"1984 + 30", Anniversary Symposium
Legacy of Shuichi Nosé's Work :

"A Unified Formulation of the Constant Temperature Molecular Dynamics Methods"

&

"A Molecular Dynamics Method for Simulations in the Canonical Ensemble"

Wm G. Hoover and Carol G. Hoover
Ruby Valley Nevada USA

Keio University
Mita Campus, 10-11 November 2014

A Legacy of Shuichi Nosé's 1984 Work

1. Nosé's Amazing Logarithmic Hamiltonian
2. Meeting Shuichi at Orly/CECAM in 1984
3. Sabbatical at Keio University 1989-1990
4. Fractals and Dimensionality Loss
5. ϕ^4 Model for Heat Conductivity
6. Nonequilibrium Hamiltonian Simulations
7. More Thermostats and 2014 Snook Prize

1. Equilibrium ← Nosé-Hoover MD : Hamiltonian Motion Equations for the Canonical Ensemble !

Shuichi Nosé's Good Idea :

$$\mathcal{H}_N = \Sigma\,(p^2/2ms^2) + \Phi(q) + NDkT\,\ln(s) + (p_s^{\,2}/2M) ;$$

"Scale the time", multiplying time derivatives by s and replace { (p/s) → p } . Then { (dp/dt) = F – ζp } where (dζ/dt) = Σ [(p²/mkT) – 1]/τ² .

Carl Dettmann's Better Idea : $\mathcal{H}_D \equiv s\mathcal{H}_N \equiv 0$

Exactly the same **NH equations of motion result, but without any time-scaling .**

1. Equilibrium ← Nosé-Hoover MD

Best Idea : The continuity equation shows that Gibbs' canonical distribution, $f \propto e^{(-\mathcal{H}/kT)}$, is a stationary solution of the equations of motion :

$$\{ (dp/dt) = F(q) - \zeta p \} .$$

provided that the friction coefficient ζ is generated by the integral feedback equation :

$$d\zeta/dt = [< (p^2/mkT) > - 1] / \tau^2 \rightarrow (\partial f/\partial t) = 0 .$$

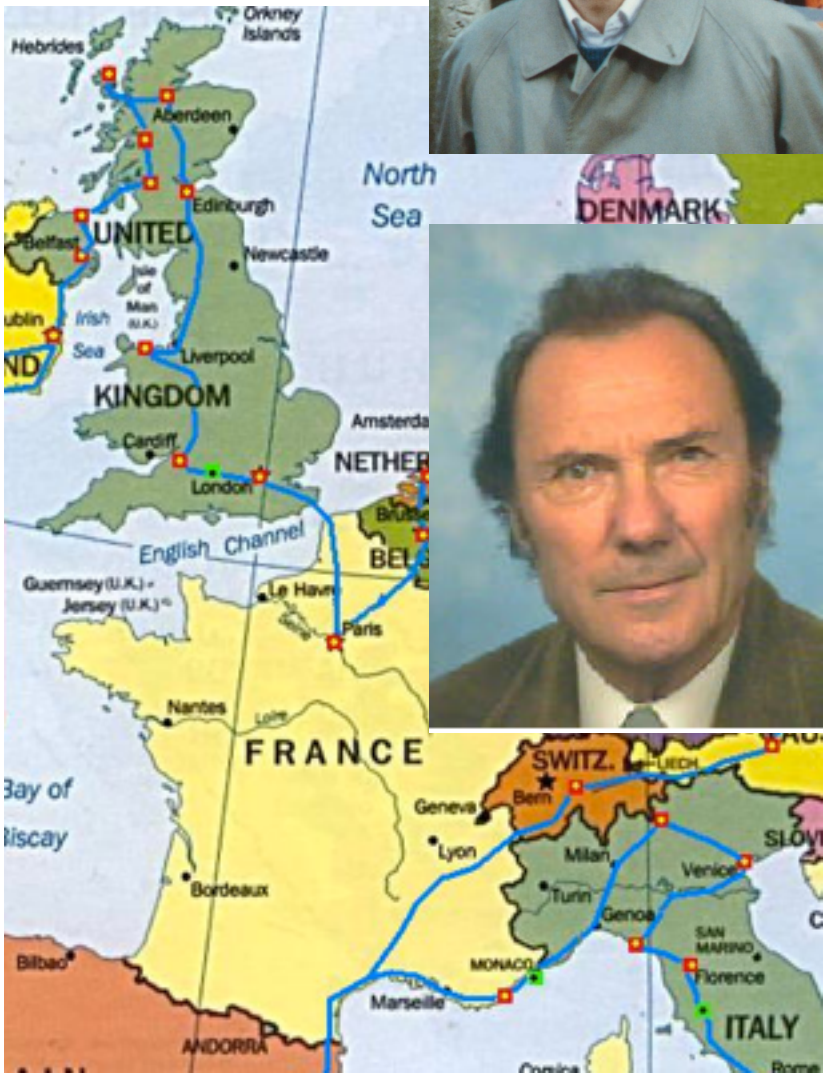
These motion equations are deterministic and time-reversible, *not* Hamiltonian. Nosé's "time-scaling variable" s has *disappeared* .

1. There are Nonequilibrium Possibilities

Shūichi Nosé
Keio University
Yokohama
1987

2. Meeting Shuichi at CECAM in 1984 and Philippe Choquard at Lausanne

What is “s” ?



3. Sabbatical at Keio, 1989-1990

3. May 1990 Snapshot, Nestlé House

Keio University 1989-1990

Shūichi Nosé 1951-2005

Gary Morriss & Carl Dettmann

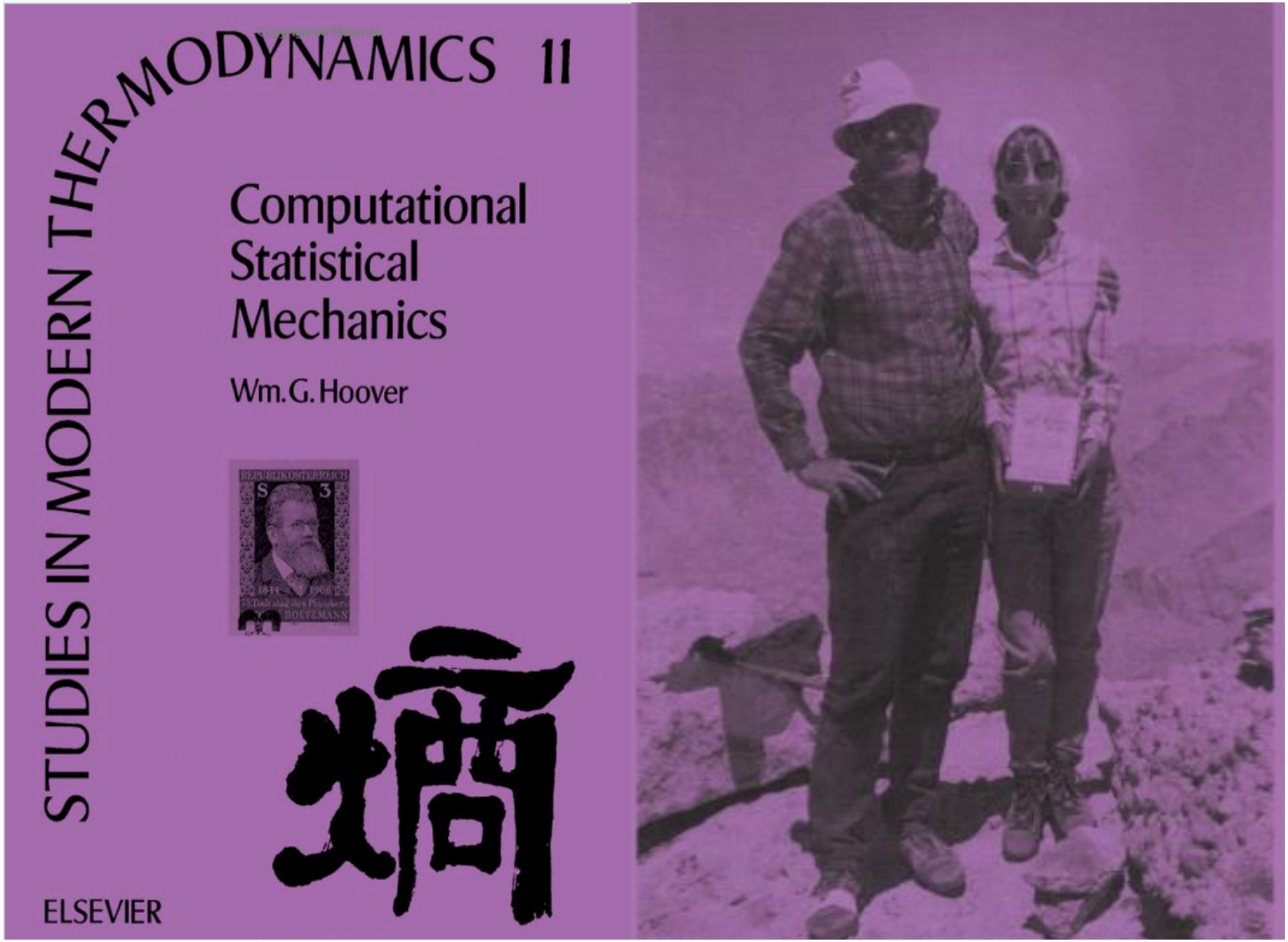
[Improved Hamiltonian in 1996]

Nosé's New Hamiltonian Generates Gibbs' Canonical Ensemble :

$$\mathcal{H} = \sum (p^2/2ms^2) + [\ \Phi(q) + NkT \ln s + (P_s^2/2M)\ ]$$

$$\{\ m\ddot{q} = F(q) - \zeta m\dot{q}\ ;\ \dot{\zeta} = [\ (K/K_0) - 1\ ]/\tau^2\ \}$$

3. Sabbatical at Keio 1989-1990



Generalizations of Nosé-Hoover MD

Bauer, Bulgac, and Kusnezov considered a much more general situation, including one, two, or more "friction coefficients" { ζ } , enough to generate Brownian Motion with time-reversible motion equations .

Their focus was Equilibrium .

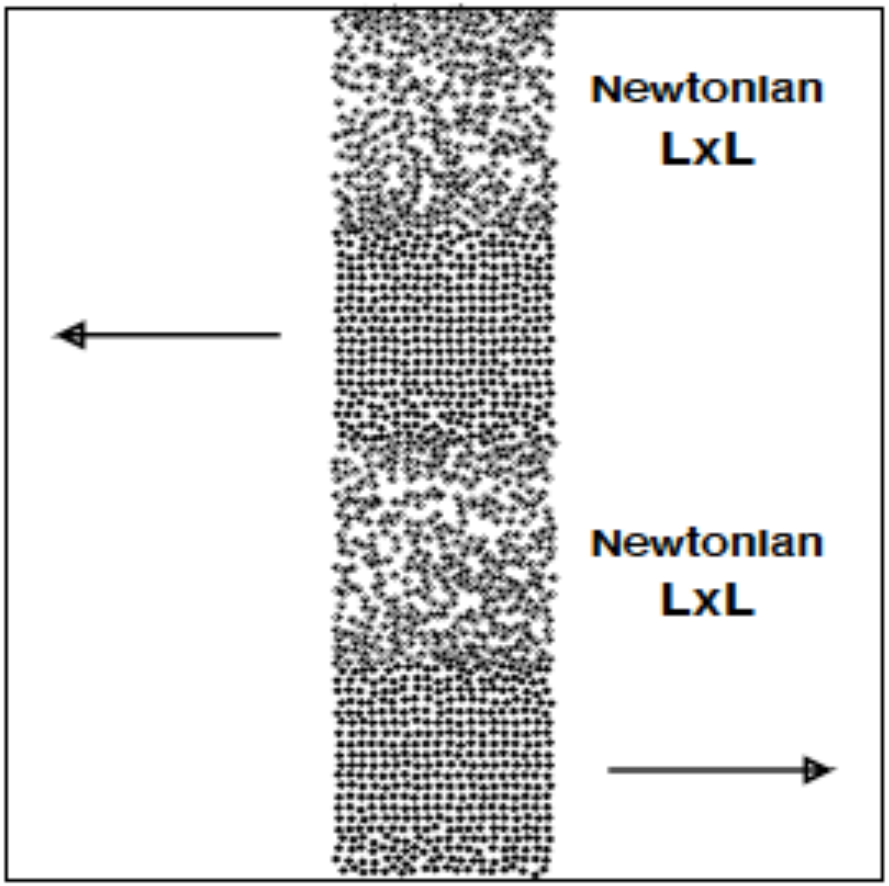
Our focus is Nonequilibrium .

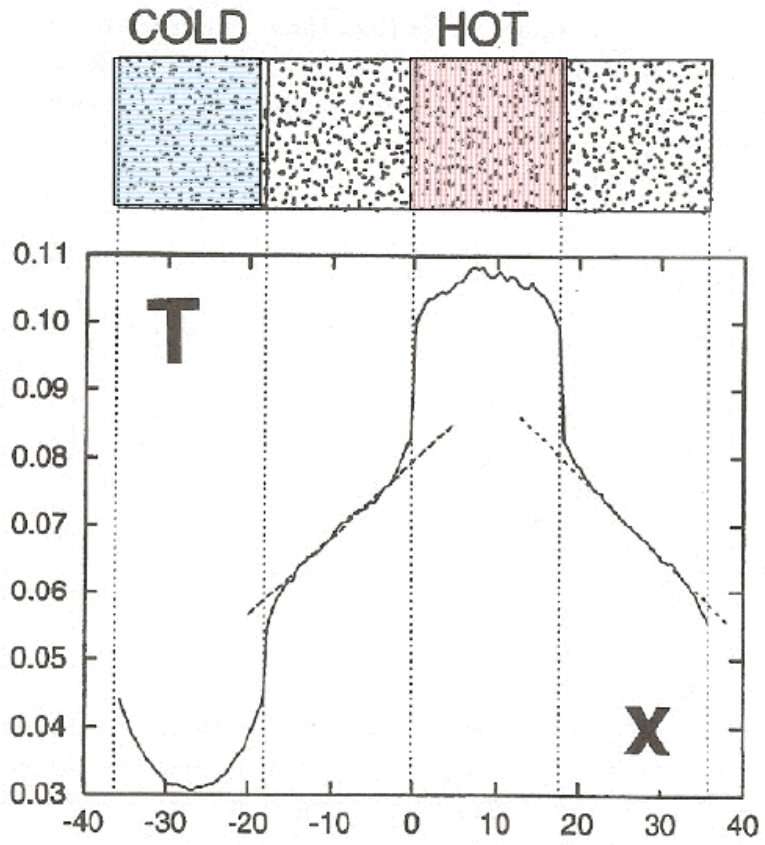
4. Fractals and Dimensionality Loss in Nonequilibrium Simulations

Shūichi Nosé
Keio University
Yokohama
1987

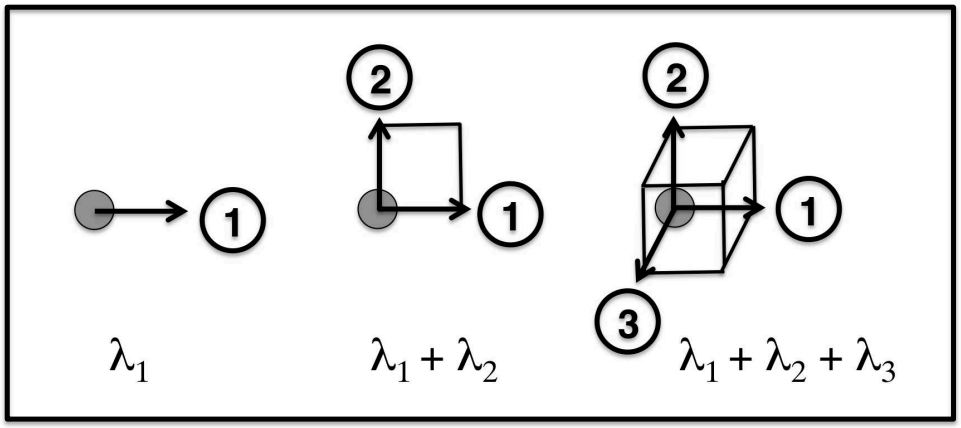
Shūichi Nosé
Keio University
Yokohama
1987

4. Pictures of Shear and Heat Flow using Nosé-Hoover thermostats



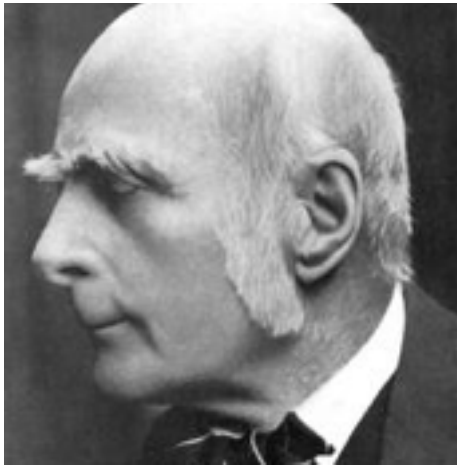


4. Fractals. { λ } → Dimensionality Loss

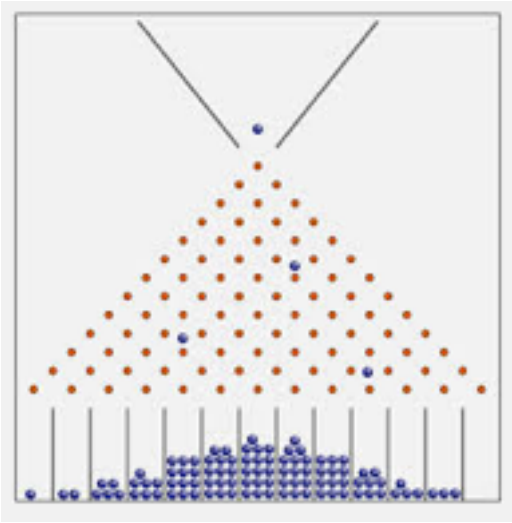


By following the motion of N satellite systems orthonormally constrained about an N-dimensional reference system, the N Lyapunov exponents are given by forces needed to maintain orthonormality. The algorithm was developed by Benettin's group.

4. Interesting Example of Lyapunov Fractal Instability → vanishing phase volume

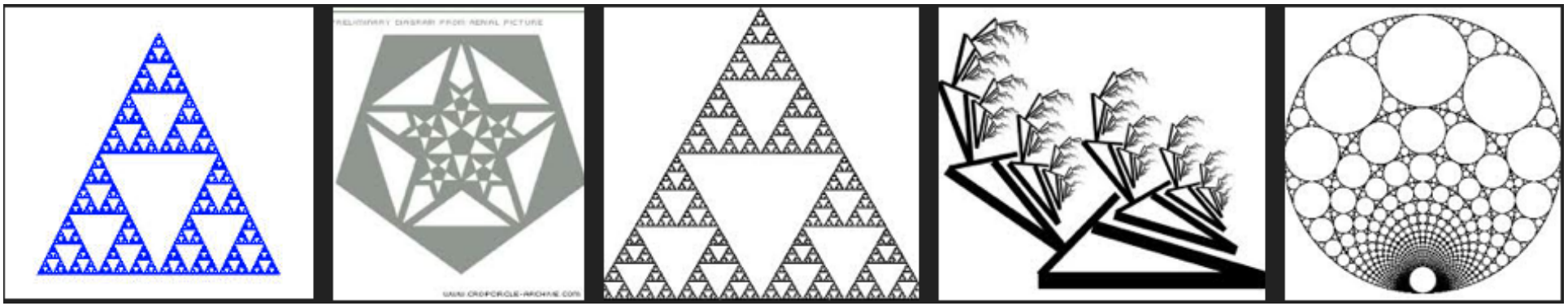


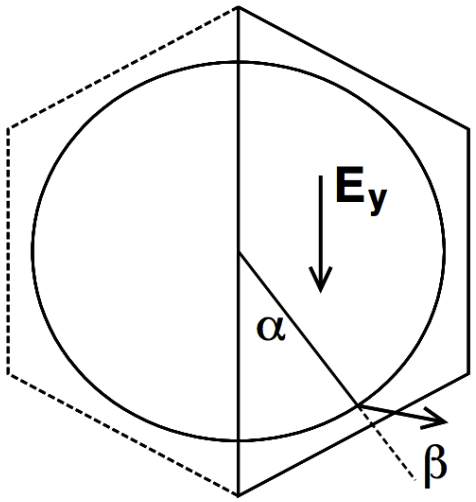
Isokinetic Galton Board : gravitational Work is converted to extracted Heat *via* frictional ζ .

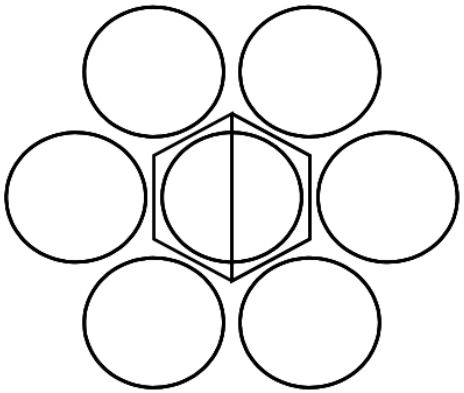


Cross sections of phase space at Fields of strength E = 1, 2, 3, and 4 . There can be a mix of conservative + dissipative parts of phase space .

4. Classical Textbook Fractals (with holes)



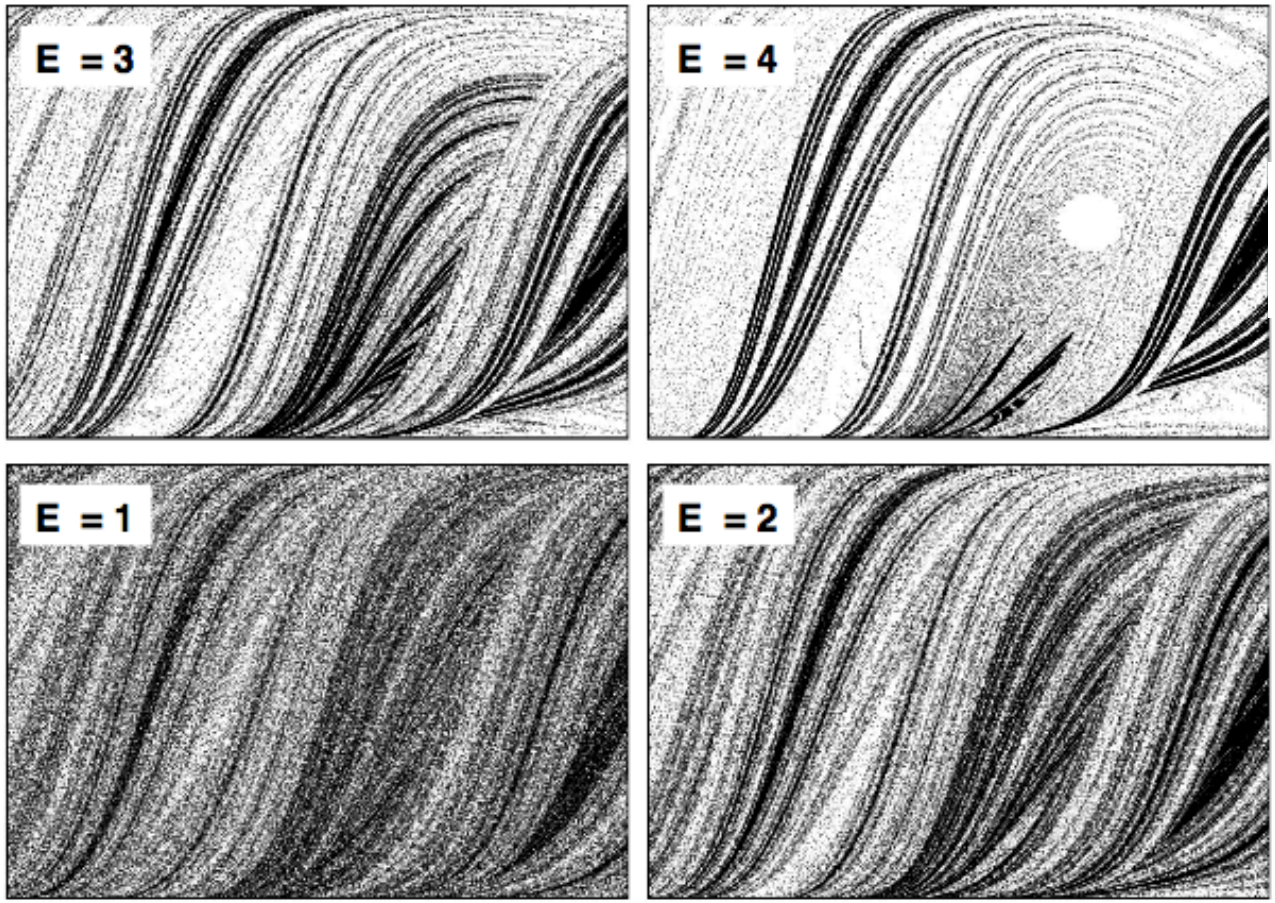


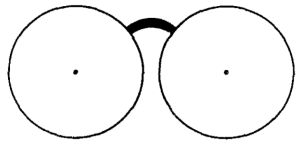


Isokinetic Galton Board Generates Fractal Phase-space Cross Sections

4. MultiFractal Galton Board Sections

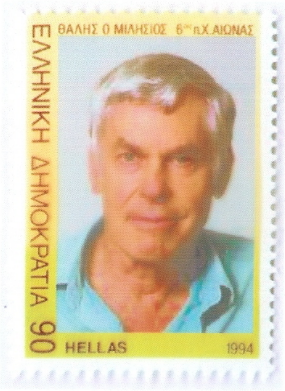
[-1 < sin(β) < +1 as function of 0 < α < π]

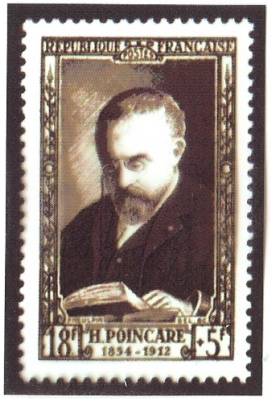




4. Fractals and Dimensionality Loss

Generic Nonequilibrium Phase Space Flow





4. Second Law of Thermodynamics

- **Fractal Distributions give Time's Arrow :**
- **Nonequilibrium states are rare .**
- **Nonequilibrium entropy diverges .**
- **Reversed nonequilibrium trajectories are**
- **more unstable, and hence unobservable .**

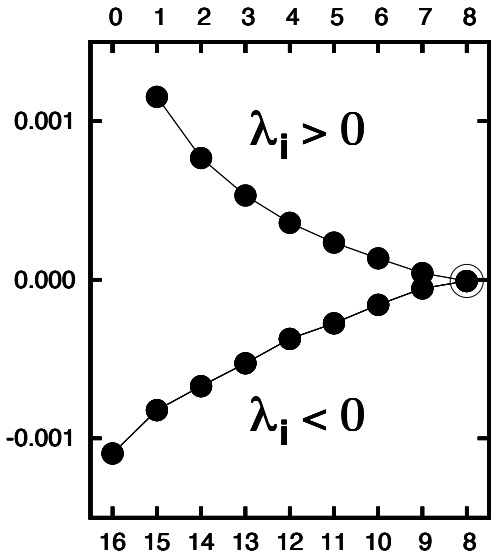
$$d(\ln f)/dt = \dot{S}/k = -\sum \lambda = \sum \zeta > 0 .$$

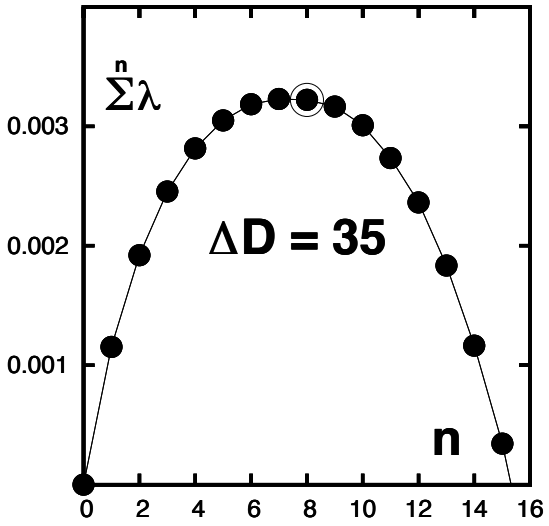
$$\Rightarrow d(\ln f)/dt = - d(\ln \otimes)/dt < 0 !$$

5. An Interesting ϕ^4 Example of NH Fractal Lyapunov Instability & Dimensionality Loss

ϕ^4 Heat Flow (Hooke's Law + quartic tethers)

The dimensionality loss, 35/50, implies zero phase volume with entropy of minus infinity.

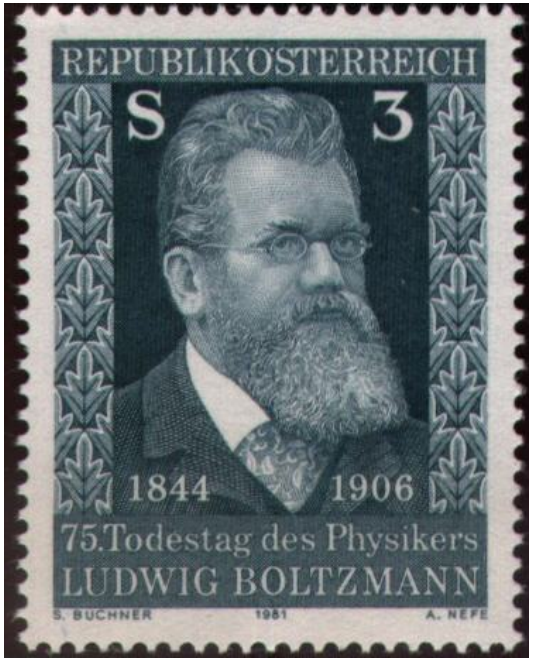




Aoki + Kusnezov in Venice

6. Nonequilibrium Simulations using Hamiltonian Mechanics ?

The Kinetic Temperature , T ≡ < mv^2/k > , can be constrained by using a Lagrange Multiplier → an *Isokinetic* Hamiltonian :

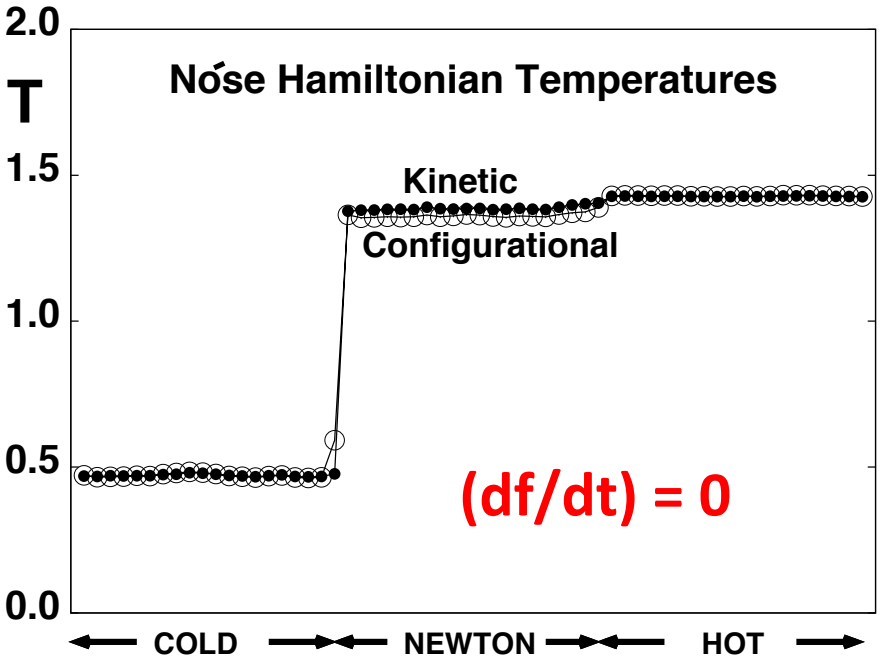


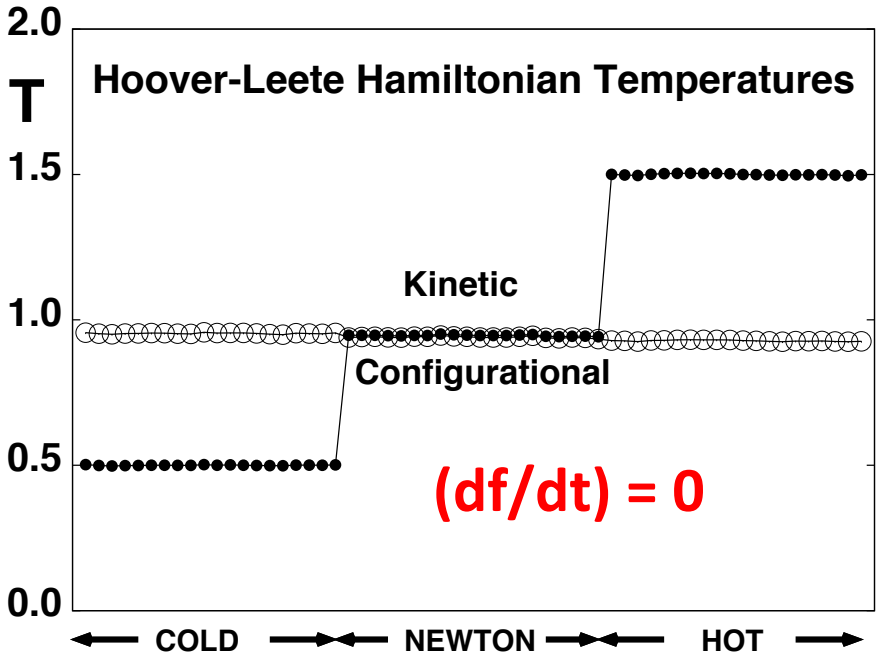
$$\mathcal{H} = 2[\,(K(v)K(p)\,]^{1/2} - K(v) + \Phi(q)$$

Here K(v) is a *fixed* kinetic energy .

An Alternative to $\mathcal{H}_{\text{Nosé}}$.

6. Puzzling Hamiltonian Thermostating ?

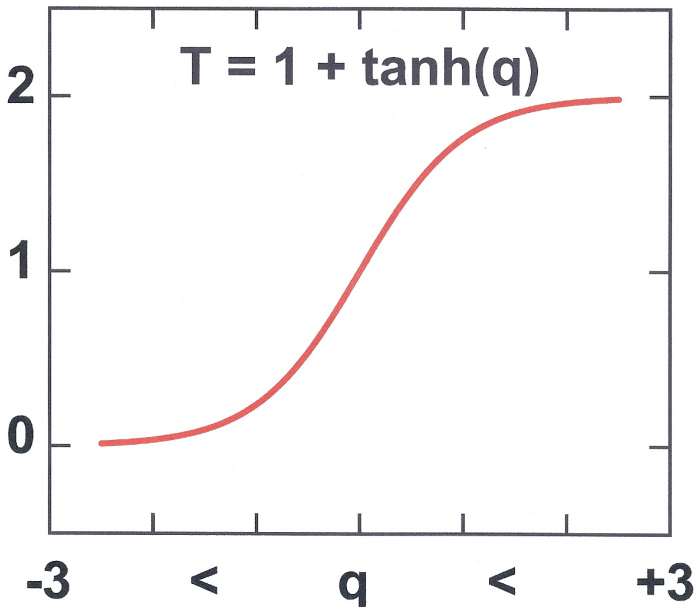




Despite tremendous temperature gradients there is no heat flow in these 60-particle ϕ^4 chains. The results are similar for the canonical and the kinetic thermostats. The ϕ^4 interparticle forces are harmonic, with quartic tethers.

7. Ergodicity *and* Multiple Temperatures for a Thermostated Harmonic Oscillator

***Two* Friction Coefficients give an *Ergodic* four-dimensional Gaussian when $\varepsilon = 0$ *; Multifractal* Distributions for $\varepsilon > 0$.**



$$\dot{q} = p \ ;$$

$$\dot{p} = -q - \zeta p - \xi p^3 \ ;$$

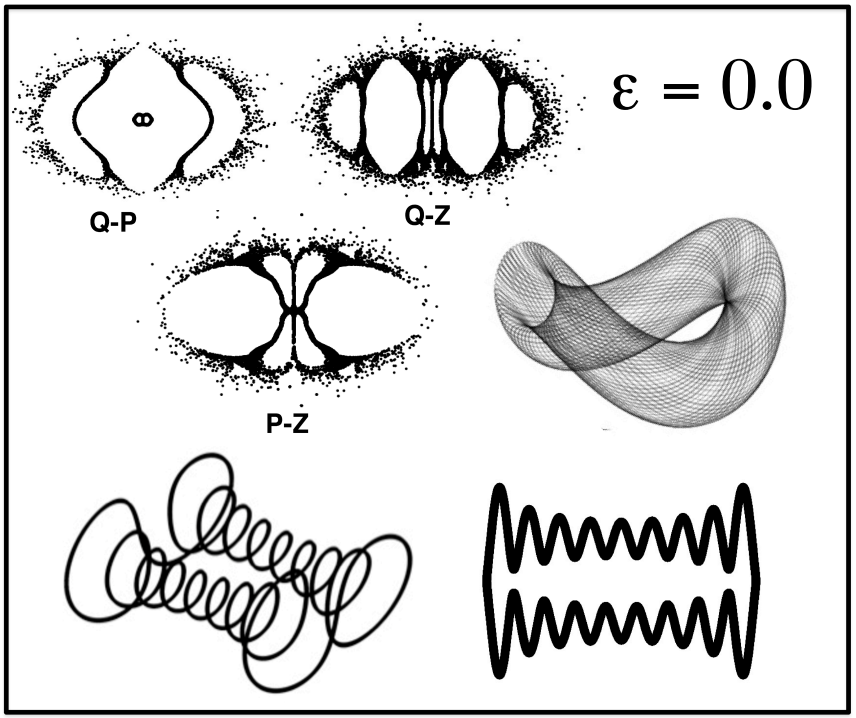
$$\dot{\zeta} = p^2 - T\left(q\right) \ ;$$

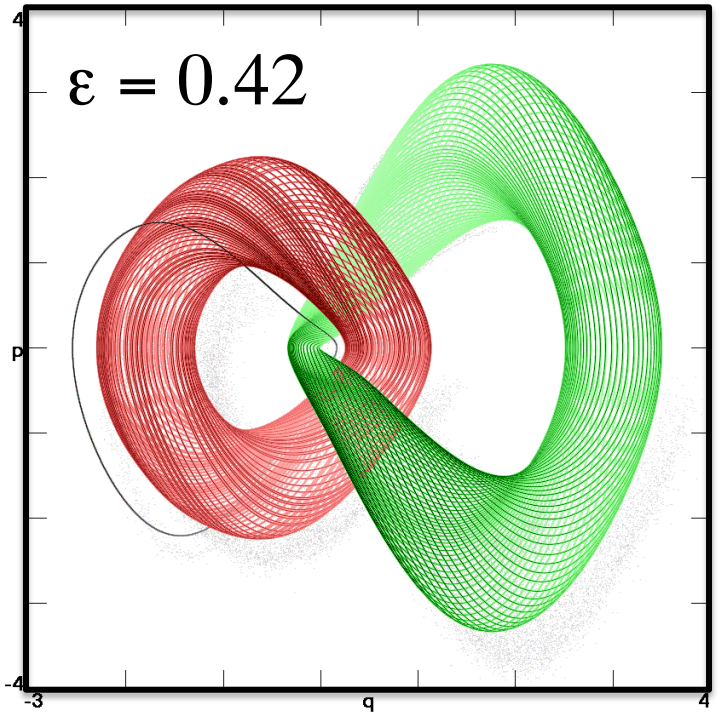
$$\dot{\xi} = p^4 - 3p^2 T\left(q\right) .$$

$$T\left(q\right) = 1 + \varepsilon \tanh\left(q\right) .$$

7. Nosé-Hoover Oscillators with Conservative and Dissipative Phase-Space Objects

$$\dot{q} = p \; ; \; \dot{p} = -q - \zeta p \; ; \; \dot{\zeta} = p^2 - T \; ; \; T = 1 + \varepsilon \tanh(q)$$



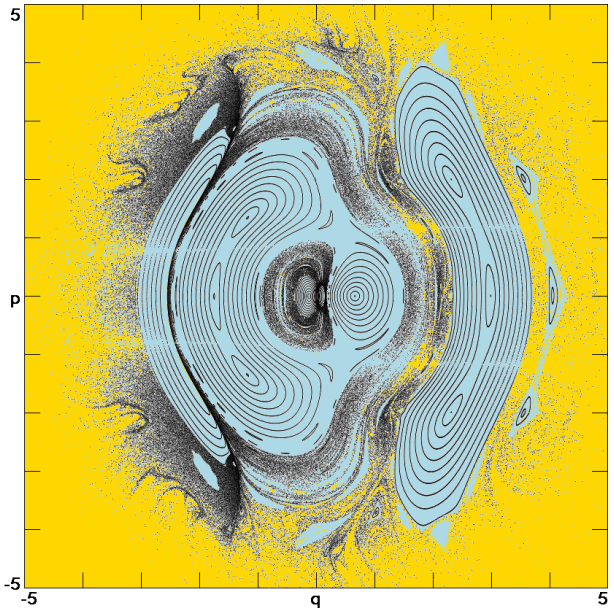


Sprott, Hoover, and Hoover, Physical Review E 89, 042914 (2014)

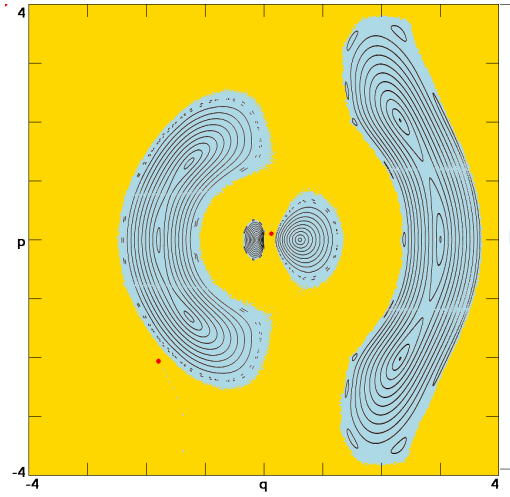
7. Nosé-Hoover Oscillators with Conservative and Dissipative Phase-Space Objects from Clint Sprott

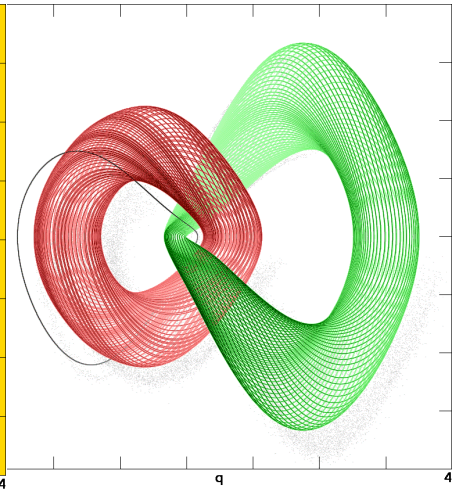
$$\dot{q} = p \; ; \; \dot{p} = -q - \zeta p \; ; \; \dot{\zeta} = p^2 - T \; ; \; T = 1 + \varepsilon \tanh(q)$$

$\varepsilon = 0.38, \zeta = 0$



$\varepsilon = 0.42, \zeta = 0$





(pq) sections
128 initial conditions
Transition at $\varepsilon = 0.4054$

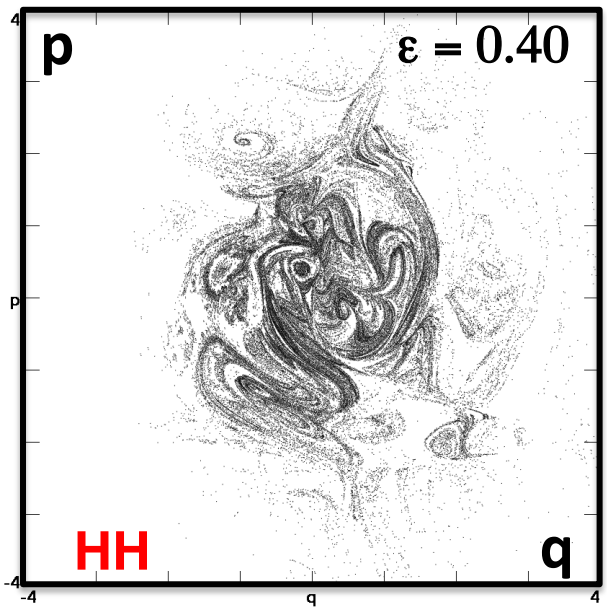
3 interlocking trajectories

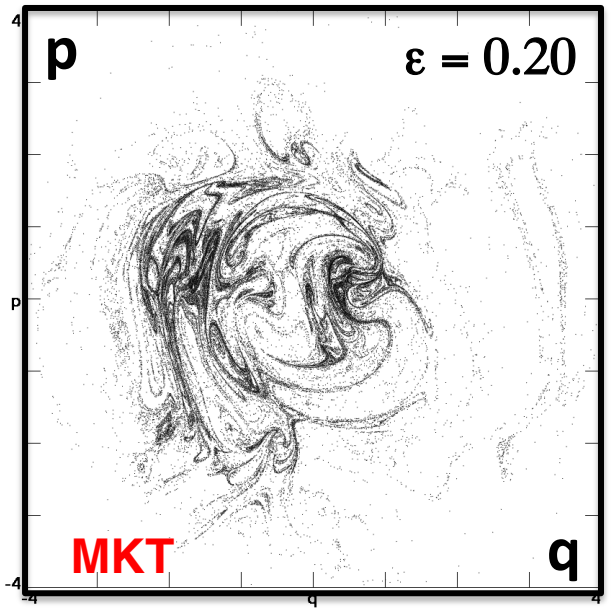
7. Robust Heat Transfer - Doubly Thermostated Oscillators

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

$$\dot{q} = p \; ; \; \dot{p} = -q - \zeta p \; ; \; \dot{\zeta} = p^2 - T - \zeta\xi \; ; \; \dot{\xi} = \zeta^2 - T \; ; \; \textbf{MKT}$$

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





These thermostated oscillators are fractal, but still ergodic, when $\varepsilon > 0$!

Patra + Bhattacharya's Idea [arXiv 1407.2353]

Patra - Bhattacharya

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

Hoover - Holian

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

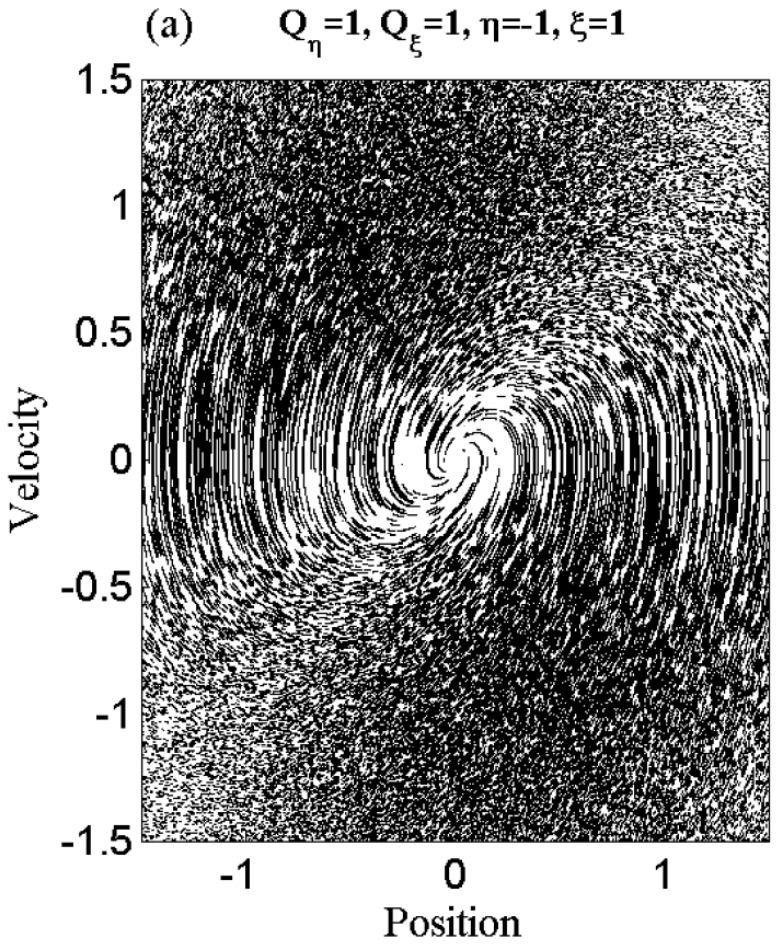
Martyna - Klein – Tuckerman (ergodic ?)

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

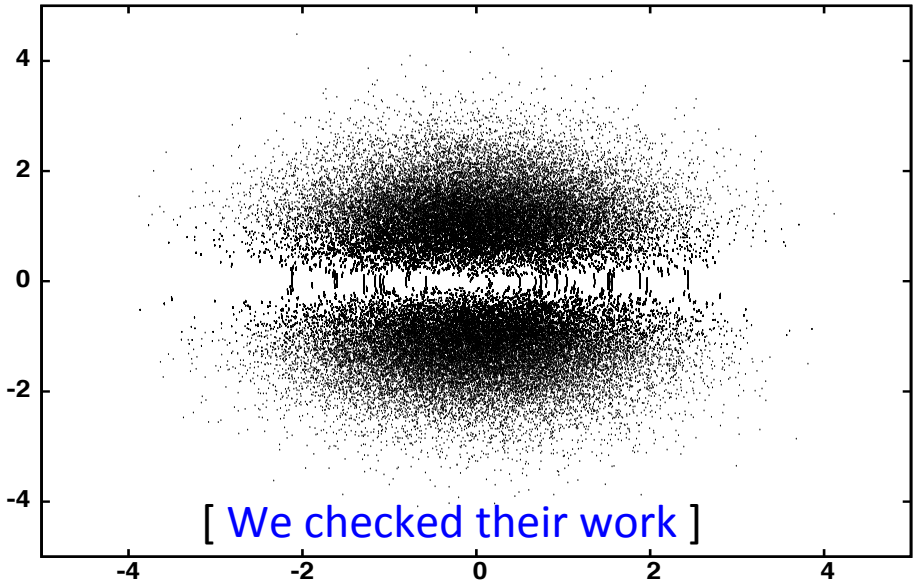
The 2014 Ian Snook Prize will be awarded for the most convincing paper addressing the MKT ergodicity for $\varepsilon = 0$.

The MKT thermostated oscillators are ergodic when $\varepsilon = 0$! Are you prepared to prove it? $500.00 US .

Martyna – Klein – Tuckerman Chain Thermostat



(q, p, -1, +1) section



[We checked their work]

Puneet Kumar Patra and Baidurya Bhattacharya, "Nonergodicity of the Nosé-Hoover Chain Thermostat in Computationally Achievable Time", Physical Review E 90, 043303 (2014)

"The [MKT] thermostat therefore does not generate the canonical distribution or preserve quasi-ergodicity for the Poincaré Section".

Summary of Nosé's Legacy

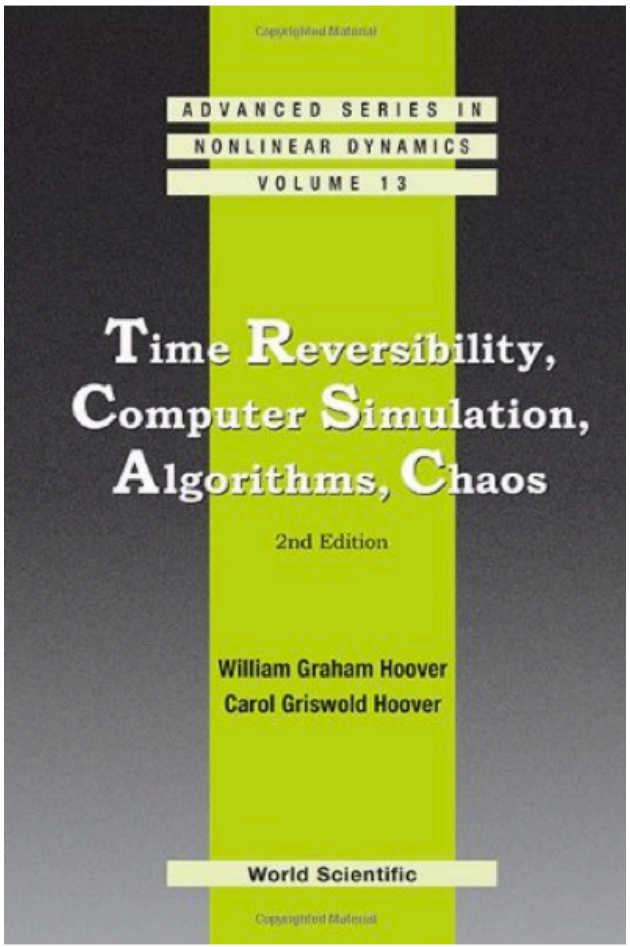
- Gibbs' Statistical Mechanics is directly linked to Hamilton's Dynamics .
- Thermostats use only a single degree of freedom, the coefficient ζ .
- Nonequilibrium steady states are multifractal .
- Entropy production from nonequilibrium processes is easy to compute : $d(\ln f)/dt = d(S/k)/dt = \zeta$.
- Multifractal symmetry breaking gives Second Law .

For additional details see www.williamhoover.info

Simulation and Control of Chaotic Nonequilibrium Systems

is our current project, which should be completed by this year's end, in plenty of time for our next meeting !

Thanks, Morishita+Isobe-sans !



30 Years After Shuichi Nosé's 1984 Work*

1984: Meeting Shuichi Nosé in Paris at a CECAM Workshop
1987: MultiFractal Thermostated Systems Far from Equilibrium
1989: Sabbatical at Keio, working with Kawai, Boku, Ihara
1990: Bauer, Bulgac, Kusnezov generalizations of Nosé-Hoover
1992: Martyna, Klein, Tuckerman Chain Thermostat
1996: Simultaneous $< p^2 >$ and $< p^4 >$ control
1996: Dettmann Hamiltonian $\mathcal{H}_D = s\mathcal{H}_N = 0$!
1997: Configurational Temperature (of 1952)
2000: Aoki and Kusnezov ϕ^4 model for heat conduction
2006: Memorial Meeting for Shuichi Nosé (1951-2005)
2008: Hamiltonian Thermostated Chains
2014: Patra-Bhattacharya Thermostat

*** "A unified formulation of the constant temperature molecular dynamics methods"**
"A molecular dynamics method for simulations in the canonical ensemble"