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2024 Snook Prize Problem: Ergodic Algorithms' Mixing Rates

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Abstract: In 1984 Shuichi Nosé invented an *isothermal* mechanics designed to generate Gibbs' canonical distribution for the coordinates $\{q\}$ and momenta $\{p\}$ of classical N-body systems [1, 2]. His approach introduced an additional time-scaling variable s that could speed up or slow down the $\{q,p\}$ motion in such a way as to generate the Gaussian velocity distribution $\propto e^{-p^2/2mkT}$ and the corresponding potential distribution, $\propto e^{-\Phi(q)/kT}$. (For convenience here we choose Boltzmann's constant k and the particle mass m both equal to unity.) Soon William Hoover pointed out that Nosé's approach fails for the simple harmonic oscillator [3]. Rather than generating the entire Gaussian canonical oscillator distribution, the Nosé-Hoover approach, which includes an additional friction coefficient ζ with distribution $e^{-\zeta^2/2}/\sqrt{2\pi}$, generates only a modest fractal chaotic sea, filling a small percentage of the canonical (q,p,ζ) distribution. In the decade that followed this thermostatted work a handful of ergodic algorithms were developed in both three- and four-dimensional phase spaces. These new approaches generated the entire canonical distribution, without holes. The 2024 Snook Prize problem is to study the efficiency of several such algorithms, such as the five ergodic examples described here, so as to assess their relative usefulness in attaining the canonical steady state for the harmonic oscillator. The 2024 Prize rewarding the best assessment is United States \$1000, half of it a gift from ourselves with the balance from the Poznań Supercomputing and Networking Center.

Key words: ergodicity, fractals, Gibbs' canonical distribution, Lyapunov instability

I. The Nosé and Nosé-Hoover Thermostatted Oscillators

Up until 1984 "molecular dynamics" meant the numerical simulation of many-body motion obeying classical isoenergetic motion equations, usually Newton's, Lagrange's, or Hamilton's. On the other hand experimental data are often based on temperature and pressure as independent variables, isothermal and isobaric rather than isoenergetic. In pursuing the goals of an isothermal or isothermal-isobaric classical mechanics, *temperature*, the mean-squared one-dimensional momentum, $T \equiv \langle p^2 \rangle$, is specified rather than a constant energy. It is natural to impose an isokinetic constraint like this with integral feedback. Shuichi Nosé did so; he developed an isokinetic-isothermal mechanics shaped by a "time-scaling" variable s. Because s appeared squared in the denominator of Nosé's motion equations, and was typically small, Nosé's equations were too stiff to be of practical value [3–5]. Hoover avoided this stiffness problem by following a smaller "scaled momentum" (p/s) rather than (p/s^2). The resulting Nosé-Hoover motion equations for a harmonic oscillator became [3–5]:

$$\{ \dot{q} = p \,; \dot{p} = -q - \zeta p \,; \, \dot{\zeta} = p^2 - T \} \text{ [NH]}.$$

Numerical work using the classic fourth-order Runge-Kutta integrator with timestep $dt = 0.001$ revealed an infinite variety of one-dimensional periodic orbits and two-dimensional tori, with these features threading through a three-dimensional chaotic sea [4]. These 1986 results were various and most amazing, giving rise to hundreds of two-dimensional computer-generated plots covering nearly all of the horizontal surfaces in Professor Posch's Vienna office at Boltzmanngasse 5. A decade later this variety grew qualitatively when temperature varied with coordinate [6], $T(q) = 1 + \epsilon \tanh(q)$. The temperature gradient (dT/dq) promotes heat flux, adding fractal distributions and dissipative one-dimensional limit cycles to the mix. With ϵ small a chaotic fractal sea can result, depending upon choices of the maximum temperature gradient $(dT/dq)_{q=0} = \epsilon$ and the initial conditions. In no case were the solutions ergodic. Instead one-, or two-, or "fractal"-dimensional distributions, with dimensionalities mostly between two and three, result.

In what follows we describe two ergodic Harmonic-Oscillator algorithms in three-dimensional (q, p, ζ) space and three such ergodic algorithms in four-dimensional (q, p, ξ, ζ) space. This richness of approaches raises a question

$$\text{“}Which\ of\ these\ approaches\ is\ best\ ?\text{”}$$

Answering this question is the 2024 Snook Prize Problem. Here we follow the algorithm descriptions by suggesting several possible routes to answers.

II. Two Oscillator Algorithms Ergodic in Three Dimensions

II. 1. The 0532 Oscillator Model, Ergodic in Three Dimensions

Because a distribution is uniquely described by its various moments,

$$\langle p^2 \rangle = T,\ \langle p^4 \rangle = 3T^2,\ \langle p^6 \rangle = 15T^3,\ \langle p^8 \rangle = 105T^4,\ \ldots,$$

in the one-dimensional canonical case, it is "natural" to consider algorithms with more than one moment controlled by integral constraints. In fact, a brute-force Monte Carlo exploration of such models turned up the apparently ergodic "0532 Model" motion equations [7]:

$$\{\ \dot q = p\ ;\ \dot p = -q - \zeta(0.05p + 0.32p^3)\ ;$$
$$\dot\zeta = 0.05(p^2 - 1) + 0.32(p^4 - 3p^2)\ \}\ [0532].$$

This model is an example of "weak control" where a single control variable ζ controls a linear combination of two Gaussian velocity moments, the second and the fourth.

II. 2. Bang-Bang Oscillator Control, Ergodic in Three Dimensions

Tapias, Bravetti, and Sanders were awarded the 2016 Snook Prize for their discovery of a "Logistic Thermostat". They applied it to the harmonic-oscillator problem and concluded that for small Q Gibbs' canonical distribution was reproduced [8]:

$$\{\ \dot q = p\ ;\ \dot p = -q - (T/Q)\tanh(\zeta/2Q)p\ ;$$
$$\dot\zeta = p^2 - T\ \}\ [\text{TBS}].$$

Sprott [9] recognized that the small-Q limit can be written in terms of the sign function $\text{sign}(\zeta)$, -1 for negative and $+1$ for positive values of the friction coefficient ζ. The control force with just two values is also called "bang-bang" control. Sprott discusses numerical implementation of this novel control idea [9] using a hyperbolic tangent representation of the control, $\text{sign}(\zeta) \simeq \tanh(500\zeta)$ along with an adaptive Runge-Kutta integrator, with the timestep dt doubling or halving whenever the mean-squared difference $\Delta q^2 + \Delta p^2 + \Delta\zeta^2$ between a single step with dt and two steps with $(dt/2)$ slips outside of a specified narrow error range. Sprott's figures establish the ergodicity of this computational implementation of the TBS thermostat.

Three interesting and perhaps more elegant, four-equation approaches include two independent control variables to implement quadratic or quartic constraints. We consider the three algorithms in the following section.

III. Three Oscillator Algorithms Ergodic in Four Dimensions

In an effort to achieve ergodicity, accessing the entire Gibbs' canonical distribution, a variety of approaches were implemented in the 1990s. Simultaneous control of the fourth moment using another friction coefficient ξ, so that $\langle p^4 \rangle = 3T^2$, can generate the entire Gaussian distribution of velocities. The momentum moments (1 for the second moment and three for the fourth) for a one-dimensional harmonic oscillator, with $\dot q = p\ ;\ \dot p = -q$ at unit temperature, can be controlled with two "friction coefficients", ξ and ζ, in any one of the following three relatively simple ways. Perhaps simplest is the simultaneous control of the second and fourth moments of momentum as are imposed by the Hoover-Holian motion equations [10]. Simultaneous control of the second and fourth moments is realized by introducing a second friction coefficient ξ.

$$\{\ \dot q = p\ ;\ \dot p = -q - \xi p^3 - \zeta p\ ;$$
$$\dot\xi = p^4 - 3p^2\ ;\ \dot\zeta = p^2 - 1\ \}\ [\text{HH}(1)]\ [10].$$

Considerable stimulating and pioneering work by Bauer, Bulgac, and Kusnezov resulted in generalizing linear combinations of moments, including forces cubic in the friction coefficient. This higher power was found to improve ergodicity. Perhaps the simplest special-case example is the doubly-thermostatted BBK algorithm:

$$\{\ \dot q = p\ ;\ \dot p = -q - \xi p^3 - \zeta^3 p\ ;$$
$$\dot\xi = p^4 - 3p^2\ ;\ \dot\zeta = p^2 - 1\ \}\ [\text{BBK}(1)]\ [11\text{–}14].$$

In a simpler effort to achieve ergodicity, implementing quadratic forms accessing the entire Gibbs' canonical distribution, Martyna, Klein, and Tuckerman introduced "chains" of thermostats in the 1990s. In the simplest of these a second thermostat variable, ξ, is used to control the first, ζ. From the standpoint of elegance the following two-thermostat chain is probably the simplest four-equation approach to ergodicity in a four-dimensional space [15]

$$\{ \dot q = p \ ; \ \dot p = -q - \zeta p \ ; \ \dot \xi = \zeta^2 - 1 \ ; \\ \dot \zeta = (p^2 - 1 - \xi\zeta \ \} \ [\mathrm{MKT(1)}] \ [15].$$

In all three of these quadratic or cubic or quartic cases, HH, BBK, and MKT, the stationary probability density is Gaussian for (q, p, ξ). The stationary distribution is also Gaussian in ζ for HH and MKT, but not for BBK. That latter case includes $e^{-\zeta^4/4}$ in the probability density, which could be viewed as Gaussian in $\zeta^2/\sqrt{2}$.

To see that the full probability density f is stationary, proportional to $e^{-\zeta^4/4}$, it is only necessary to do a little algebra (the continuity equation) to show that the net flux into and out of an infinitesimal volume element $\otimes = dqdpd\zeta$ leaves the probability density unchanged [3]:

$$(\partial f/\partial t) \equiv -\partial(f\dot q)/\partial q - \partial(f\dot p)/\partial p + \\ -\partial(f\dot \xi)/\partial \xi - \partial(f\dot \zeta)/\partial \zeta \equiv 0.$$

In these three example problems the distributions of q and p can be extended from unit temperature to a general temperature T while leaving ξ and ζ dimensionless. It is easy to see that the modifications chosen here leave f stationary:

$$\{ \dot q = p \ ; \ \dot p = -q - (\xi p^3/T) - \zeta p \ ; \ \dot \xi = (p^4 - 3p^2 T)/T^2 \ ; \\ \dot \zeta = (p^2 - T)/T \ \} \ [\mathrm{HH(T)}] \ [10],$$

$$\{ \dot q = p \ ; \ \dot p = -q - (\xi p^3/T) - \zeta^3 p \ ; \ \dot \xi = (p^4 - 3p^2 T)/T^2 \ ; \\ \dot \zeta = (p^2 - T)/T \ \} \ [\mathrm{BBK(T)}] \ [11\text{–}14],$$

$$\{ \dot q = p \ ; \ \dot p = -q - \zeta p \ ; \ \dot \xi = \zeta^2 - 1 \ ; \\ \dot \zeta = (p^2 - T)/T - \xi\zeta \ \} \ [\mathrm{MKT(T)}] \ [15].$$

In all three cases the probability density for the coordinate q and momentum p are Gibbs' canonical distribution with Gaussian distributions for ζ and ξ :

$$f(q, p, \xi, \zeta) \propto e^{-(q^2+p^2)/2T} e^{-\xi^2/2} [\ e^{-\zeta^2/2} \text{ or } e^{-\zeta^4/4} \ ].$$

Just as before the full distribution $f(q, p, \xi, \zeta)$ is stationary provided that the flux in a four-dimensional volume element leaves the probability density unchanged [3]:

$$\partial(f\dot q)/\partial q + \partial(f\dot p)/\partial p + \partial(f\dot \xi)/\partial \xi + \partial(f\dot \zeta)/\partial \zeta \equiv 0.$$

Just as before the acronyms (HH, BBK, MKT) indicate the sources of the motion equations to papers by Hoover and Holian; Bauer, Bulgac, Ju, and Kusnezov; and Martyna, Klein, and Tuckerman. The BBK(T) equations have a quartic distribution for ζ, $e^{-\zeta^4/4}$. In all these cases prodigous numerical work established the ergodicity of the motion equations, indicating that the long time limiting distribution, independent of the initial conditions, includes complete Gaussian distributions for each of the four independent variables.

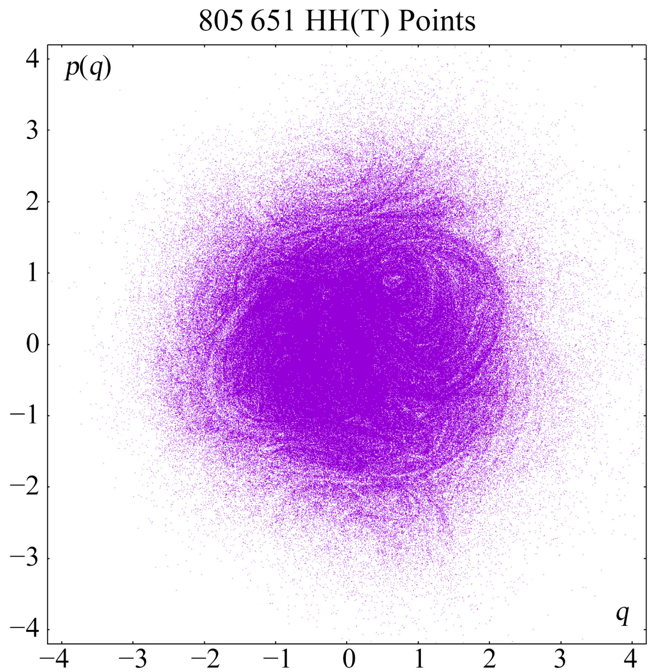

Fig. 1. Benchmark solution of the HH(T) equations with the explicit nonequilibrium $T(q)$ detailed in Sec. I. 15-hour half-trillion-timestep simulations. 805 651 $p(q)$ points selected from every fifth timestep with $|\xi|$ and $|\zeta|$ simultaneously less that 0.005. $\epsilon = 0.25$ so that $T = 1 + (1/4)\tanh(q)$ and $dt = 0.001$

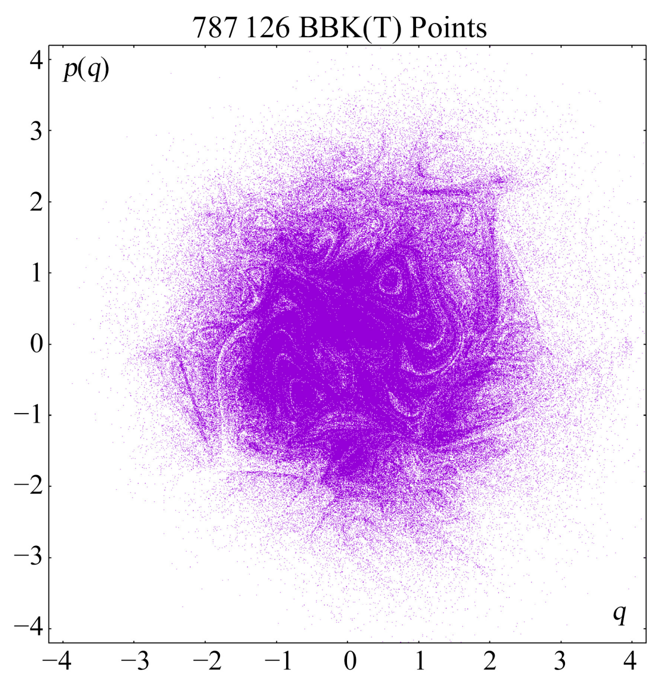

Fig. 2. Benchmark solution of the BBK(T) equations with the nonequilibrium $T(q)$ detailed in Sec. I. 15-hour half-trillion-timestep simulations. 787 126 $p(q)$ points selected from every fifth timestep with $|\xi|$ and $|\zeta|$ simultaneously less that 0.005. $\epsilon = 0.25$ so that $T = 1 + (1/4)\tanh(q)$ and $dt = 0.001$

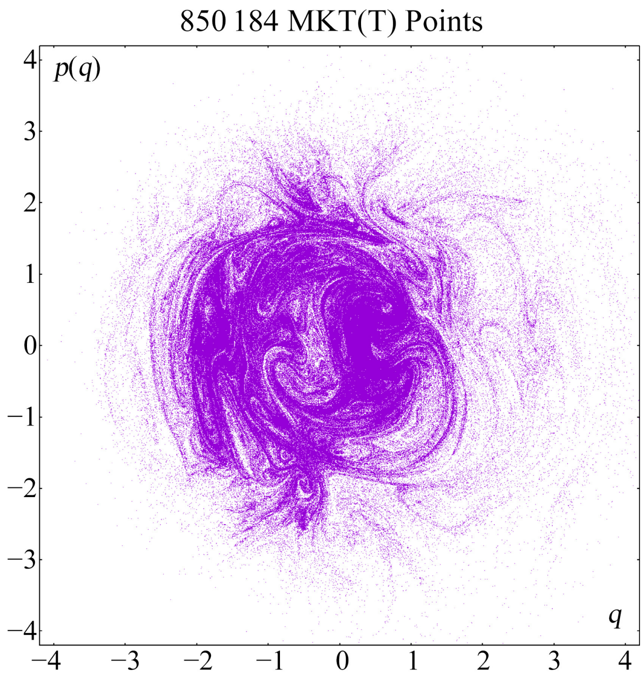

Fig. 3. Benchmark solution of the MKT(T) equations with the nonequilibrium $T(q)$ detailed in Sec. I. 15-hour half-trillion-timestep simulations. 850 184 $p(q)$ points selected from every fifth timestep with both $|\xi|$ and $|\zeta|$ simultaneously less that 0.005. $\epsilon = 0.25$ so that $T = 1 + (1/4)\tanh(q)$ and $dt = 0.001$

We benchmark the set of three nonequilibrium motion equations with an explicit temperature dependence in Figs. 1–3. In each case we avoid displaying one-dimensional trajectory segments near the $\xi = \zeta = 0$ plane by skipping four timesteps after each one displayed that satisfies $|\xi| < 0.005$ and $|\zeta| < 0.005$. The three simulations in the figures all used the initial conditions $(q, p, \xi, \zeta) = (0, 4, 0, 0)$.

IV. Estimating Phase-Space Mixing Rates

Straightforward computation should reveal the rate at which particular thermostats generate the canonical distribution. Moments of the oscillator coordinates and the friction coefficients from a few or many initial conditions are straightforward to compare. For the specified temperature of unity nearly all the measure of the various Gaussian distributions is confined to a hypercube with sidelength 12: $e^{-6^2/2} = 10^{-7.82}$ and $e^{-6^4/4} = 10^{-141}$.

The Lyapunov exponents are another tool for measuring the mean exponential spreading rate of probability in phase space. Sample values for the largest Lyapunov exponent are easy to find in the literature for the five ergodic thermostats and the Nosé-Hoover sea.

Finally, the time-dependent entropy can be followed by computing and extrapolating probability sums, $\sum P \ln(P)$, over the three or four-dimensional phase spaces, just as in the calculation of information dimension for the underlying differential equations [16]. The figures show very nicely that there are æsthetic sides to the study of these four-dimensional thermostatted flows, mostly unexplored. We are happy to consult with researchers interested in creating an understanding of the relative Mixing Rates of the various ergodic few-dimensional algorithms described here. In closing we thank Kris Wojciechowski for his encouragement and support.

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