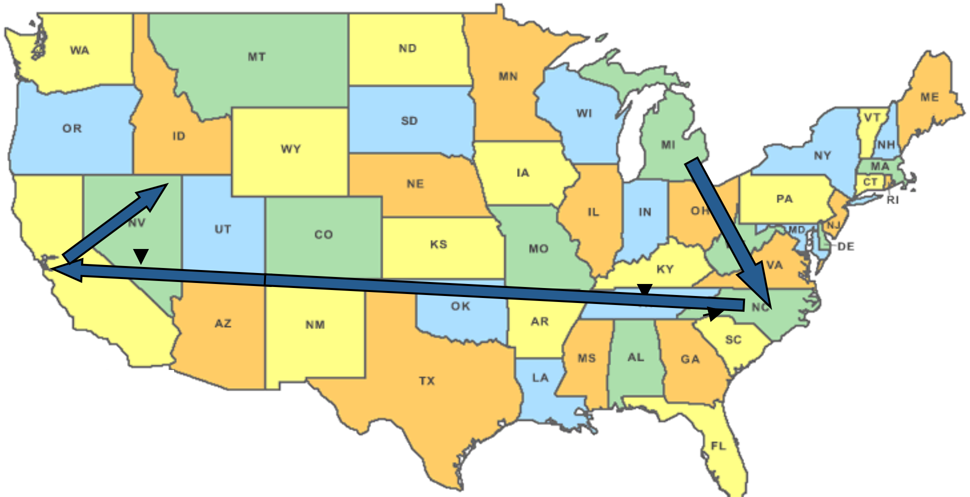
Nosé, Posch, Patra, Sprott

Wm G Hoover & Carol G Hoover
[no longer at UCDavis & LLNL!]



Ruby Valley Research Institute
Highway Contract 60, Box 601
Ruby Valley 89833 Nevada USA

Ruby Valley Neighbors

Local Ruby Valley Industry

MICRO-BREWED IN NEVADA'S HIGH COUNTRY

RUBY MOUNTAIN

BREWING COMPANY

VIENNA STYLE

LAGER

Nosé, Posch, Patra, and Sprott

by William Graham Hoover, Ruby Valley Nevada
From the perspective of a University of California Professor working at the Lawrence Livermore Lab

1. 1984 Shuichi Nosé*, Paris, Harald/Franz
2. 1996 Brad Holian and Ergodicity
3. 1997 Posch and Nonequilibrium Fractals
4. Clint Sprott and Color Graphics
5. 2014 Patra and Bhattacharya
6. 2010 Sergi and Ezra
7. 2001 Sergi and Ferrario
8. The Present and the Future
9. The 2015 Ian Snook Prize $500 + $555.55 US

* [The unexpected consequences of a Canadian Post-doctoral fellowship for a Japanese PhD From Kyoto, Shuichi Nosé]

#1: Shuichi Nosé published two amazing papers in 1984 !

Canonical (isothermal) dynamics from Hamiltonian (isoenergetic) mechanics .

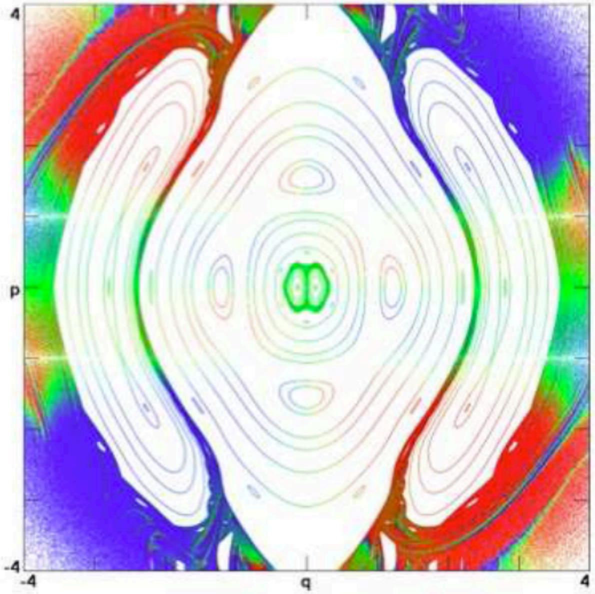
Academy of Applied Science (NH) → Paris to attend Carl Moser's CECAM meetings

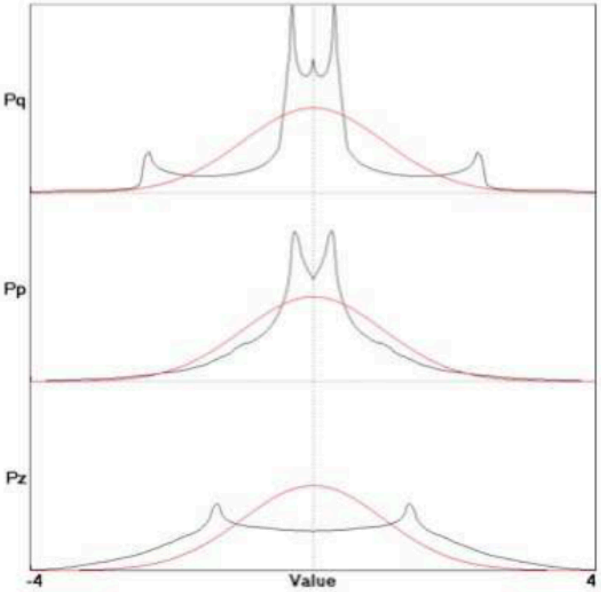
Met Shuichi Nosé and Harald Posch → Sabbaticals in Yokohama and Wien

#1: Nosé's canonical harmonic oscillator (6% Chaotic)

$$2H = q^2 + (p/s)^2 + z^2 + kT \ln (s^2)$$

$$dq/dt = p \,;\, dp/dt = -q - zp \,;\, dz/dt = (p^2/T) - 1$$





#2. Brad Holian (Berkeley → LANL) and Ergodicity*

$$dq/dt = p \; ; \; dp/dt = -q - zp - xp^3$$

$$dz/dt = (p^2/T) - 1 \; ; \; dx/dt = (p^4/T^2) - 3(p^2/T)$$

Local Lyapunov exponent shows longtime divergence

* W. G. Hoover and B. L. Holian, "Kinetic Moments Method for the Canonical Ensemble Distribution", Physics Letters A **211**, 253-257 (1996) .

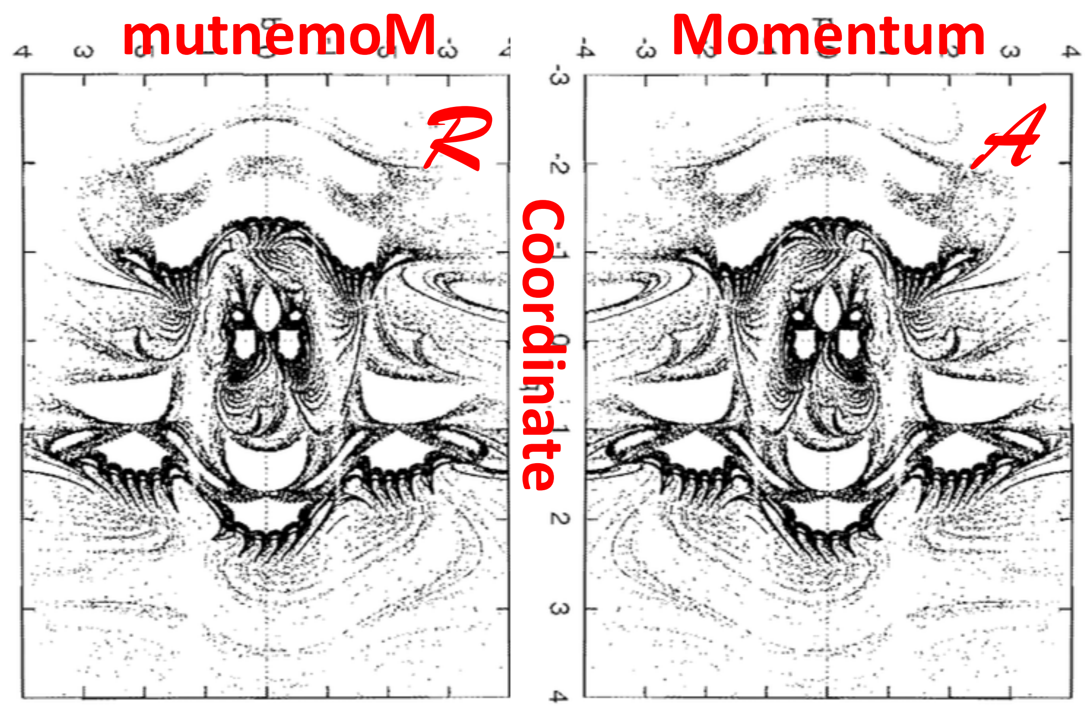
#3: Nosé's thermostat → Repellor-to-Attractor Flows

Dissipation ← Time-Reversible Deterministic Mechanics

Simplest Case : Oscillator with a Temperature Gradient :

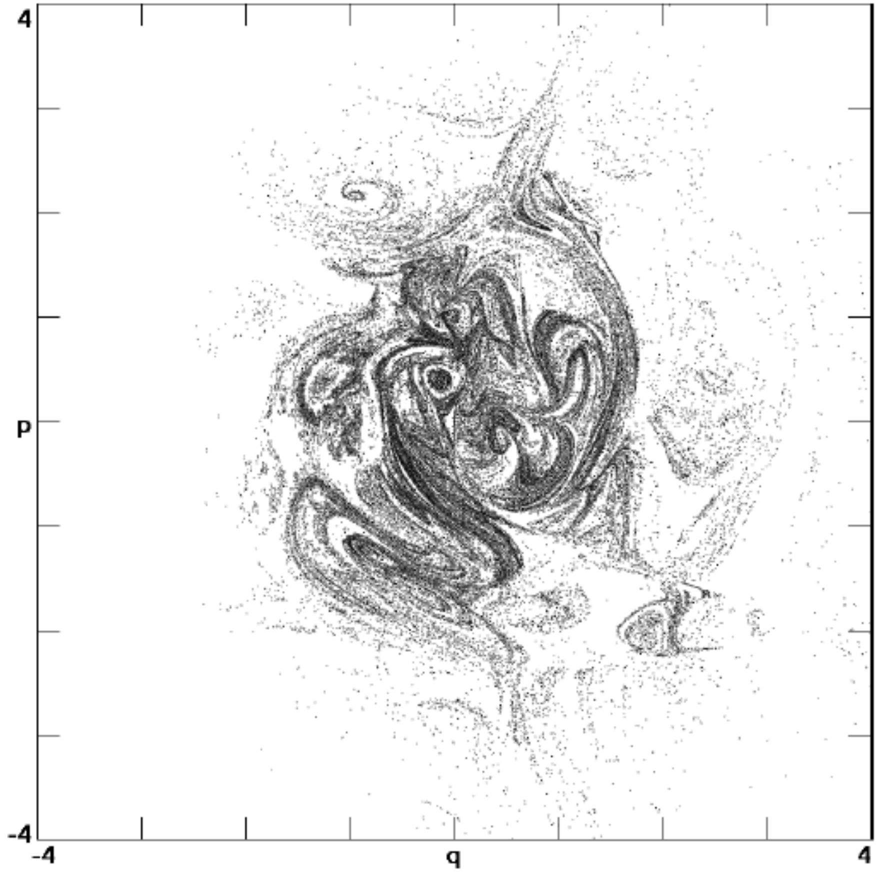
$$T(q) = 1 + 0.4 \tanh(2q)$$

Obeys Second Law and generates very nice fractals



Harald Posch's 65th Birthday -- Wien 2007

#3,4: 1997 Nonequilibrium Steady States with Heat Transfer*



$dz/dt = (p^2/T) - 1$;

$dx/dt = (p^4/T^2) - 3(p^2/T)$

Double Poincaré section

With both z and x = 0

Fractal dimensions :

Kaplan-Yorke : 3.687

Correlation : 3.38

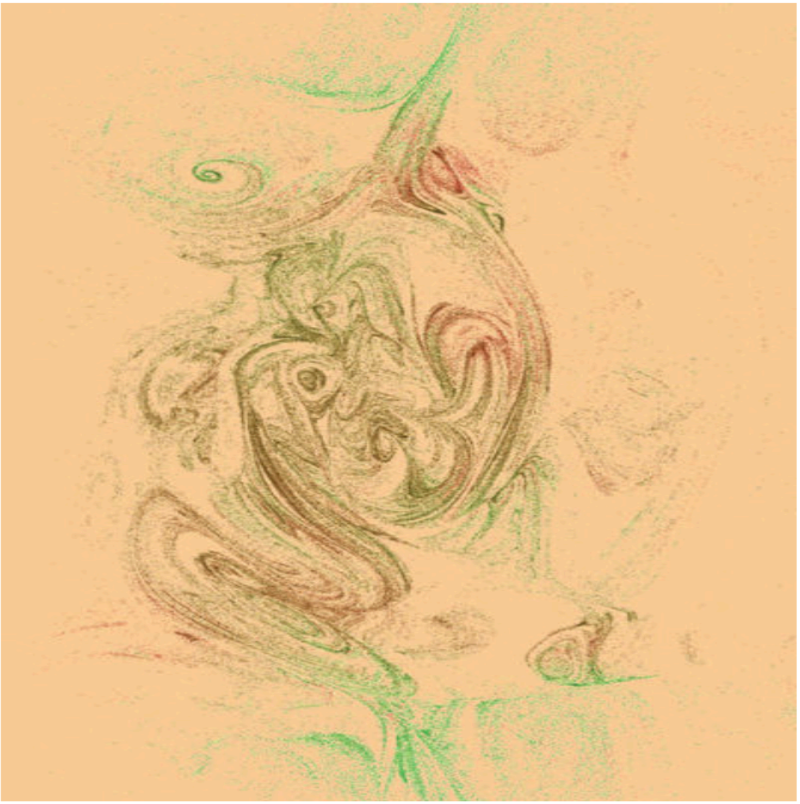
$T(q) = 1 + 0.4 \tanh(q)$

* H. A. Posch and W. G. Hoover, “Time-Reversible Dissipative Attractors in Three and Four Phase-Space Dimensions”, Physical Review E **55**, 6803-6810 (1997) .

* J. C. Sprott, W. G. Hoover, and C. G. Hoover, “Heat Conduction, and the Lack Thereof, in Time-Reversible Dynamical Systems: Generalized Nos´e-Hoover Oscillators with a Temperature Gradient”, Physical Review E **89**, 042914 (2014) ,

#4: 1997 and Nonequilibrium Steady States with Heat Transfer

[Courtesy of Julien Clinton Sprott]



$dz/dt = (p^2/T) - 1$;
$dx/dt = (p^4/T^2) - 3(p^2/T)$

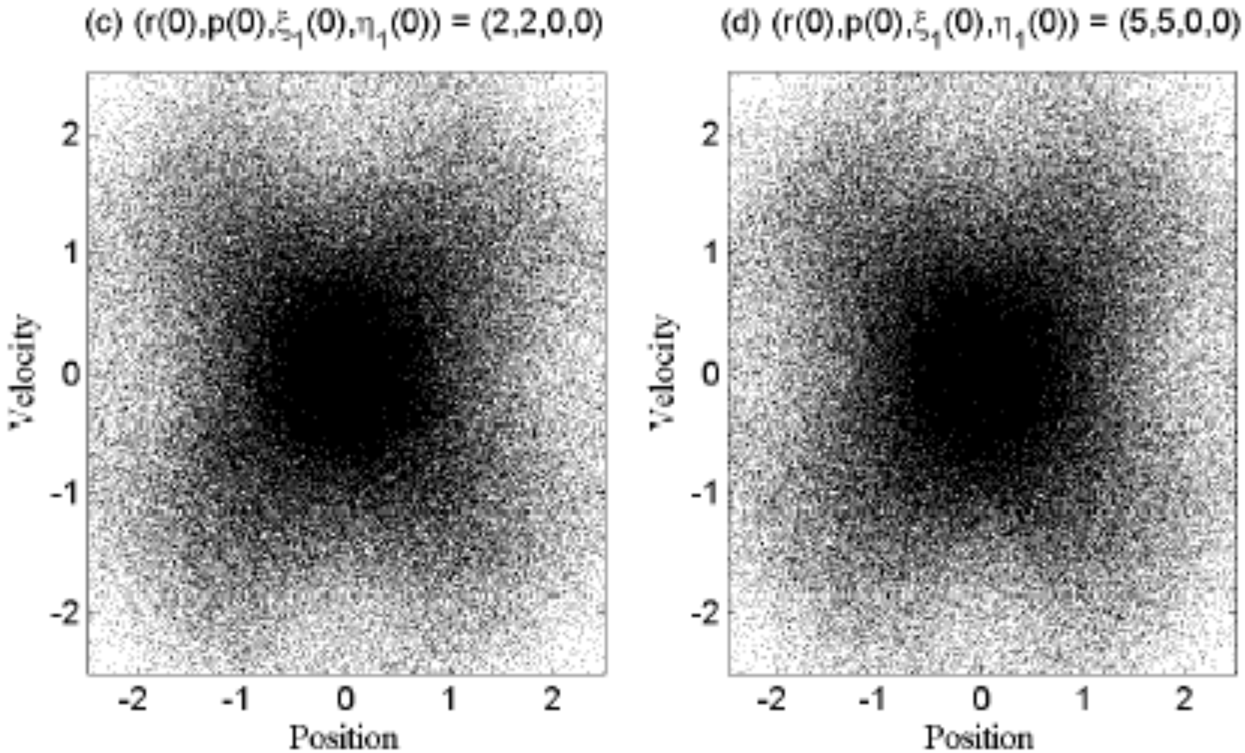
Double Poincaré section
With both z and x = 0

Fractal dimensions :
Kaplan-Yorke : 3.687
Correlation : 3.38

$T(q) = 1 + 0.4 \tanh(q)$

#5: 2014 Puneet Patra and Baidurya Bhattacharya* **

$$dq/dt = p - xq \; ; \; dp/dt = -q - zp$$
$$dz/dt = p^2 - 1 \; ; \; dx/dt = q^2 - 1$$



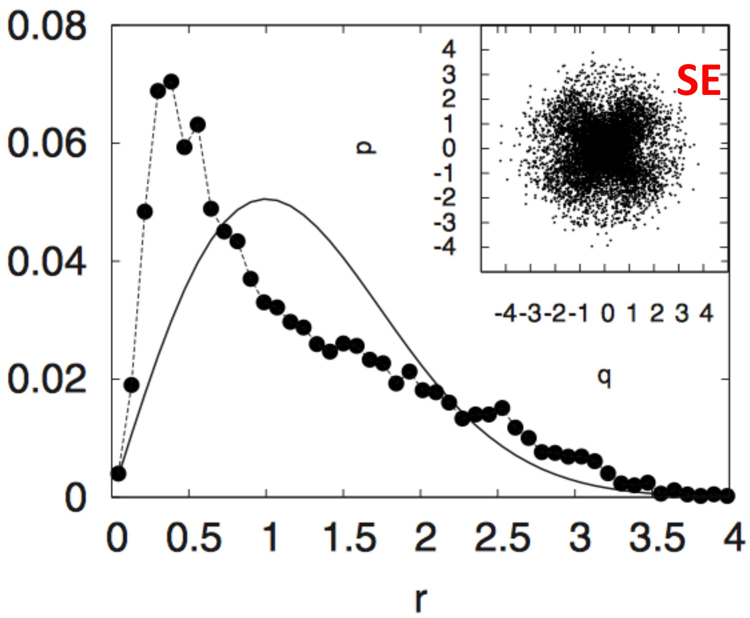
* P. K. Patra and B. Bhattacharya, “A Deterministic Thermostat for Controlling Temperature Using All Degrees of Freedom”, Journal of Chemical Physics **140,** 064106 (2014) .

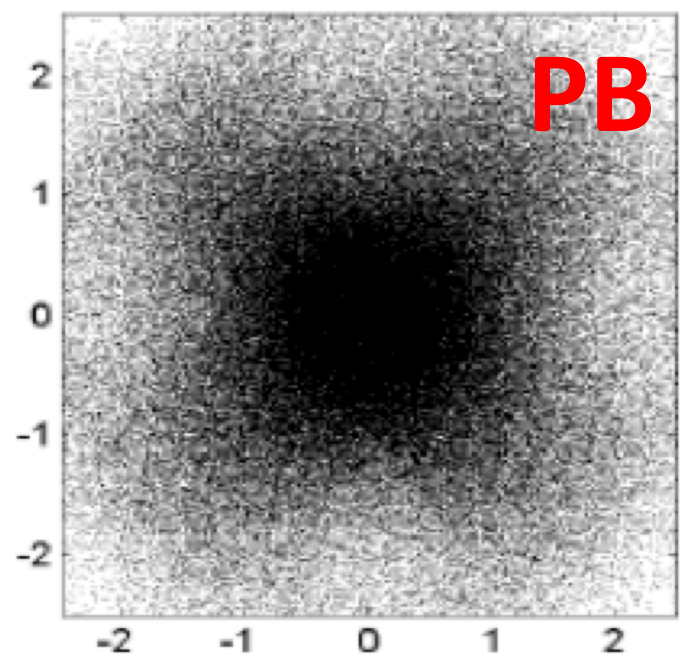
** P. K. Patra and B. Bhattacharya, “Improving the Ergodic Characteristics of Thermostats Using Higher Order Temperatures”, arxiv : 1411:2194, (2014) Figure 2 .

#6: 2010 Sergi and Ezra* = Patra and Bhattacharya !

dq/dt = p – xq ; dp/dt = – q – zp
dz/dt = p^2 – 1 ; dx/dt = q^2 – 1

PHYSICAL REVIEW E **81**, 036705 (2010)





* A. Sergi and G. S. Ezra, “Bulgac-Kusnezov-Nosé-Hoover Thermostats”, (2010) Figure 2 .

#7: 2010 Sergi and Ferrario "Ergodic" *

dq/dt = p + zp ; dp/dt = - q - zp ; dz/dt = p^2 - 1 - qp

$$\dot{q} = \frac{p}{m}\left(1 + \tau \frac{p_\eta}{M_\eta}\right), \qquad (24)$$

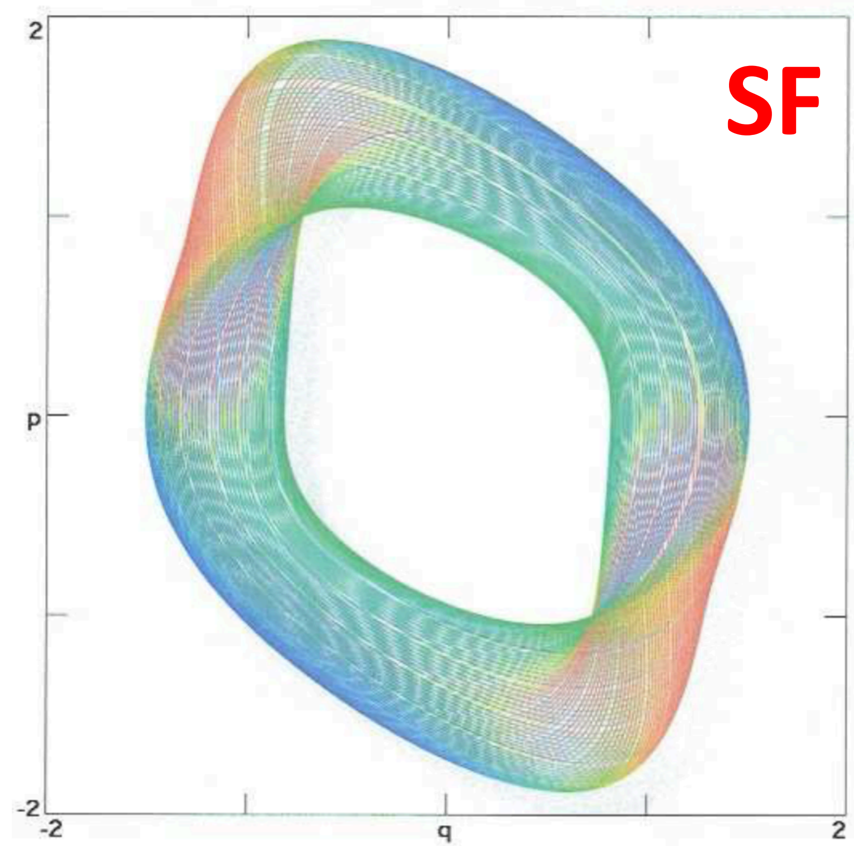
$$\dot{\eta} = \frac{p_\eta}{M_\eta}, \qquad (25)$$

X X

$$\dot{p} = -\frac{\partial \Phi}{\partial q} - p\frac{p_\eta}{M_\eta}, \qquad (26)$$

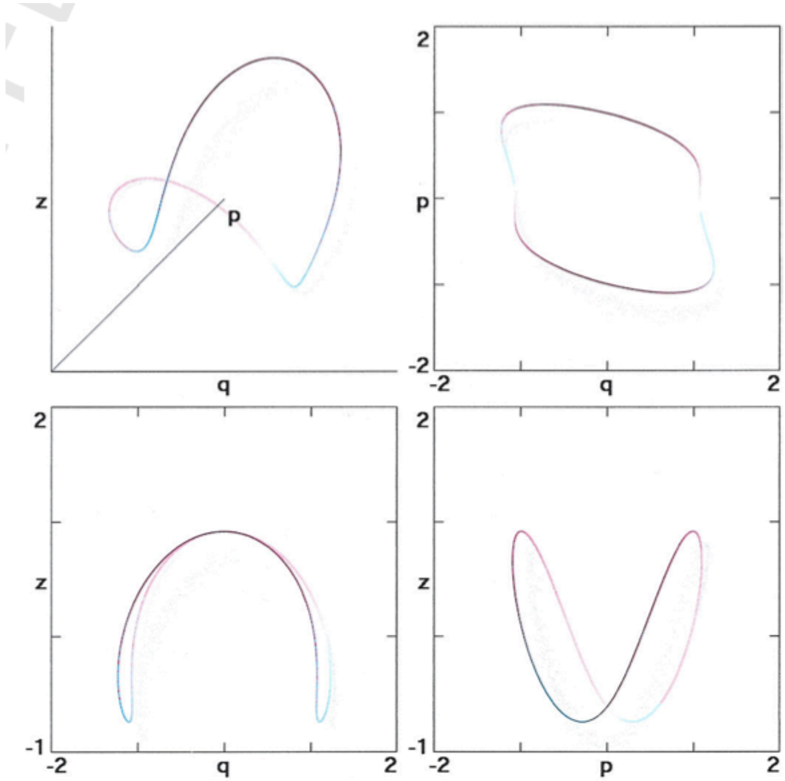
$$\dot{p}_\eta = \frac{p^2}{m} - k_B T - \tau \frac{p}{m}\frac{\partial \Phi}{\partial q}. \qquad (27)$$

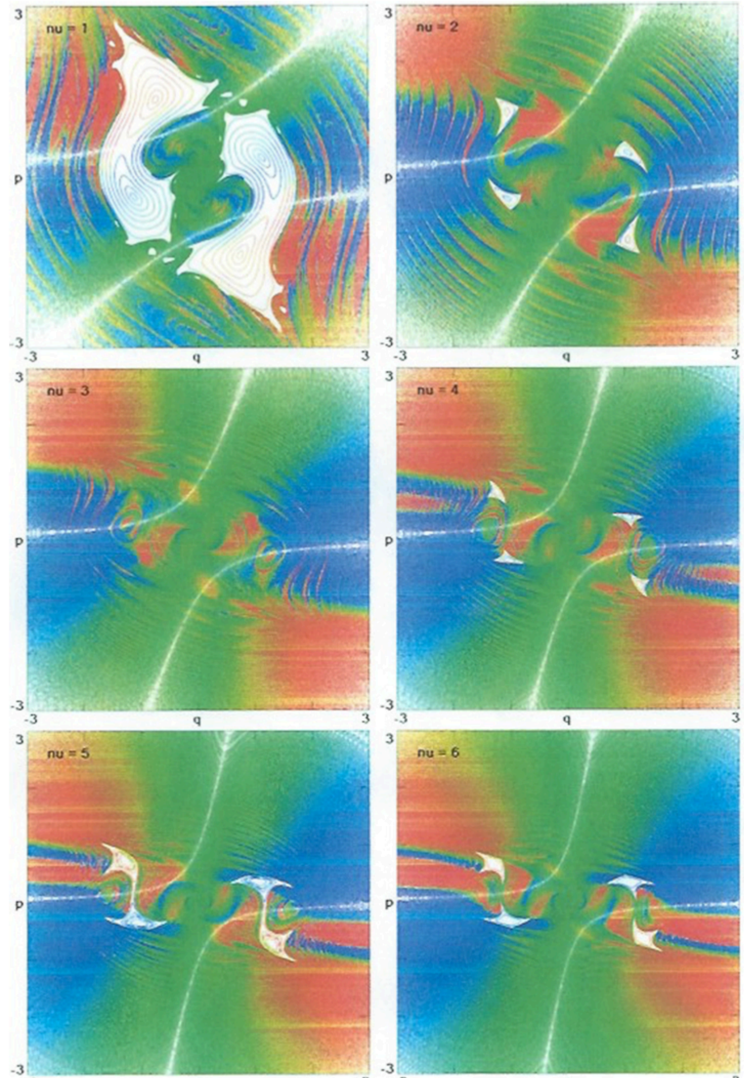
Whenever "tau > 0.50" → "Ergodicity"



* A. Sergi and M. Ferrario, "Non-Hamiltonian Equations of Motion with a Conserved Energy", Physical Review E **64**, 056125 (2001), Equations 24, 26, and 27 .

#7,8: 2015 *





At 2.903521 there is a conservative torus present so that the problem is not ergodic. Physics Letters A (in press, 2015 *) .

* W. G. Hoover, J. C. Sprott, and P. K. Patra, arXiv 1503.06749 "Ergodic time-reversible chaos for Gibbs' canonical oscillator"

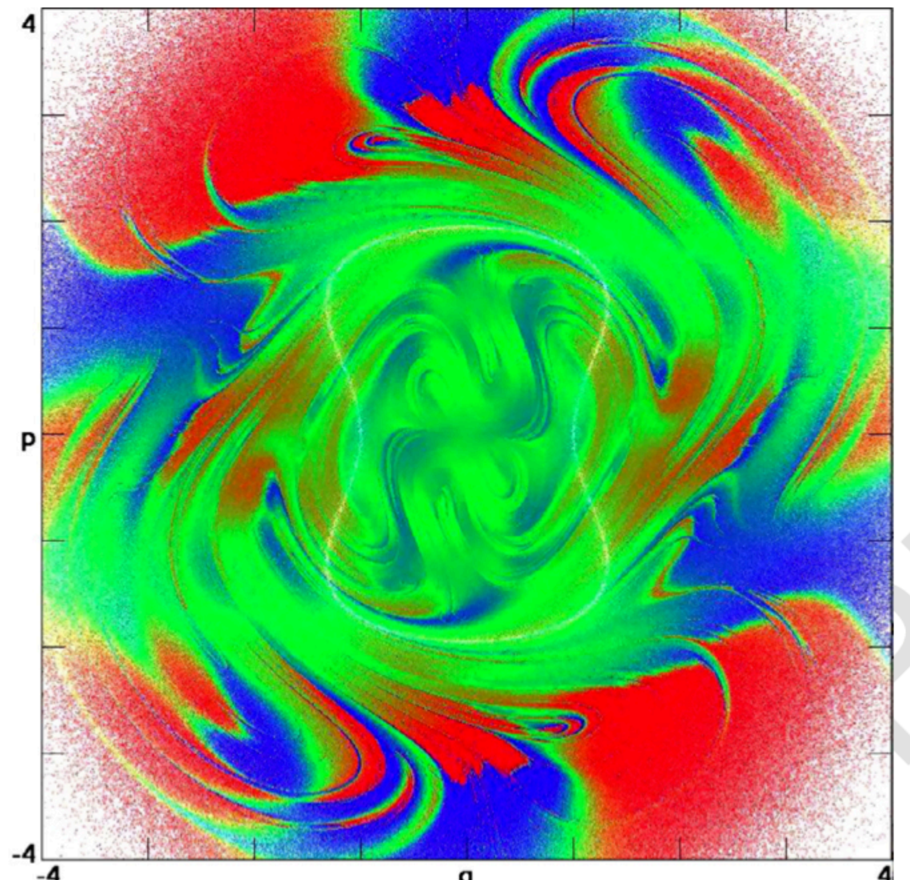
#8: 2010 Sergi and Ferrario "Ergodic"

A weak-control method which works (CNSNS in press *)

$$dq/dt = p - 0.827z^3q \; ; \; dp/dt = -q - 0.273z^3p^3$$

$$dz/dt = 0.827(q^2 - 1) + 0.273(p^4 - 3p^2)$$

This is a little unaesthetic as it affects q as well as p .



*** W. G. Hoover, J. C. Sprott, and C. G. Hoover, "Ergodicity of a Singly-Thermostated Harmonic Oscillator" = arXiv 1504.07654, rejected by Ben Naim at Physical Review E**

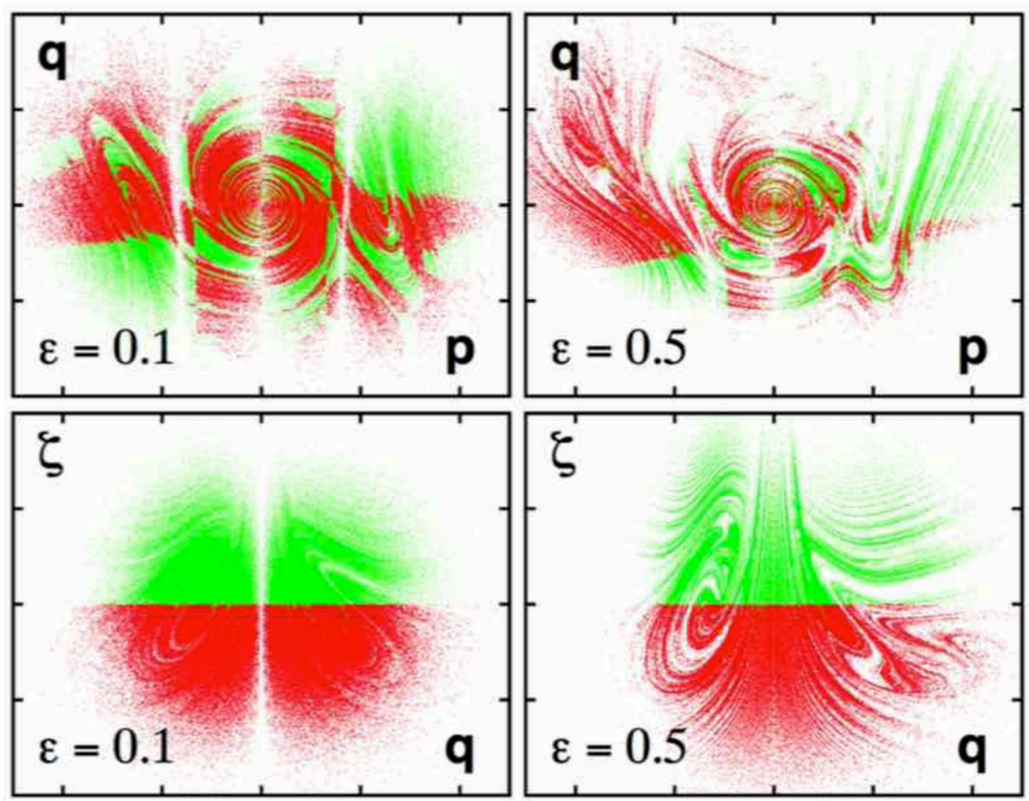
#8: after 2010 Sergi and Ferrario "Ergodic" *

A better weak-control method which works (MS in press) :

$$dq/dt = p \; ; \; dp/dt = -q - 0.05zp - 0.32zp^3$$

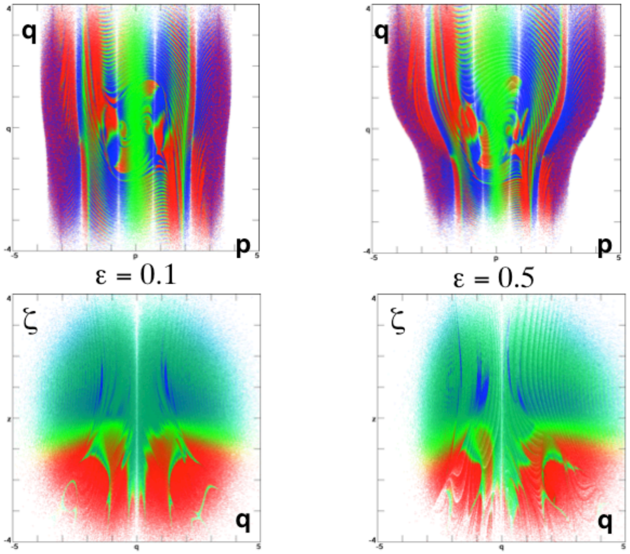
$$dz/dt = 0.05(p^2 - 1) + 0.32(p^4 - 3p^2)$$

This is a solution to a problem raised by Nosé's work in 1984



* W. G. Hoover, C. G. Hoover, and J. C. Sprott, ``Nonequilibrium Systems : Hard Disks and Harmonic Oscillators Near and Far From Equilibrium" = arXiv:1507.08302 .

1-8: Moral : Collaborations : Are a Good Thing !



Clint Sprott

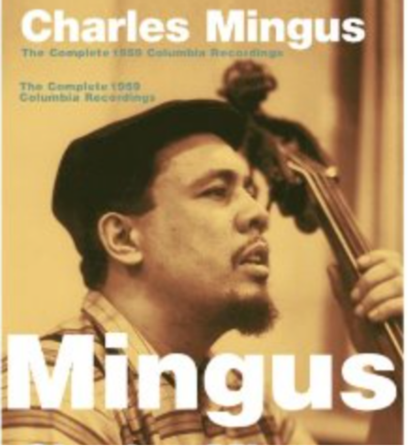
Puneet Patra

Old Faithful and the Baidurya Bhattacharyas

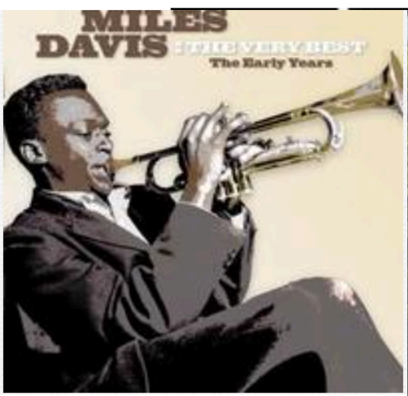
9: 2015 Ian Snook Prize :

$1000 US for the most interesting Ergodic Time-Reversible Map Of Unit Square Into Itself

Computational Methods in Science and Technology 21 (3) [2015] at cmst.eu



← 1996



2007 with Ian & Marie →