2024 Snook Prize Winner: Mixing Rates of Ergodic Algorithms

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Abstract: The Snook Prizes (2014–2024) were stimulated by Shuichi Nosé's IBM–Japan prize award for time-reversible dynamics generating the canonical distribution [?]. The 2024 Snook Prize has been awarded to Clint Sprott for his exploration of six thermostatted harmonic oscillators at unit temperature that produce ergodic Gaussian distributions of position q and momentum p. The simplest example of a bang-bang controller with a signum nonlinearity reaches equilibrium most quickly as measured by the time-dependent kurtosis, $K_p(t) = \langle p^4 \rangle / \langle p^2 \rangle^2$.

Key words: Snook prize, ergodicity, Gibbs' canonical distribution, mixing

I. Introduction

In 1985 the Nosé–Hoover system was proposed [?] as a model of a harmonic oscillator in equilibrium with a heat bath at constant temperature T:

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -q - \zeta p \\ \dot{\zeta} &= p^2 - T. \end{aligned} \tag{1}$$

The thermostat variable ζ controls the damping of the oscillator such that the time-averaged mean square momentum $\langle p^2 \rangle = T$. However, the resulting chaotic orbit is not ergodic in the sense that it does not visit the entire (q, p) phase space. Instead, many initial conditions lead to quasi-periodic orbits embedded in the chaotic sea.

Nevertheless, hundreds of papers have been published over the past forty years using this technique along with many modifications of Eq. (1) intended to make the system more nearly ergodic. The most successful of these models are the 0532 system [?], the Tapias, Bravetti, and Sanders (TBS) system [?], the Hoover–Holian (HH) system [?], the Bauer, Bulgac, and Kusnezov (BBK) system [?], the Martyna, Klein, and Tuckerman (MKT) system [?], and the most recent signum thermostat system [?] given by

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -q - a\,\mathrm{sgn}(\zeta) p \\ \dot{\zeta} &= p^2 - T. \end{aligned} \tag{2}$$

where $\mathrm{sgn}(\zeta) = \zeta / |\zeta|$ is the signum function. All of these systems appear to be fully ergodic with a canonical (Gaussian) distribution of q and p.

In the 2024 Snook Prize Problem [?], we asked "which of these approaches is best" in the sense of converging most rapidly to the Gibbs' canonical distribution. We were pleased when Prof. Sprott accepted the challenge.

II. Method

In his prize-winning paper [?], Sprott calculated the time-dependent kurtosis $K_p(t) = \langle p^4 \rangle / \langle p^2 \rangle^2$ [and similarly $K_q(t)$] for each of the six systems with 10^5 initial conditions uniformly distributed in angle $0 < \phi < 2\pi$ over the constant energy circle given by $q_0^2 + p_0^2 = 2T$. For each case, the kurtosis increases from its initial value of

$K(0) = \langle \sin^4 \phi \rangle / \langle \sin^2 \phi \rangle^2 = 1.5$ to its asymptotic value of $K(\infty) = 3$ as expected for a Gaussian distribution. The convergence time t_c was arbitrarily defined as the earliest time at which K_q and K_p simultaneously fall within 1% of 3.0. Sprott assumed $T = 1$ and determined that the minimum t_c in Eq. (2) occurs for $a \cong 4$. The TBS system also has an adjustable parameter Q for which the minimum t_c occurs for $Q \cong 0.2$ with $T = 1$.

III. Results

Sprott then calculated t_c for each of the six cases, giving the results summarized in Table 1 with a statistical uncertainty of about 1%. The signum thermostat had the smallest value of $t_c \simeq 159$ independent of T, although only slightly less than the 4-dimensional MKT chain thermostat. He also showed that the largest Lyapunov exponent (LE) does not correlate with t_c in any obvious way.

System	Ref	t_c	LE
0532	[?]	632	0.1440
TBS	[?]	1608	0.1446
HH	[?]	1309	0.0680
BBK	[?]	406	0.0796
MKT	[?]	162	0.0665
signum	[?]	159	0.5050

Tab. 1. Convergence time and largest Lyapunov exponent for six ergodic models.

Figure **??** shows how K_q and K_p approach 3.0 for the best signum thermostat with $a = 4$, and it is typical of the cases shown in his paper.

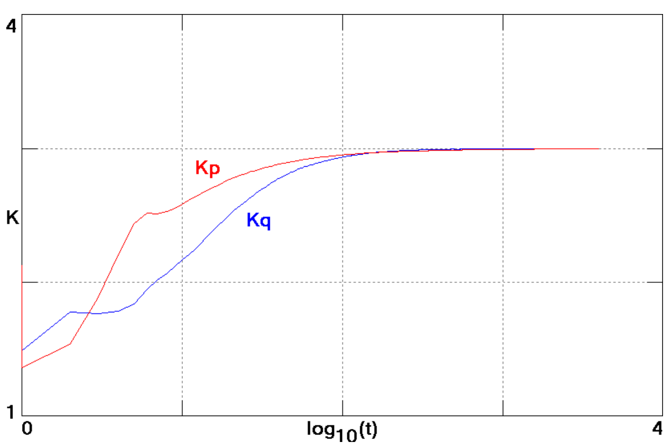

Fig. 1. Kurtosis versus time for the signum thermostatted system in Eq. (2) with $a = 4$.

IV. Conclusion

Perhaps it is unsurprising that a thermostat that switches abruptly and fully between two extreme states would achieve equilibrium the fastest, although this is not a foregone conclusion. We congratulate Prof. Sprott for proposing this elegant system and convincingly demonstrating its superiority over systems earlier proposed and studied.

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Bill and Carol Hoover met in 1973 in Livermore California. Bill was a Professor with a joint appointment teaching courses in the University of California's Department of Applied Science at the Davis Campus' Livermore Branch while serving as a physicist at the Livermore Laboratory. Carol was a student at the Department and a plasma physicist at the Livermore Laboratory. Carol earned her PhD in 1978. A decade later the Hoovers reconnected socially and married in preparation for joint sabbatical work with Shuichi Nosé, Taisuke Boku, and Toshio Kawai at the Yokohama Campus of Keio University. They developed million-atom molecular dynamics simulations at Keio and continued small-system work with Brad Holian at Los Alamos and Harald Posch at the University of Vienna. The Hoovers have published hundreds of research papers in computational statistical mechanics and eight books, beginning with *Molecular Dynamics* in 1986 and most recently, in 2023, *Elegant Simulations, from Simple Oscillators to Many-Body Systems*, coauthored with Clint Sprott (University of Wisconsin). The Hoovers moved from California to Nevada in 2005, and have continued their research work in retirement there in the ranching settlement of Ruby Valley in Elko County.