oscillator seeks out an attractive dissipative limit cycle. The likewise irreversible, but thoroughly conservative, Newtonian shockwave eventually generates a reversible near-equilibrium pair of rarefaction fans. Both problem types illustrate interesting features of Lyapunov instability. This instability results in the exponential growth of small perturbations,  $\propto e^{\lambda t}$  where  $\lambda$  is a “Lyapunov exponent”.

**Key words:** time reversibility, irreversibility, heat conduction, shockwaves, thermodynamics’ Second Law

## I. Reversibility of Dissipative and Conservative Mechanics

Classical mechanics is *time-reversible* in the sense that a movie of the motion, run backwards, obeys exactly the same motion equations as does the original forward version. Classical mechanics is an excellent model for conservative systems free of the real-life dissipative effects of friction, viscosity, and heat conduction. In order to model dissipative phenomena on an atomistic scale *nonequilibrium* molecular dynamics includes *control variables* in the equations of motion. These variables use feedback to impose local values of the temperature and pressure which drive nonequilibrium flows. Thousands of implementations of this approach have been stimulated by Shuichi Nosé’s pioneering 1984 work [1, 2]. We will explore the time reversibility of an application of his work here.

Nosé’s 1984 papers generalize Hamiltonian mechanics with a frictional variable  $\zeta$  controlling the kinetic temperature  $T$  of one or more particular degrees of freedom:

$$\zeta \longrightarrow kT = \langle p^2/m = mv^2 \rangle.$$

Here  $k$  is Boltzmann’s constant,  $m$  the mass of a particle, and  $mv = p$  the momentum of a controlled degree of freedom. For simplicity in what follows we set both  $k$  and  $m$  equal to unity. Hoover applied Nosé’s idea to the simplest special case, a one-dimensional harmonic oscillator, in 1985 [3], later extending that work in 1986 with Posch and Vesely [4]. Numerical solutions of the thermostatted oscillator’s equations of motion (with  $k$  and  $m$  unity now),

$$\{ \dot{q} = p; \dot{p} = -q - \zeta p; \dot{\zeta} = p^2 - T \},$$

can be reversed in either of two ways, by [1] changing the signs of the time and timestep,  $t$  and  $dt$ , or [2] by changing

the signs of  $p$  and the control variable  $\zeta$ . Both ways simply reverse the time dependence of the coordinate:  $q(+t) \rightarrow q(-t)$ .

## II. One-Dimensional Heat-Conducting Oscillator

In 1997 Posch and Hoover generalized the oscillator problem, specifying a coordinate-dependent temperature  $T(q) = 1 + \epsilon \tanh(q)$ . This temperature profile has a maximum temperature gradient,  $(dT/dq) = \epsilon$  at  $q = 0$ . Particular choices of  $\epsilon$  generated a variety of  $(q, p, \zeta)$  “strange attractors” [fractal distributions in  $(q, p, \zeta)$  space]. Fig. 5, a cross-section through a fractal attractor, gives an impression of the complicated structures resulting from relatively simple ordinary differential equations. The fractional dimensionalities of these attractor distributions were all between 2 and 3. Other initial conditions or choices of  $T(q)$  resulted in one-dimensional limit cycles rather than fractals [5]. More recently, in 2014, Sprott and the Hoovers found initial conditions,  $(q, 0, 0)$ , with  $T(q) = 1 + 0.42 \tanh(q)$ , which generate two distinct families of conservative tori (with the initial values  $q = -2.3$  and  $3.5$ ) [6]. The tori are interlinked and coexisting stably with a one-dimensional dissipative limit cycle. The cycle can be generated easily with initial values  $(q, p, \zeta) = (-2, -2, 0)$  and a fourth-order Runge-Kutta timestep  $dt = 0.01$ . Fig. 2 in Reference 6 shows the three interlinked phase-space structures. We reproduce it here as Fig. 1.

In this rich collection of one-dimensional limit cycles, two-dimensional tori, and fractional-dimensional strange attractors the simplest special case is arguably  $T(q) = 1 + \tanh(q)$ . The coordinate-dependent temperature varies from 0 to 2 as  $q$  varies from  $-\infty$  to  $+\infty$ . We believe that the basin of attraction for this case is the entire three-

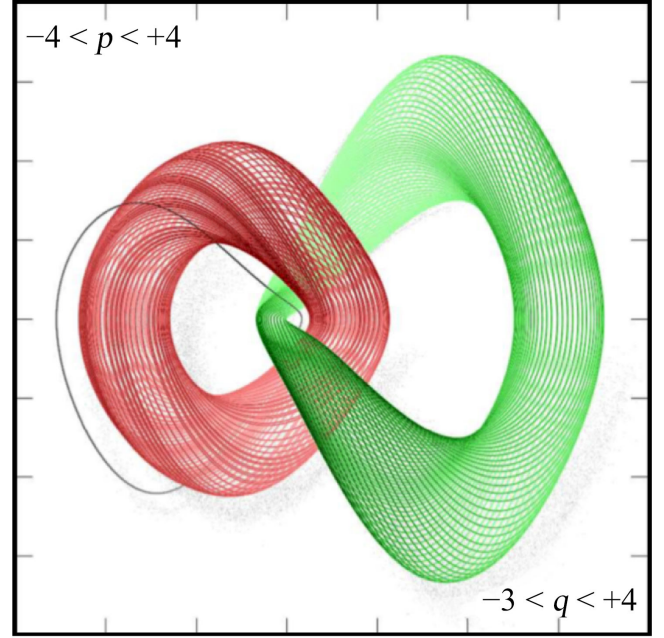


Fig. 1. Two conservative tori are interlinked with a dissipative limit cycle [6]. All three stationary solutions of the oscillator equations for  $T(q) = 1 + 0.42 \tanh(q)$  can be generated with initial values  $(q, p, \zeta) = (-2, -2, 0)$ ,  $(-2.3, 0, 0)$  and  $(+3.5, 0, 0)$ . If instead  $T(q) = 1 + \tanh(q)$  all initial conditions lead to the limit cycle illustrated in Figs. 2–4

dimensional phase space. To support this idea we chose a square  $200 \times 200$  grid of  $(q, p, \zeta)$  points in the  $\zeta = 0$  plane with  $q$  and  $p$  ranging from  $-4.975$  to  $+4.975$  in steps of  $0.05$ . For each of these 40,000 initial conditions we generated an orbit of length  $100\tau$ , and plotted the  $(q, p)$  val-

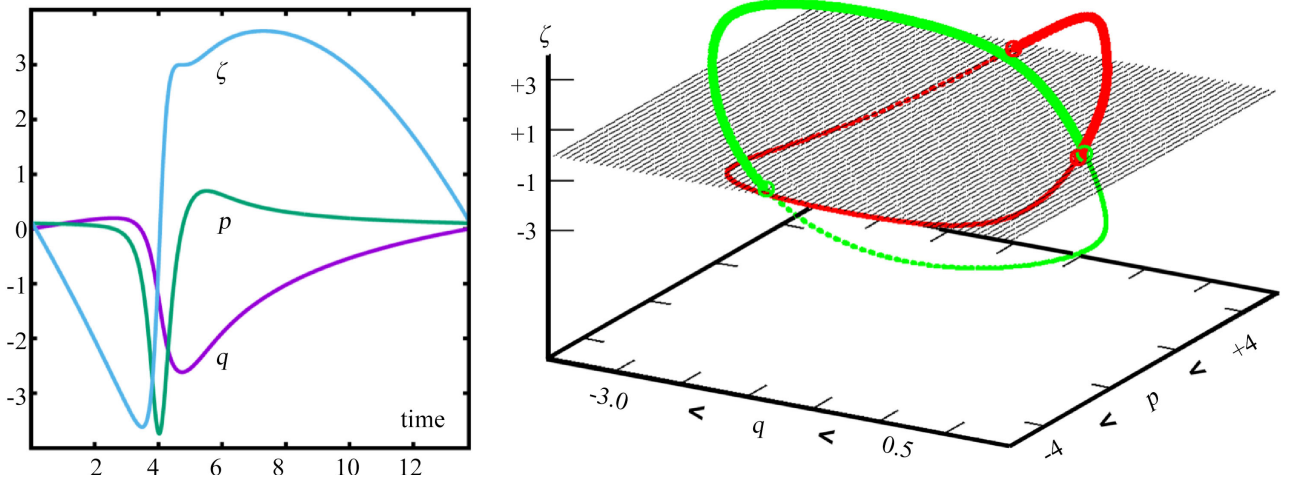


Fig. 2. Stable and unstable limit cycles for a heat-conducting one-dimensional harmonic oscillator. At the left the time dependence of coordinate  $q$ , momentum  $p$ , and friction coefficient  $\zeta$ , purple, green, and blue respectively, for the conducting oscillator with period  $\tau = 13.7494$ . At the right are three-dimensional plots of the attractive orbit (green), with initial condition  $\{q, p, \zeta\} = \{0, 0.1050726, 0.1455481\}$  and the corresponding *unstable* repulsive orbit (red), with  $p$  and  $\zeta$  changed in sign. The mean value of the (hot to cold) heat current is  $\langle (p^3/2) \rangle = -0.74383$ . The red and green circles indicate the four crossings of the orbits with the  $\zeta = 0$  grey plane

ues whenever  $\zeta$  changed sign. Every one of these long orbits ended up crossing at the two penetration points plotted in green in Fig. 2. For each orbit we used a timestep of  $\tau/10000$  where the cycle period is  $\tau = 13.7494$ . Let us explore that solution in more detail, based on fourth-order Runge-Kutta numerical simulations.

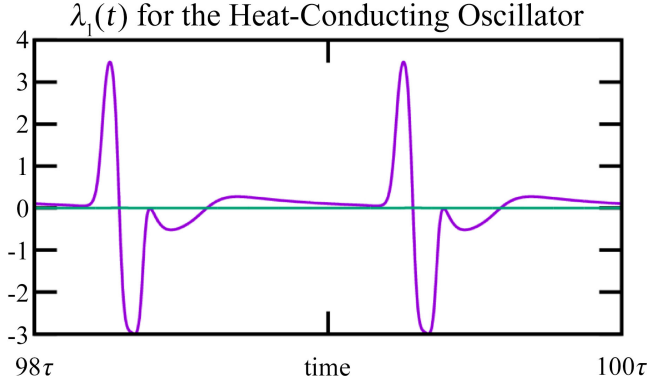


Fig. 3. Time dependence of the local Lyapunov exponent for the oscillator during its 99th and 100th period of oscillation. The local value is purple. The green time average of  $\lambda_1(t)$  vanishes, corresponding to the lack of averaged strain along the trajectory

From the phase-space analog of Liouville's continuity equation the mean value of the friction coefficient  $\zeta$  necessarily corresponds to the time-averaged loss rate of phase volume,  $\otimes = dqdpd\zeta$ :

$$\begin{aligned} \langle (\otimes/\otimes) \rangle &= \langle (\partial\dot{q}/\partial q) + (\partial\dot{p}/\partial p) + (\partial\dot{\zeta}/\partial \zeta) \rangle = \\ &= \langle 0 - \zeta + 0 \rangle = -1.325. \end{aligned}$$

In a single period the comoving phase volume decreases by a factor of  $e^{\langle \zeta \rangle \tau} = e^{1.325 \times 13.7494} \simeq 10^8$ . The maximum temperature gradient,  $(dT/dq)$ , is unity, at  $q = 0$ . The mean heat current, averaged over time,  $\langle (p^3/2) \rangle$ , is  $-0.74383$ , and the net transport of kinetic energy  $\langle p^2/2 \rangle$  is from right to left, consistent with thermodynamics' Second Law.

The Lyapunov exponents, three of them in a three-dimensional phase space, measure the comoving expansion rates of the phase volume  $\otimes$ :

$$(\dot{\otimes}/\otimes) = \lambda_1(t) + \lambda_2(t) + \lambda_3(t).$$

The one-dimensional limit cycle's largest Lyapunov exponent has an average value of zero, as shown in Fig. 3. The vanishing mean value of  $\lambda_1$  corresponds to the averaged lack of relative motion of two adjacent trajectory points along the attractive one-dimensional trajectory.  $\lambda_2$  and  $\lambda_3$  have negative averages,  $-0.110$  and  $-1.215$ , describing the net rates of convergence of nearby trajectories in the two directions perpendicular to the limit cycle.

For the special case  $T(q) = 1 + \tanh(q)$  the longtime solution of the motion equations forward in time is the unique attractive periodic orbit shown (green) in the right panel of Fig. 2. The period  $\tau$  is  $13.7494$  with  $-2.616 < q < +0.198$ . The reversed orbit, with the same range of  $q$  visited in the opposite time direction, is half the attractor/repellor pair.

The repellor is only observable briefly due to its inherent Lyapunov instability, proportional to  $e^{\lambda_1(t) \times t} \simeq e^{+1.215t}$ . We expect to see the exponential growth of an original one-step roundoff error grow to observability in just a few oscillator periods. We examine that next.

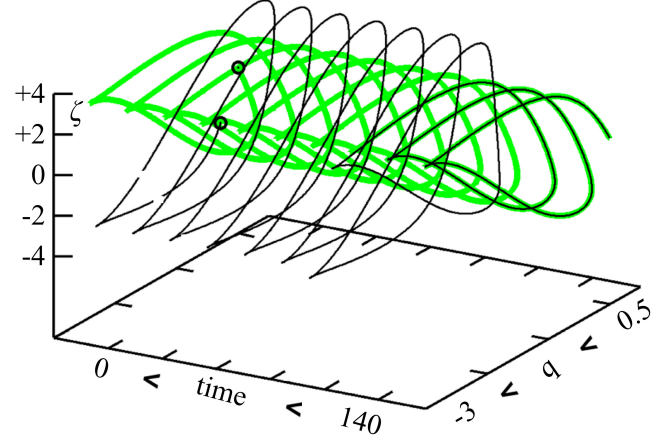


Fig. 4. Evolution of ten  $(q, \zeta)$  orbits beginning at the initial upper black circle with the conditions of Fig. 2. At time  $t = 137.494$  the sign of the timestep is reversed. The reversed trajectory (black) traces back accurately for nearly three reversed orbits before making a rapid switch to the stabilized repellor, following it to the lower black circle at  $t = 0$

### III. Stability and Instability of Periodic Oscillator Orbits

Fig. 4 illustrates the stability of the attractive limit-cycle orbit,  $\{\lambda_i\} = \{0, -0.110, -1.215\}$  and the instability of its time reversal,  $\{\lambda_i\} = \{+1.215, +0.110, 0\}$  with a two-stage simulation. First we follow ten circuits of the attractor in green, using a million quadruple-precision fourth-order Runge-Kutta timesteps of  $dt = 10^{-5}\tau = 0.000137494$ , implying a local integration error of order  $dt^5/120 \simeq e^{-49}$  at each step. We then reverse time,  $+dt \rightarrow -dt$ , converting the stable attractor to the unstable reversed repellor. Unlike the stable attractor the repellor is unstable, with a positive Lyapunov exponent  $\lambda_1 = 1.215$ . This suggests that the reversal should become visibly inaccurate at a time of order  $49.3/1.215 \simeq$  three or four periods. This agrees well with the reversed black trajectory of Fig. 4, which follows the reversed  $(q, p, \zeta)$  orbit (stabilized by the negative  $dt$ ) for between six and seven periods, ending up at the lower black circle:

$$\{q = 0, p = -0.1050726, \zeta = -0.1455481\}.$$

The largest Lyapunov exponent is relatively easy to measure. Follow two neighboring trajectories, the “reference” and the “satellite”, adjusting the satellite location by rescaling its separation from the reference,  $\delta_{t+dt} \rightarrow \delta_o$ , at the conclusion of each time step. This rescaling precisely counters the exponential growth which would occur in the absence

of rescaling. The local Lyapunov exponent follows from the rescaling operation:

$$\lambda_1 dt = -\ln(\delta_{\text{after}}/\delta_o) \rightarrow \lambda_1(t) = (-1/dt) \ln(\delta_{t+dt}/\delta_o).$$

A convenient choice for  $\delta_o$  is 0.00001. Fig. 3 shows the time variation of the largest Lyapunov exponent  $\lambda_1$ , which lies in the range  $-3.00 < \lambda_1(t) < +3.48$  with a mean value of zero, corresponding to the (lack of) growth rate of perturbations parallel to the trajectory.

#### IV. Time Reversibility and Loschmidt's Paradox

A classic physics puzzle addresses the surprising coexistence of macroscopic irreversibility with microscopic time reversibility. In 1876 Loschmidt pointed out that any solution of the equations of motion which is time reversible and demonstrates the production of entropy can be made to violate the Second Law of Thermodynamics by analyzing the reversed motion. Simply stated, time-reversible mechanics necessarily violates the Second Law in one of the two time directions. We have already seen that time-reversible Nosé-Hoover mechanics, with control of the kinetic temperature, obeys the Second Law. This is not only possible, but inevitable, for computational models of the heat-conducting oscillator. With  $dt$  positive, attractive distributions such as the oscillator limit cycle are inevitably observed. Repellers are not, due to their vanishing probabilities.

The exploration of a simple one-body time-reversible model [7], and its relation to entropy production in a many-body system with heat flow [8], clarified the reversibility paradox in 1987. The “Galton Staircase” pictures a reversibly thermostatted particle in a downhill steady state, driven by a periodic sinusoidal potential superimposed on a constant downhill field. As the particle falls more than it climbs, the model generates a fractal (fractional dimensional) phase-space distribution in its three-dimensional phase space  $(q, p, \zeta)$ . The resulting zero-volume attractive fractal, when reversed, corresponds to the extreme rarity of states violating the Second Law of Thermodynamics by converting heat to work. The mirror-image repulsive fractal, corresponding to an upward moving particle violating the Law has, like the attractor, zero volume, but is repulsive and of zero probability. The “attractor” is attractive, with probability one. This difference in behavior occurs because Lyapunov instability is *not* time-reversible.

In the Galton staircase a particle travelling uphill, as described by the repeller states, violates the Law by converting kinetic energy to potential. Repulsion, coupled with zero volume, makes these fractal repeller states unobservable. The conducting oscillator of Figs. 2–4 offers a simple analog for a particle transporting energy from hot to cold rather than transporting mass through motion driven by a gravitational field. Both systems resolve Loschmidt's Paradox by introducing time-reversible variables controlling temperature. It is the extreme unobservable rarity of repeller states, the fractal set for uphill motion in the Galton Staircase, and here the repulsive one-dimensional repeller limit

cycle in three-dimensional space, that forces motions to obey the Second Law. Staircase simulations reveal the exponential growth of the separation from the fractal repeller and an irresistible attraction to the repeller's mirror-image attractor. Likewise the conducting oscillator with  $T = 1 + \tanh(q)$  follows the attractive limit cycle of the figures, rather than the cycle's mirror image repulsive twin, which repels rather than attracts.

Holian, Hoover, and Posch [8] stressed that similar irreversible behavior occurs in the reversible simulations of thermostatted nonequilibrium manybody systems. They described a heat-conducting system in contact with two reservoirs, one hot and the other cold. Such a system loses phase volume when it satisfies Fourier's Law, transmitting heat from the hot reservoir (with an entropy production  $Q/T_H$ ) to the cold (with an entropy loss  $Q/T_C$ ) which necessarily exceeds the gain. The result is a phase-volume loss exponential in the time. Just as in the Galton Staircase mass-flow problem heat flow *from hot to cold* results in fractal phase-space structures. Both fractal types have zero volume, with zero probability of observing the repeller and with inevitable longtime probability one for the attractor.

#### V. An Illustrative Fractal for the Conducting Oscillator

To help visualize the attractors and repellers that characterize nonequilibrium systems we consider here a fractal resulting from dissipation controlled by a *pair* of control variables.  $\xi$  controls the fourth moment of the velocity distribution while  $\zeta$  controls the second. Because fractal distributions are difficult to visualize in their entirety they are typically described by projections or cross sections. The four-dimensional conducting oscillator introduced by Posch and Hoover [5] provides a variety of thought-provoking fractal structures. As an example, for the same temperature profile considered here,  $T = 1 + \tanh(q)$ , see Fig. 5. The additional phase-space dimension results from using two control variables rather than one. The doubly-thermostatted oscillator requires the solution of four ordinary differential equations:

$$\{ \dot{q} = p; \dot{p} = -q - \xi p^3 - \zeta p; \dot{\xi} = p^4 - 3p^2 T; \dot{\zeta} = p^2 - T \}.$$

These motion equations are fully ergodic for the special case in which  $T = 1$ . That is, all possible values of the four variables occur and with the known distribution:

$$4\pi^2 \text{prob}(q, p, \xi, \zeta) = e^{-(q^2 + p^2 + \xi^2 + \zeta^2)/2}.$$

#### VI. Two-Dimensional Strong Shockwaves Do Not Reverse

We have seen that Nosé-Hoover temperature control provides a probabilistic mechanism for irreversibility, the formation of attractor-repeller pairs in phase space which stabilize the attractor and destabilize the repeller, both through Lyapunov instability. We have recently detected a related mechanism, but free of control variables, demonstrating the

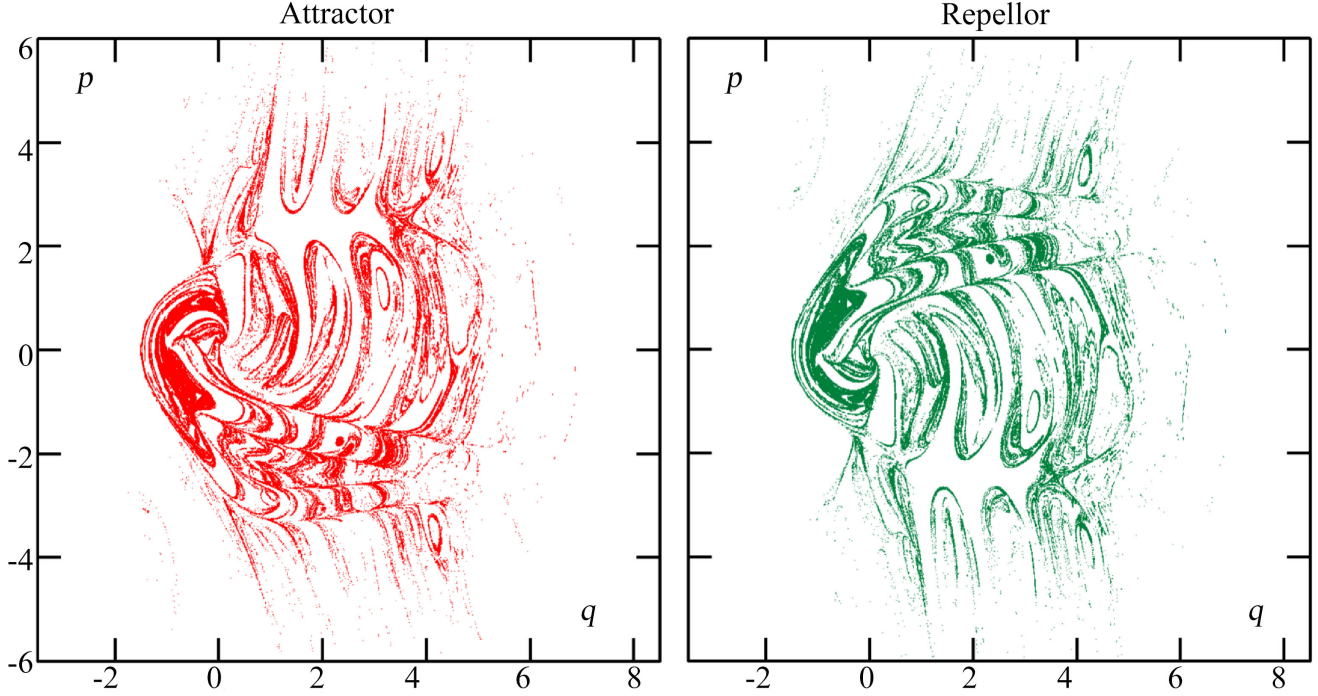


Fig. 5. This double cross section is generated by plotting  $(q, p)$  trajectory points whenever the two thermostat values are near zero. The figure includes ten million points satisfying the condition  $\xi^2 + \zeta^2 < 0.0001$ . Fourth-order Runge-Kutta integration with  $dt = 0.001$  was used

irreversibility of purely Newtonian mechanical systems, illustrated here with an atomistic model generating strong shockwaves. Shockwaves are localized regions, usually just a few atomic diameters in width, within which density, pressure, energy, and temperature all undergo substantial increases. We consider a model here where the temperature changes by a factor of 100 and the density doubles. Shockwaves are relatively easily treated computationally because they are bounded by equilibrium thermodynamic states. To ease the computational burden we consider the shockwave compression of two-dimensional soft-disk particles in two space dimensions. The sudden compression occurs in the  $x$  direction. The purely-repulsive pair potential is chosen for simplicity,  $\phi(r < 1) = (10/\pi)(1 - r)^3$ . The initial near-zero-pressure state is a nearly perfect square lattice, with lattice spacing of unity. The small initial displacements in the range  $\pm 0.05$  correspond to a temperature of order 0.001.

Consider the head-on collision of two  $N$ -body mirror-image zero-pressure zero-energy blocks of material with opposite velocities [9–11], shown in Fig. 6. Here  $N = 35 \times 24 = 840$ . With periodic boundaries in  $y$  the two colliding  $N$ -body blocks steadily convert their kinetic energy to heat. At any stage in the simulation a reversed solution will show, briefly, antithermodynamic behavior, converting some of the internal energy of the stagnating blocks back into the original directed kinetic energy,  $(p_x^2/2) = (0.875^2/2)$  per particle.

Berni Alder and Marvin Ross emphasized the highly irreversible nature of shockwaves [12] as follows: “the most irreversible way to go from one thermodynamic state to another”. A simple example of this transformation is illustrated

in Fig. 6, where  $70 \times 24 = 1680$  particles undergo twofold compression and then expand to form a symmetric pair of rarefaction fans. The initial condition for this example is a neighboring mirror-image pair of colliding square-lattice blocks, both at the stress-free density of unity. The left half travels rightward and the right half leftward. Periodic boundaries are imposed in the  $y$  direction, at the top and bottom of the two colliding 840-body blocks. The dynamics is purely Newtonian. The difference between the steady shockwaves forward in time and the unsteady rarefaction (rather than shocks) waves in the reversed time direction of Fig. 7 shows that the shockwaves are irreversible. In fact the irreversible Navier-Stokes equations of motion predict that a reversed shockwave will immediately widen and slow, transforming into an unsteady rarefaction fan [9, 10].

Fig. 7 was constructed by reversing the velocities of all particles in Fig. 6 at the time of maximum twofold compression. Notice that the snapshot second from the bottom of Fig. 7, where the flow has been reversed so that the configuration is only halfway to maximum compression, resembles closely that second from the bottom in Fig. 6, where the flow is forward, and halfway to the time of maximum compression. This apparent reversibility suggests that the initial single-step Runge-Kutta integration error,

$$dt = 0.01 \rightarrow 0.01^5/5! = e^{-27.8} \text{ or}$$

$$dt = 0.005 \rightarrow 200^{-5}/5! = e^{-31.3},$$

expands exponentially to become of order unity at  $t = 27.8/\lambda$  or  $31.3/\lambda$  in these two typical cases.



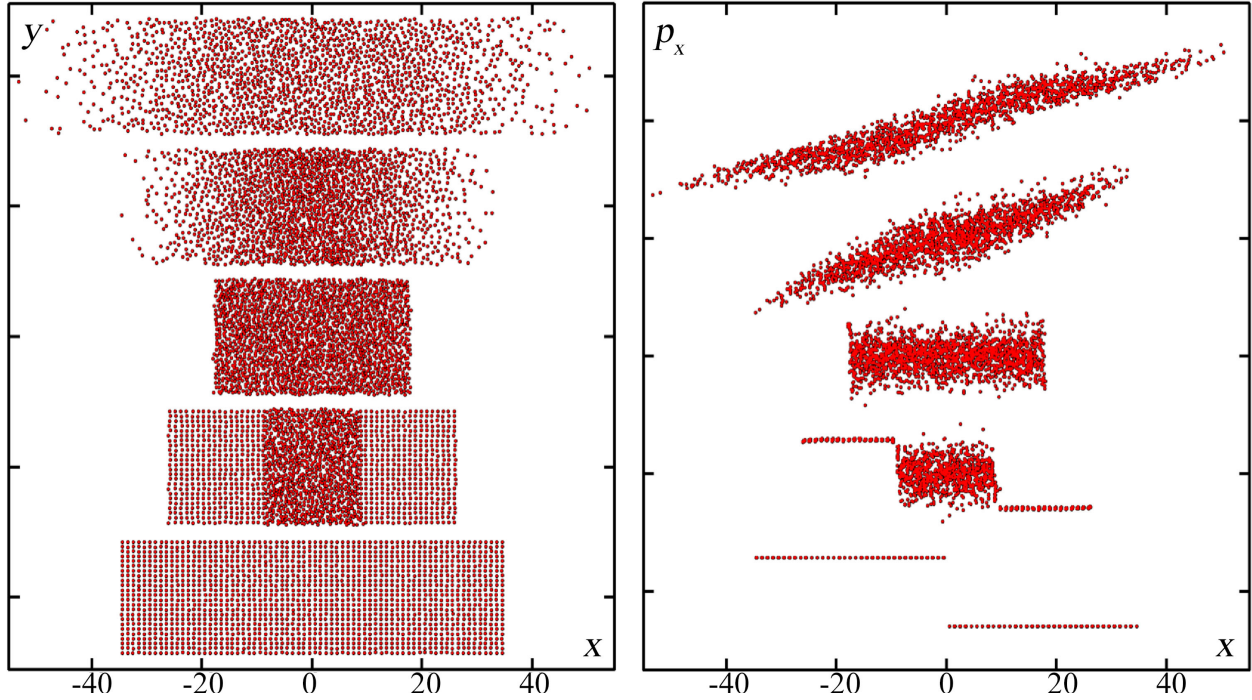


Fig. 6. At the left we see five particle plots, at times 0, 10, 20, 30, and 40 from bottom to top, during the twofold shock compression ( $0 < t < 20$ ) and subsequent generation of rarefaction waves ( $t > 20$ ) simulated by the head-on collision of  $2 \times 840 = 1680$  soft disks. The initial square-lattice coordinates (at bottom left) and horizontal velocities  $u_p = u_s/2 = \pm 0.875$  (at bottom right) are selected so as to generate twofold shock compression, doubling the density to generate a hot fluid, reaching it with the coordinates and velocities in the middle view of Fig. 6 and the bottom view of Fig. 7. Initially the lattice symmetry is broken with random displacements of  $x$  and  $y$  in the range from  $-0.05$  to  $+0.05$ . The top two plots show the growing twin rarefaction fans launched from the edges of the hot dense fluid. At the right the evolving horizontal velocity components are shown at the same five equally-spaced times, from 0 to 40. The rarefaction fans at times 30 and 40 are expanding at about the speed of sound. The smooth short-ranged repulsive pair potential governing the Newtonian dynamics is  $\phi(r < 1) = (10/\pi)(1 - r)^3$ . The fourth-order Runge-Kutta integrator with  $dt = 0.01$  was used for Figs. 6 and 7

Attempting to confirm and elaborate this estimate we constructed reference and satellite trajectories, for a range of timesteps from  $n = 1$  through  $n = 7$ :

$$dt = 0.1/2^n ; n = 1 \rightarrow dt = 0.05 \dots n = 7 \rightarrow \\ \rightarrow dt = 0.00078125 ,$$

rescaling their reference-to-satellite separation to 0.00001 at the end of each timestep. Typical resulting values of the local-in-time Lyapunov exponent  $\lambda_1(t) \simeq 1.8$  are shown in Figs. 8 and 9. The complete set of 6720 two-block motion equations is included in the Lyapunov calculation. The signs of all the velocity components are changed at time 20 in Fig. 8 and at time 10 in Fig. 9, with the particle coordinates pictured as the latter figure's inset.

Fluctuations of the local exponent  $\lambda_1(t)$  can be substantially reduced by smoothing, averaging the nearest 100 local values. In Fig. 8 this average is plotted in red. With  $dt$  positive the exponent  $\lambda_1(t)$  is uniformly positive, changing sign with the velocity reversal. The reversed reference and satellite trajectories attract for a while, as expected, but only for a while, for a time of order 3 with  $dt = 0.01$  and 5 with  $dt = 0.00078125$ . Because integration errors are magnified exponentially, as described by the Lyapunov expo-

nent,  $\lambda_1 \simeq 1.8$ , there is a systematic timestep dependence of the time “ $t_{\text{rev}}(dt)$ ”. The exponent is reversed for a time proportional to the logarithm of the number of timesteps,  $\propto \ln(1/dt)$ . Roughly speaking,  $t_{\text{rev}}(dt)$  increases by about 0.4 for each halving of the timestep. See Fig. 9. A set of seven computations with  $0.05 \leq dt \leq 0.0078125$  suggests the phenomenological relation

$$e^{1.8t_{\text{rev}}(dt)} \simeq dt^{-?} \rightarrow 1.8t_{\text{rev}} \simeq -? \ln(dt) .$$

In Fig. 9  $t_{\text{rev}}$  varies from about 3 to about 5 as the timestep decreases by a factor of 64.

The logarithmic relationship between timestep and reversal time is consistent with the exponential amplification of few-step integration errors. A similar rough relationship holds for the limit-cycle problem of Figs. 2–4. Capturing a reversed trajectory with visual accuracy up to a time  $t_{\text{rev}}(dt)$  requires a simulation effort varying as  $(t_{\text{rev}}/dt)$ .

We are pleased to offer a reward for further investigation of these problem types: a special \$1000 “Snook Prize”, in honor of our late colleague Ian Snook, who died in 2013. Application for this Prize requires the submission of an appropriate acceptable electronic manuscript addressing shock-wave reversibility to [link](http://cmst.eu)<sup>1</sup> prior to year's end of 2023.

<sup>1</sup> <http://cmst.eu>

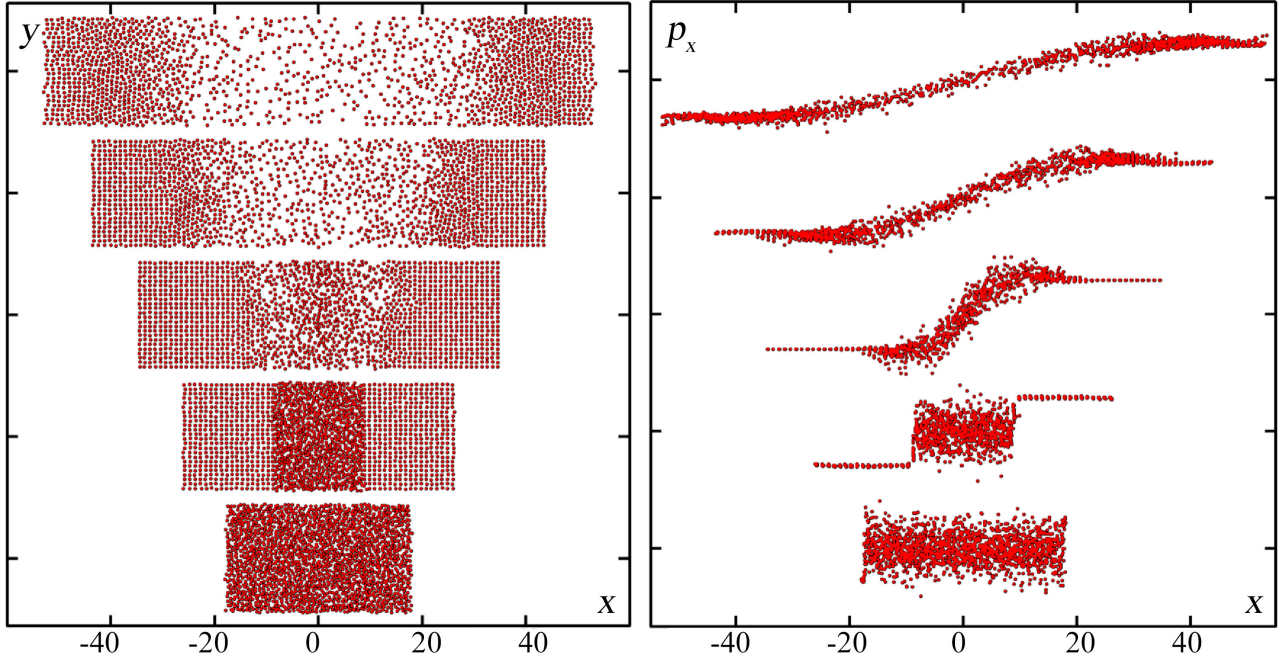


Fig. 7. Velocity reversal following the twofold shock compression of 1680 soft disks. The initial velocities  $\pm 0.875$  at the left and right, resulted in a head-on collision. The initial particle coordinates at the base of this figure correspond precisely to the maximum-compression middle view of Fig. 6. The initial velocities were changed in sign so that the next-to-bottom snapshot here corresponds closely to a reversal of the next-to-bottom view of Fig. 6. Soon after, Lyapunov instability, with  $\lambda_1 \simeq 2$ , prevents additional reversed configurations at time 20, 30, and 40. Just as in Fig. 6 particle positions appear at the left with corresponding horizontal velocity components at the right

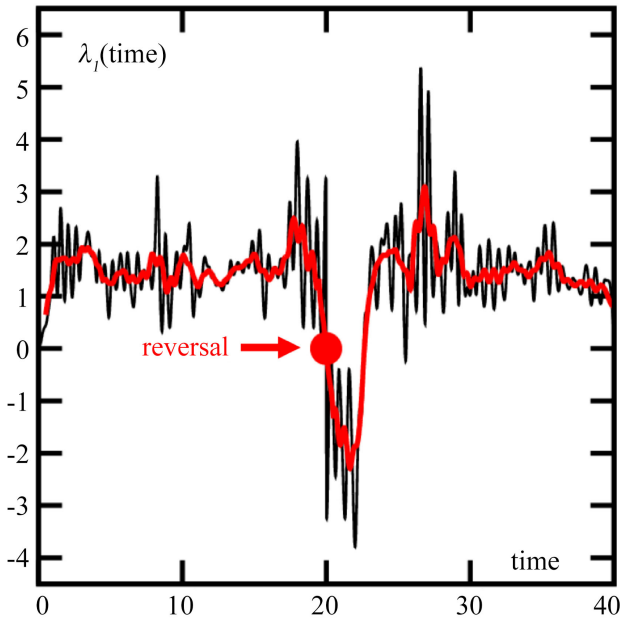


Fig. 8. The local Lyapunov exponent for the time-reversal of Fig. 6. The reversal, at time 20, is indicated by a filled red circle. The red curve corresponds to a smoothed exponent averaged over unit time, 100 time steps with the step  $dt = 0.01$ . Notice that the Lyapunov exponent is of order  $\pm 2$  in the shocked dense fluid or in the cold initial solid, suggesting an observable lack of reversibility when the amplified roundoff error reaches the amplitude of Lyapunov instability, a time of order 14 for  $dt = 0.01$ :  $0.01^5 e^{\lambda_1(t) \times t} / 120 \simeq \simeq 1 \rightarrow t \simeq 14$

## VII. Summary and Prognosis

Our first problem, the thermostatted generation of a heat current, stabilized by Nosé-Hoover mechanics, demonstrates that such dissipative examples, despite their time reversibility, stabilize mass, momentum, and energy flows consistent with the Second Law of Thermodynamics. The mechanism for this dissipative irreversibility is the formation of fractal phase-space distributions with mirror-image fractal pairs of distributions. With these pairs the attractor has probability one while the repeller has probability zero, even for a small system, the heat-conducting oscillator. This same explanation of thermostatted irreversibility holds for manybody systems, as was suggested in Refs. 7 and 8.

The purely-Newtonian shockwave problem illustrates a different, but related, mechanism for irreversibility. Though “mechanism” is conceptual, its realization is necessarily computational. Lyapunov instability destroys a time-reversed system’s memory by magnifying computational noise. Soon the amplified roundoff error becomes of order unity. Our shockwaves simulations show that this time is of order  $t \simeq 3$  to 5, just a few collision times. At that time the reversed flows are destabilized by the preponderance of entropy-producing flows over entropy-reducing flows, giving a purely Newtonian resolution of Loschmidt’s paradox. No thermostating control variable is required. But still it is likely that the probability of going forward with an entropy-producing shock exceeds that of its reversal in a singular way. The preponderance of states generating entropy, in the shock, over those which would reduce it in the reversed

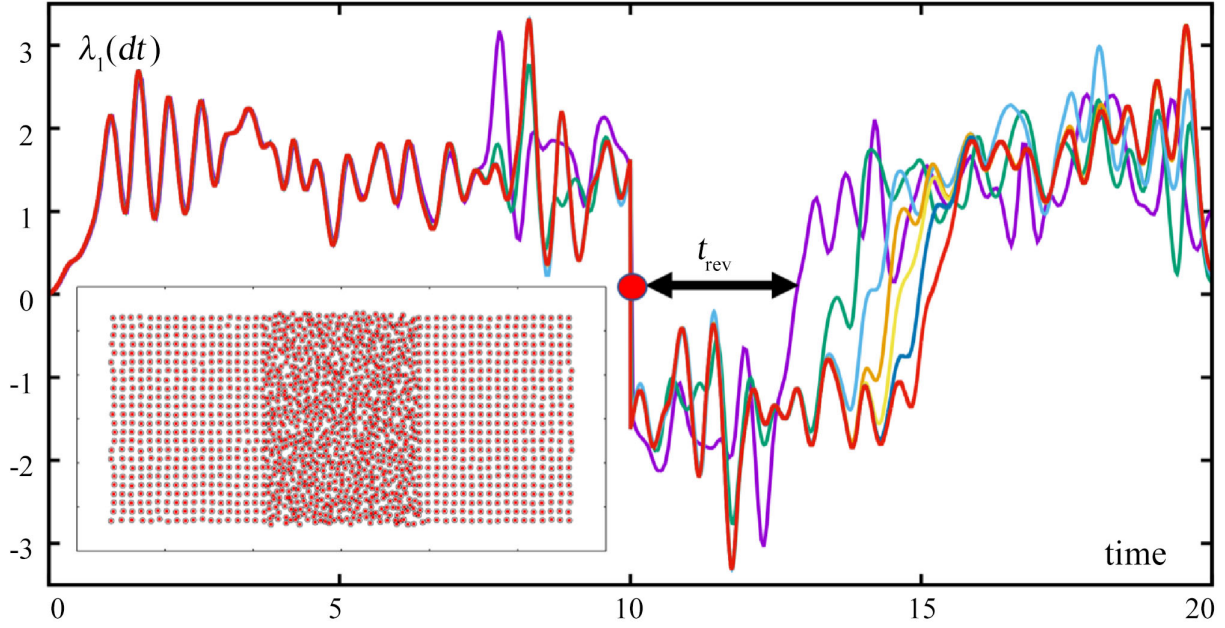


Fig. 9. The largest Lyapunov exponent,  $\lambda_1 \simeq 1.8$  for seven simulations with  $dt = 0.1/2^n$  reflects the velocity sign change at time 10. The accuracy of the reversal persists for a time  $t_{rev}$  varying as  $\ln(1/dt)$ , consistent with the Lyapunov amplification of integration errors to visible size. The inset snapshot corresponds to the  $t = 10$  configuration of 1680 soft-disk particles undergoing twofold shock compression up until the reversal time indicated by the red dot

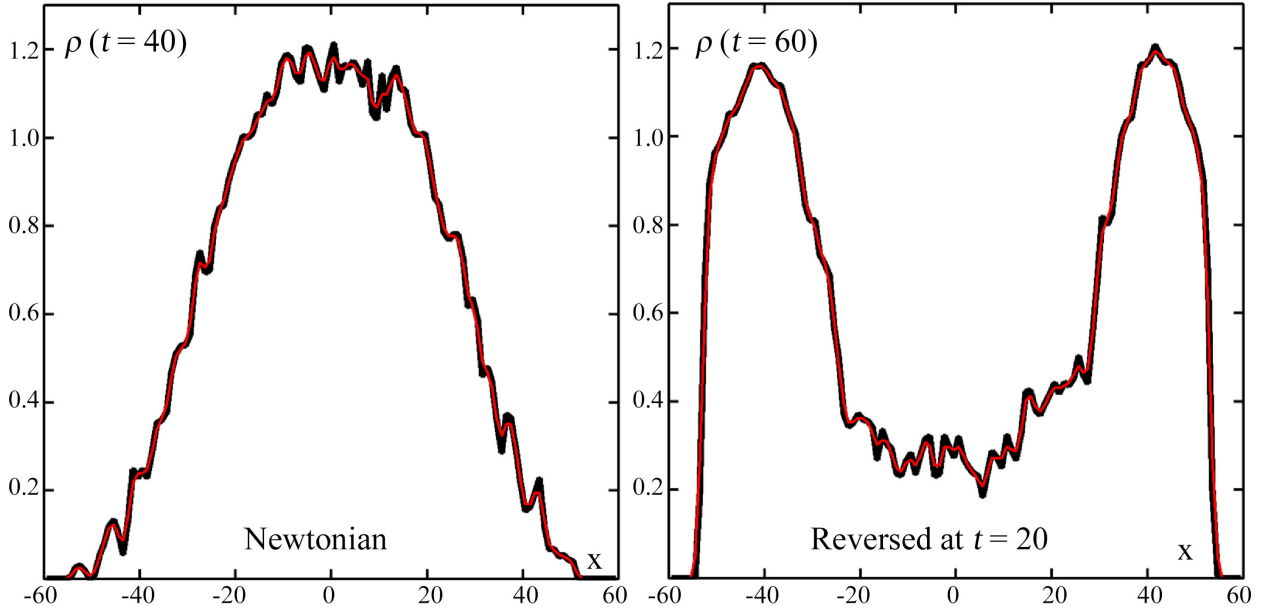


Fig. 10. Smoothed-particle density profiles, Newtonian at the left and reversed at the right. These profiles correspond to the topmost configurations of Figs. 6 and 7. Similar profiles of  $P_{xx}$  and  $P_{yy}$  show that the pressure is nearly isotropic. The thick black and red lines correspond to smoothed-particle ranges of 2 and 3 respectively

shock, requires no modification of the Newtonian motion equations.

In making the connection between computational simulations and continuum mechanics smooth-particle averaging is an indispensable tool. To illustrate this idea let us calculate density profiles  $\rho(x)$  for the topmost snapshots in

Figs. 6 and 7. Imagine the density of every particle to be spread out in  $x$  over a range  $h$  according to a normalized weight function  $w(r)$  with finite range and two continuous derivatives:

$$r < h \longrightarrow w(r, h) = [5/4hL_y][1 - (r/h)]^3[1 + 3(r/h)]$$

[Lucy's weight function].



Summing the weights contributed by each of the particles to every grid point in the set  $\{x_g\}$  produces the smoothed density profiles shown in Fig. 10 with  $h = 2$  and  $h = 3$ . The grid spacing is unity so that every particle contributes to four or 6 nearby grid points for these two values of  $h$ . We see that neither profile matches the uniform density at the base of Fig. 6. The regular square-lattice structure near both ends of the hot shocked fluid (near  $x = \pm 20$ , at the base of Fig. 7 and the middle of Fig. 6) is less susceptible to the smoothing loss of memory due to Lyapunov instability.

Smooth-particle averaging can be applied to any of the atomistic functions of coordinates and momentum. Plots of the pressure tensor indicate isotropy with  $P_{xx} \simeq P_{yy}$ . Research into the details of the atomistic distribution functions could elucidate further the mechanism responsible for the exponentially greater density of phase flows obeying the Second Law to those flouting it. There remains much to do in understanding the failure of Loschmidt's cogent idea – questioning the ability of mechanics to provide an understanding of thermodynamics.

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