Nonequilibrium Molecular Dynamics, Fractal Phase-Space Distributions, the Cantor Set, and Puzzles Involving Information Dimensions for Two Compressible Baker Maps

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Abstract—Deterministic and time-reversible nonequilibrium molecular dynamics simulations typically generate “fractal” (fractional-dimensional) phase-space distributions. Because these distributions and their time-reversed twins have zero phase volume, stable attractors “forward in time” and unstable (unobservable) repellors when reversed, these simulations are consistent with the second law of thermodynamics. These same reversibility and stability properties can also be found in compressible baker maps, or in their equivalent random walks, motivating their careful study. We illustrate these ideas with three examples: a Cantor set map and two linear compressible baker maps, N2(q, p) and N3(q, p). The two baker maps’ information dimensions estimated from sequential mappings agree, while those from pointwise iteration do not, with the estimates dependent upon details of the approach to the maps’ nonequilibrium steady states.

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1. NONEQUILIBRIUM MOLECULAR DYNAMICS GENERATES FRACTALS

The computers developed for the National Laboratories were first applied to manybody problems in the 1950s. At Los Alamos in 1953, Fermi, Pasta, and Ulam [1] described the incomplete equilibration of one-dimensional waves in anharmonic chains. Soon afterward, at Livermore, Berni Alder and Tom Wainwright simulated the motion of systems of several hundred hard disks and spheres [2]. At Brookhaven George Vineyard and his coworkers studied “realistic” atomistic models of the impact of high-energy radiation on models of simple metals shortly thereafter [3]. All of these atomistic simulations were developed based on classical Newtonian mechanics with short-ranged pairwise-additive forces. “Large” simulations involved several hundred discrete particles. A generation later simulations with millions of particles were possible. Figure 1 shows a typical simulation from our 1989–1990 visit to Japan. These indentations of amorphous Stillinger—Weber silicon, using two different indenter models, generate plastic flow near the indentors [4]. Trillion-atom simulations are feasible in 2020.

In 1984 Shuichi Nosé had announced a revolutionary method for imposing specified temperatures and pressures on molecular dynamics simulations [5, 6]. His modification of Hamiltonian mechanics was designed to replicate Gibbs’ isothermal and isobaric ensembles. Equilibrium distributions had been formulated by Gibbs’ statistical mechanics prior to the close of the 19th century. To match Gibbs’ results Nosé found it necessary to introduce a “scaled” time which had the drawback of introducing wild fluctuations in the dynamics. Hoover helped develop these ideas into practical
numerical algorithms [7] which avoided time-scaling. The simplest problem to which the Nosé–
Hoover approach can be applied is the harmonic oscillator with unit mass, force constant, and
temperature:

\[ \dot{q} = p; \quad \dot{p} = -q - \zeta p; \quad \dot{\zeta} = p^2 - 1 \ [ \text{NH}] \]

Here \((q,p)\) are the oscillator coordinate and momentum. The time-averaged kinetic temperature,
\(\langle p^2 \rangle\), is controlled (“thermostatted”) by the time-reversible friction coefficient \(\zeta\). The reader can
verify, as was pointed out in Ref. [7], that applying the steady-state continuity equation for the
flow in \((q,p,\zeta)\) space gives Gibbs’ canonical distribution for the oscillator together with a Gaussian
distribution for the friction coefficient \(\zeta\):

\[ (\partial f/\partial t) = 0 = -\partial(f\dot{q})/\partial q - \partial(f\dot{p})/\partial p - \partial(f\dot{\zeta})/\partial \zeta \leftrightarrow f(q,p,\zeta) \propto e^{-(q^2+p^2+\zeta^2)/2}. \]

This idea and its isobaric analog have become standard approaches to equilibrium molecular
dynamics simulations for a wide variety of systems both large and small.

Although pairwise-additive potentials might seem an oversimplification, work earning Nobel
Prizes in chemistry (1986 and 2013), carried out by Dudley Herschbach and Martin Karplus
and their colleagues, showed otherwise [8]. Straightforward classical solutions of pairwise-additive
motion turned out to be quite useful in interpreting and predicting the properties of molecules both
simple (hydrogen and various alkali halides) and complex (proteins). In most isoenergetic dynamics
motion equations,

\[ x_{t+dt} = 2x_t - x_{t-dt} + dt^2(F_x/m)_t \leftarrow \ddot{x} = (F_x/m). \]

Similar time-reversible algorithms have been developed for isothermal and isobaric systems [9].

Though not time-reversible, fourth-order Runge–Kutta integration of the system of first-order
motion equations,

\[ \{ \dot{x} = (p_x/m); \quad \dot{p}_x = F_x \}, \]

provides better accuracy at a fixed time step \(dt\), particularly for the velocities. Typical equilibrium
simulations, based on Newtonian or Hamiltonian or Nosé–Hoover mechanics, use periodic boundary
conditions. Series of such simulations can be used to generate “equations of state”, temperature
and pressure as functions of energy and density.

Nonequilibrium simulations such as Vineyard’s radiation-damage studies, or the simulation of
planar shockwaves, require the implementation of special boundary conditions capable of imposing
velocity and temperature differences across systems of interest. An early discovery motivating
quantitative atomistic simulations was the finding that the width of strong shockwaves is on the
order of the size of molecules so that details can be modelled reasonably well with only a few
thousand particles. The atomistic and continuum descriptions of strong shockwaves were in rough,
ten percent, agreement with one another [10].

By 1987 a significant difference between equilibrium and nonequilibrium steady states had come
to light. Simple nonequilibrium simulations were shown to produce fractal (fractional-dimensional)
phase-space distributions, with a negligible phase-space volume relative to corresponding higher-
dimensional equilibrium Gibbs’ distributions, such as the microcanonical and canonical ensem-
bles [11–13]. About the simplest steady-state mechanical problem results when heat is driven
through a Nosé–Hoover harmonic oscillator exposed to a temperature gradient [14, 15]. Where the
maximum value of the temperature gradient is \(\epsilon\), the three motion equations (for the coordinate \(q\),
the momentum \(p\), and the current-driving friction coefficient \(\zeta\)) are as follows:

\[ \dot{q} = p; \quad \dot{p} = -q - \zeta p; \quad \dot{\zeta} = p^2 - T(q); \quad T(q) = 1 + \epsilon \tanh(q) \ [ \text{NH}] \]

Here again, the oscillator mass, force constant, and mean temperature have all been chosen
equal to unity, but the temperature gradient can generate nonequilibrium steady states. The three
coupled equations give rise to a wide variety of solutions. Three such solutions, all for a maximum
temperature gradient \(\epsilon = 0.42\), are shown in Fig. 2. There we see a dissipative limit cycle as well
as two conservative tori. Chaotic solutions are also accessible to the model. More complicated
mechanical models, with two friction coefficients, $\zeta$ and $\xi$, and the same coordinate dependence of the temperature, $T(q) = 1 + \epsilon \tanh(q)$, can generate ergodic fractal distributions. In ergodic systems the same longtime steady-state solutions obtained apply for any initial condition (“almost any” for the mathematically minded). Two examples are shown in Fig. 3. The Hoover–Holian [16] and Martyna–Klein–Tuckerman [17] motion equations which generated them are as follows:

$$\dot{q} = p; \dot{p} = -q - \zeta p - \xi p^3; \dot{\zeta} = p^2 - T(q); \dot{\xi} = p^4 - 3p^2 T(q); \text{ [ HH ];}$$

$$\dot{q} = p; \dot{p} = -q - \zeta p; \dot{\zeta} = p^2 - T(q) - \xi \zeta; \dot{\xi} = \zeta^2 - T(q); \text{ [ MKT ].}$$

At equilibrium, with $T \equiv 1$, the two Hoover–Holian thermostat variables control both the second and the fourth moments of momentum. The Martyna–Klein–Tuckerman $\xi$ controls the distribution of the other thermostat variable $\zeta$. Detailed investigations of these oscillator problems at equilibrium show that both the HH and the MKT dynamics give the same ergodic distribution, including Gibbs’ canonical Gaussians in both $q$ and $p$.

$$f(q, p, \zeta, \xi) \propto e^{-(q^2 + p^2 + \zeta^2 + \xi^2)/2}.$$
Fig. 2. Three stationary solutions for the Nosé–Hoover oscillator with maximum temperature gradient $\epsilon = 0.42$. Unlike the Borromean rings each of the three solutions here is linked to the other two. See Ref. [15] for more details. The two tori are produced using the initial conditions $(q, p, \zeta) = (-2.3, 0, 0)$ and $(3.5, 0, 0)$. The limit cycle is produced using the initial condition $(-2.7, 0, 0)$.

Fig. 3. Two fractal $p(q)$ sections near the $\zeta = \xi = 0$ plane for (left) the Hoover–Holian oscillator with $\epsilon = 0.40$ and for (right) the Martyna–Klein–Tuckerman oscillator with $\epsilon = 0.20$. See Section 5.7.2 of W.G. Hoover and C.G. Hoover’s *Simulation and Control of Chaotic Nonequilibrium Systems* (World Scientific, Singapore, 2015). The initial conditions are $(q, p, \zeta, \xi) = (1, 0, 0, 0)$ with every fourth-order Runge–Kutta point plotted satisfying $\zeta^2 + \xi^2 < 0.00001$. Both sections were generated with $2 \times 10^{11}$ time steps using $dt = 0.003$.

A reversed process converting heat to work, a repellor, is outlawed by both the second law of thermodynamics and by computational instability in time-reversed numerical simulations [12].

We consider fractal distributions in more detail in the following sections. We have already seen that in the 1980s nonequilibrium molecular dynamics led to the characterization of fractal (fractional-dimensional) distributions. These are qualitatively different to Gibbs’ smooth equilibrium distributions. Because the mathematics of fractals and their geometric characterization is interesting and sometimes paradoxical, we highlight stimulating research areas well-suited to student exploration in what follows. In Section II we begin with the simplest fractal, the Cantor
set, and a description of its fractal dimensionality. Section III takes up time-reversible compressible baker maps, where phase-volume changes model nonequilibrium heat transfer. The one-way nature of these maps ("Time’s Arrow") is a direct geometric analog of the second law conversion of work to heat. Finally, we consider Kaplan and Yorke’s relation linking the fractal information dimension to the Lyapunov exponents. We show that their conjectured equality between the information dimension and the Kaplan–Yorke dimension, $D_{KY} \equiv D_I$, is precisely true for one baker map, N3, and apparently false for its very similar twin, N2. This surprise was completely unexpected. It richly deserves further study.

2. THE CANTOR SET AND THE FRactal INFORMATION DIMENSION

The simplest fractal is arguably the “middle third” "Cantor set". The middle third description suggests one of the several means for constructing the set: begin with the unit interval [0 to 1]; discard the middle third [(1/3 to 2/3)] leaving two intervals, [(0/3) to (1/3)] and [(2/3) to (3/3)]; discard the middle third of those two, leaving four intervals of length (1/9); finally, imagine the limiting set of points remaining after an infinite number (ℵ₀, the number of integers) of removal stages.

A more elegant alternative description of this same Cantor set, or “Cantor dust”, is the set of numbers on the unit interval whose ternary representation is composed wholly of 0s and 2s. An example set member is the base-3 number 0.20220000... = 2/3 + 0/9 + 2/27 + 2/81 + 0 = 62/81. Because each of ℵ₀ digits of the Cantor set can be either a 0 or a 2, the (likewise infinite) number of Cantor-set members is $2^{ℵ₀} \equiv ℵ₁$. The fact that the continuum itself, when expressed in binary base-2 rather than ternary base-3, has likewise ℵ₁ members, all the binary combinations of 0s and 1s, seems paradoxical. The continuum has no holes, while the well-named Cantor dust has nothing but! Does it really make "sense" to accept the notion that the members of the continuum and the Cantor set are equinumerous? Worse still, how sound is the notion that the number of members of the continuum is invariably ℵ₁, independent of the continuum’s dimensionality, one, two, three, ...? These troubling counter-intuitive aspects of Cantor’s ideas (and the undecidability of the continuum hypothesis) suggest an aesthetic-but-inapplicable branch of mathematics. Nevertheless, let us pursue a descriptive approach to dimensionality differences among the various infinite fractal subsets of continua.

Alfréd Rényi described recipes for various fractal dimensions long ago, the fractal dimension, information dimension, correlation dimension. Expressed in terms of the probabilities \{p\} of occupying a set of bins, all of the same size $δ$, with $δ$ sufficiently small, the forms of these three are as follows:

$$D₀ = \ln(\sum [p^θ]) / \ln(1/δ); \quad D₁ = \ln(\sum [p \ln p]) / \ln(δ); \quad D₂ = \ln(\sum [p^2]) / \ln(δ).$$

The sums include all occupied bins. The probabilities are normalized, $\sum [p] = 1$, and are typically proportional to the number of counts or the fractions of the total time associated with residence in each of the occupied bins. The fractal (or capacity), information, and correlation dimension correspond to $D₀$, $D₁$, and $D₂$. The reader can verify that in the case of the Cantor set these three dimensions are all the same, $D = \ln(2) / \ln(3) = 0.630930$. Notice that reducing the bin size by a factor of three results in just twice as many occupied bins. Likewise, coarsening the bin size by a factor of three results in just half as many occupied bins. $D$ plays the role of a ( fractional) dimension: $3^D = 2 \leftrightarrow D = \ln(2) / \ln(3)$.

This simplest of fractals sets the stage for studying two interrelated families of nonequilibrium fractals even simpler than those generated by the conducting harmonic oscillator problems. The two families of simpler models are [1] stochastic random walks (usually on the unit interval from 0 to 1) and [2] deterministic time-reversible compressible maps (where we use a rotated $2 \times 2$ diamond-shaped domain in order to model time-reversibility and to enhance ergodicity). The expected equivalence of these models is itself interesting. The fact that such simple models can lead to results that are contradictory or paradoxical, despite the long history of their study, is currently in need of further pedagogical explanation. The Ian Snook Prize for 2020 [18], to be awarded to the author(s) best addressing this need, is designed to shed light on these families of fractal problems.
The information dimension $D_I = D_1$, a close relative of Gibbs’ statistical entropy, is arguably the most useful descriptor of fractal point sets or distributions. Using the $p \ln p$ formula for $\delta = 1/27$ there are eight three-digit members of the Cantor set:

$\{0.000, 0.002, 0.020, 0.022, 0.200, 0.202, 0.220, 0.222\}$.

The resulting dimensionality is $\ln(1/8)/\ln(1/27) = \ln(2)/\ln(3) = 0.630930$. For any fixed number of digits the same distribution-based result is obtained. A numerical representation of the Cantor set as an arbitrarily large set of points can be generated by choosing an initial “seed” in the set, like $C = 2/9$ or $C = 62/81$, followed by iteration of the following loop of FORTRAN pseudocode:

```fortran
call random_number(R)
if(R.lt.0.5) Cnew = (C/3)
if(R.ge.0.5) Cnew = (C/3) + (2/3)
C = Cnew
write(33,*) it,C
```

[Unit Square Generation of the Cantor Set in (R,C) Cartesian Coordinates]

Here the FORTRAN `random_number` subroutine generates series of random numbers \{ R \} uniformly distributed between zero and one. Notice particularly that exactly the same pseudocode describes a random walk with variable length steps. Half the time the walker moves left from his present position $C$ to $C/3$ corresponding to adding a ternary 0 after the “decimal” point. Otherwise, and also half the time, the walker moves to the right, corresponding to adding in a ternary 2 after the point. The overall single-step operation shifts the ternary representation of $C$ one digit to the right and then chooses randomly either 0 or 2 to precede it.

Alternatively, a deterministic two-dimensional compressible map can be constructed to generate the Cantor set in a rotated $(q, p)$ space with the constant $d$ equal to $\sqrt{2}/6$:

```fortran
if(q.lt.p) qnew = + (7*q)/6 - (5*p/6) + 5*d
if(q.lt.p) pnew = - (5*q)/6 + (7*p/6) - 1*d
if(q.ge.p) qnew = + (7*q)/6 - (5*p/6) - 5*d
if(q.ge.p) pnew = - (5*q)/6 + (7*p/6) + 1*d
q = qnew
p = pnew
```

[Diamond-Shaped Generation of the Cantor Set in (q,p) Space]

100,000 points generated with these stochastic and deterministic mappings are illustrated in Fig 4. Here and in that figure, just for convenience in the programming, the $2 \times 2$ diamond-shaped domain has extreme values of $q$ and $p$ of $\pm \sqrt{2}$. In the next section we elaborate on our preference for the rotated map of the two-dimensional $(q, p)$ domains rather than the conventional $(x, y)$ unit square.

### 3. INFORMATION DIMENSIONS FOR COMPRESSIBLE BAKER MAPS

The baker map considered by Eberhard Hopf in 1937 provides a simple deterministic model for the dissipative chaos causing irreversible behavior in the solutions of time-reversible motion equations. By 1987 several examples of thermostatted molecular dynamics led to the representation of nonequilibrium steady states as fractal structures in $(q,p)$ (coordinate, momentum) phase space [11–13]. A two-panel baker map $N_2$, incorporating twofold changes in the area $dqdp$ is the prototypical example, displayed in Figs. 5 and 6. This mapping [19–22] follows the equations

```fortran
if(q-p.le.-sqrt(2/9)) qnew = + (11/6)*q - (7/6)*p + 14*d
if(q-p.le.-sqrt(2/9)) pnew = - (7/6)*q + (11/6)*p - 10*d
if(q-p.gt.-sqrt(2/9)) qnew = + (11/12)*q - (7/12)*p - 7*d
if(q-p.gt.-sqrt(2/9)) pnew = - (7/12)*q + (11/12)*p - 1*d
```

[Nonequilibrium Two-Panel Baker Map N2]
Fig. 4. Two two-dimensional forms of the one-dimensional Cantor set are shown here. At the left, in the unit square with $0 < R, C < 1$ $R$ is chosen randomly and the $C$ coordinate follows a stochastic random walk governed by $R$. At the right, in the rotated $2 \times 2$ diamond-shaped domain the next $(q, p)$ point follows from the last according to the “diamond-shaped generation” algorithm given at the end of Section II. The figure shows a sequence of 100,000 points in both cases.

where the constant $d$ is $\sqrt{1/72}$. The map is irrotational, with unstable fixed points at the top and bottom of the diamond-shaped domain where $q$ is horizontal and $p$ vertical. The diamond-shaped domain used here, $-\sqrt{2} < q, p < +\sqrt{2}$, is purposefully rotated 45 degrees from the usual Cartesian baker map. So as to emphasize the time-reversibility of our compressible baker map N2 we choose the diamond-shaped $2 \times 2$ domain. Reversing the time corresponds to reversing the sign of the (vertical) “momentum” $p$ while keeping the horizontal “coordinate” $q$ unchanged.

This nonequilibrium baker map N2 is “time-reversible” in the sense that the inverse mapping, $N_2^{-1}$, is given by the product mapping $T \cdot N_2 \cdot T$. The time-reversal mapping $T$ simply changes the sign of the momentum, $T(q, \pm p) = (q, \mp p) = T^{-1}(q, \pm p)$. A typical long-time cumulative solution of the N2 mapping is far from homogeneous but is nonetheless ergodic, with nonvanishing density everywhere within its diamond-shaped domain. This nonequilibrium (area-changing) mapping produces no “holes” so that its capacity or box-counting or fractal dimension is 2. See the 100,000-point samples of the mapping and its inverse in Fig. 5. The N2 mapping is compressive parallel to the line $q = p$ and expansive in the perpendicular direction. Numerical work indicates that the resulting distribution of points is random in $\tilde{x}$ and remains fractal in $\tilde{y}$ where the orthogonal coordinates $(\tilde{x}, \tilde{y})$ occupy a $2 \times 2$ square centered on the origin:

$$-1 < \tilde{x} = (q - p)/\sqrt{2} ; \quad \tilde{y} = (q + p)/\sqrt{2} < +1.$$  

For convenience in the measurement of the fractal information and correlation dimensions and the construction of random walks in $y$ corresponding to the fractal direction parallel to $q = p$, it is convenient to map the $2 \times 2$ $(\tilde{x}, \tilde{y})$ square onto the unit $(x, y)$ square:

$$x \equiv (\tilde{x} + 1)/2 ; \quad y \equiv (\tilde{y} + 1)/2.$$  

Then an equivalent set of $(x, y)$ values can be generated by a random walk based on random numbers from the unit interval, $0 < \{ r \} < +1$ as follows:

```fortran
    call random_number(r)
    x = r
    call random_number(r)
    if(r.lt.(2/3)) ynew = (0+1*y)/3
    if(r.ge.(2/3)) ynew = (1+2*y)/3
```
Because the N2 mapping and this random walk generate the same long-time distributions of the compressive $y$ variable the various fractal dimensions [23–25] \{ $D$ \} (box-counting, information, Kaplan–Yorke, and correlation, ...) are simply related, $D_{\text{map}}(q,p) = D_{\text{walk}}(y) + 1$.

Careful investigations [21, 22] of the local densities of points in two-dimensional bins of area $\delta^2 = (1/3)^{2M}$, with the integer $M$ up to 20, suggested a pointwise fractal information dimension of 1.7415. But mapping regions rather than points, and starting with a uniform distribution in the diamond-shaped domain gave a totally different result! The information dimension calculated for the same N2 map according to the mapping of regions (areas) rather than by propagation of a single mapped point can be calculated analytically [24]. The result is $D_{\text{regions}}^{N2} = 1.789690$ rather than $D_{\text{points}}^{N2} = 1.7415$.

### 3.1. The Kaplan–Yorke Dimension from Lyapunov Instability

On the other hand, forty years ago Kaplan and Yorke [26] conjectured that the fractal information dimensions of solutions of typical two-dimensional maps are simply related to the solutions’ Lyapunov exponents. Because two-thirds of the N2-mapped area undergoes a 1.5-fold stretching while one-third undergoes three-fold stretching, the larger Lyapunov exponent is $\lambda_1 = (2/3) \ln(3/2) + (1/3) \ln(3) = +0.636514$. The smaller (negative) Lyapunov exponent describes the shrinking: $\lambda_2 = (2/3) \ln(1/3) + (1/3) \ln(2/3) = -0.867563$. Kaplan and Yorke reasoned that the information dimension for such a map is given by

$$D_I = 1 - (\lambda_1/\lambda_2) = 1.733680,$$

a bit less than the estimate from bin-density data [21, 22] and far from the analytic area-mapping result, 1.789690.

In our efforts to understand these differences we came upon a related N3 mapping, compared to N2 in Fig. 6. N3 is a slight elaboration of N2 and, from the standpoint of irrotational area mappings, produces the same information dimension. Here is the **FORTRAN** description of a single step in the corresponding random walk:

```fortran
  call random_number(r)
  x = r
  call random_number(r)
  if (r.lt.(2/3)) ynew = (y/3) + (0/3)
  if ((r.ge.(2/3)).and.(r.le.(5/6))) ynew = (y/3) + (1/3)
  if (r.gt.(5/6)) ynew = (y/3) + (2/3)
  y = ynew
```

![Fig. 5.](image_url) The repellor generated by N2$^{-1}$ (left) and attractor generated by N2 (right) using 100 000 iterations from the initial point $(q,p) = (0,0)$. Note that $-\sqrt{2} < q, p < +\sqrt{2}$. The map is time-reversible so that the repellor is the mirror-image (with the mirror horizontal) of the attractor. Although the fractal dimensions of the attractor and the repellor are identical, their stabilities (as given by their Lyapunov exponents from N2) are opposite as a consequence of their time-reversibility.
Throughout our numerical work we have used the handy FORTRAN random-number generator indicated here, “random_number(r)”, said to have a repeat length of order $10^{77}$ (!).

![Two and Three Panel Nonequilibrium Baker Maps](image)

**Fig. 6.** The rotationless two-panel and three-panel maps N2 and N3 are illustrated here. For more details, see our recent arXiv contributions. N2 is time-reversible with its $N_2^{-1} = T^*N_2*T$, where the time-reversal mapping $T$ changes the sign of the vertical “momentum”, $T(q, \pm p) = (q, \mp p)$. Although the two mappings are similar, N3 is not time-reversible.

To illustrate the differences in ordering of the bin populations resulting from the first four steps of the random walks equivalent to N2 and N3, we compare million-point 81-bin histograms of the two walks in Figs. 7 and 8. Evidently, the N3 mapping, starting with a uniform distribution, produces exactly the same set of bin probabilities as does N2 (though in a different order) and so the walks have exactly the same information dimensions [24], 0.789690. But in the N3 case the Lyapunov exponents and the Kaplan–Yorke dimension are different, and produce an interesting

![ln2(ρ) for four iterations of N2](image)

**Fig. 7.** The histograms resulting from four iterations of the random walk version of the N2 map in the unit square. The initial distribution of one million points was uniform in the unit interval $(0 < x < 1)$. After the first iteration, with one third of the points moving left and two thirds right the probability density is 2 for $(0 < x < 1/3)$ and $(1/3) for $(1/3 < x < 2/3)$. Two iterations give probability densities of 4 for $(0 < x < 1/9)$, 1 for $(1/9 < x < 5/9)$ and $(1/4) for $(5/9 < x < 1)$. After the fourth iteration the numbers of bins at each level of probability density, from the highest, 16, to the lowest, 1/16, are $\{ 1 \times 1, 2 \times 4, 4 \times 6, 8 \times 4, 16 \times 1 \}$, 81 in all.
surprise:
\[ \lambda_1 = \frac{2}{3} \ln(3/2) + \frac{1}{3} \ln(6) = 0.867563; \quad \lambda_2 = \frac{2}{3} \ln(1/3) + \frac{1}{3} \ln(1/3) = -1.098612. \]
\[ \rightarrow D_{KY} = 1 - (\lambda_1/\lambda_2) = 1.789690. \] [Equivalent to \( D_I \) for N3].

\[ \text{Fig. 8.} \] The histograms resulting from four iterations of the random walk version of the N3 map in the unit square. The initial distribution of one million points was uniform in the horizontal interval \((0 < x < 1)\). The histograms show the base-2 logarithms of the fraction of the points in each of 81 bins of equal width. These bin probabilities are equal here to probability densities which integrate to unity over the interval \((0 < x < 1)\).

We show five different probability-density levels from \(2^{-4}\) for the highest probability density to \(2^{-4}\) for the least probable. After the fourth iteration the numbers of bins at the five different levels, from the highest probability to the lowest, are exactly the same as those from the N2 mapping in Fig. 7.

In fact, this time the Kaplan–Yorke conjecture is true, provided one imagines that the steady state maintains the stationary value of the information dimension observed during the evolution suggested by Fig. 9! A proof or disproof of this thought would be welcome.

4. DISCUSSION AND CONCLUSIONS

The Kaplan–Yorke conjecture \( D_I \approx D_{KY} \) is forty years old. It is surprising that the apparent counterexample for the linear N2 mapping considered here evaded detection for so many years. We have seen that the generalized baker maps N2 and N3 agree with both the thermodynamic and the computational statements of the second law of thermodynamics. The baker map fractals provide exactly the same computational mechanism for dissipation as is present in many-body simulations. But our understanding remains incomplete. Why is or is not the Kaplan–Yorke approximation valid or invalid for linear maps? The puzzling difference between pointwise dimensionality and regionwise dimensionality is likewise unsettling, but is firmly established by our results.

The mathematics of fractal sets remains paradoxical and challenging. Besides the disagreement between the various versions of the information dimension the simple geometry of fractals is itself puzzling. The popular understanding of cumulus clouds as 2.5-dimensional objects suggests that fractals are isotropic. The Sierpinski carpet and sponge fractals have characteristic rotational symmetries. On the other hand, all of the fractals arising from statistical mechanics appear to be
Fig. 9. Information dimension data for the random walk problem equivalent to the N3 mapping are all consistent with the same information dimension $D_I = D_{KY} = 0.789690$ for the walk and 1.789690 for the mapping. Pointwise analyses of the N3 mapping are described here for meshes of $(1/2)^n$ (red), $(1/3)^n$ (green), and $(1/6)^n$ (black). Analogous data for the N2 mapping are displayed in Fig. 5 of Ref. [18].

5. POSTSCRIPT OF 25 APRIL 2020

We wish to thank the anonymous referee for his many thoughtful suggestions, most of which we have adopted. The abstract has been completely rewritten. Some repetitions and ambiguities have been removed. Our descriptions of the Cantor set and the geometry of time-reversible maps have both been improved. We decided not to follow the referee’s suggestion to add additional references citing work of the many that have been attracted to these and similar problems independently of our own efforts. We believe that any attempt at completeness on our part would have the unintentional effect of slighting others of our kind friends and colleagues. We have chosen to refer here only to those works that have directly influenced our own. Comparing the present version to the arXiv second version of 9 January 2020 will satisfy the curious reader as to all the changes we have made.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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