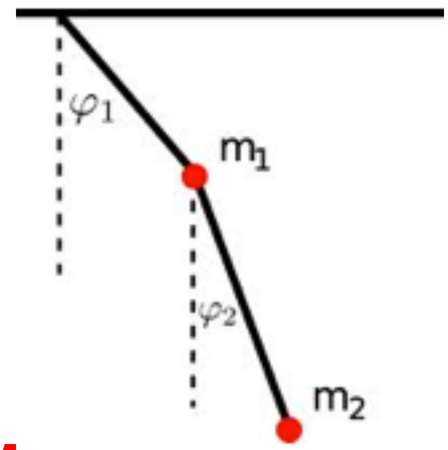
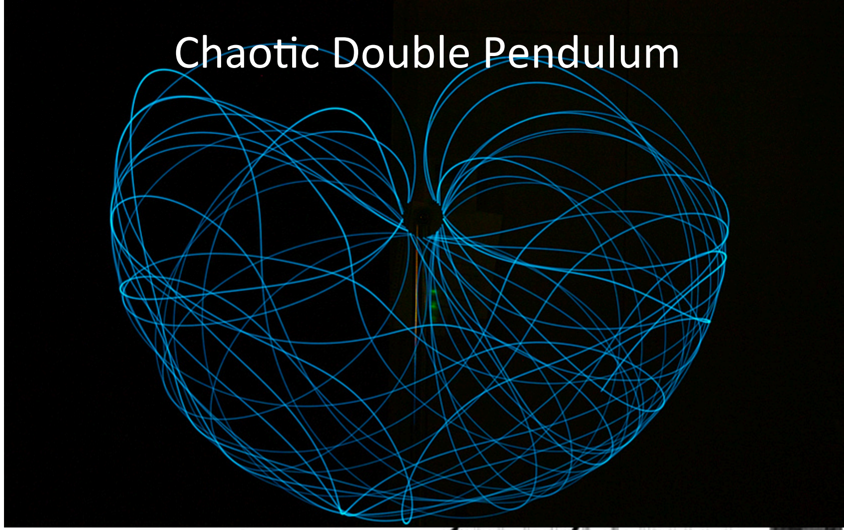
Microscopic Reversibility

versus

Macroscopic Irreversibility





Wm G Hoover and Carol G Hoover

Ruby Valley Research Institute

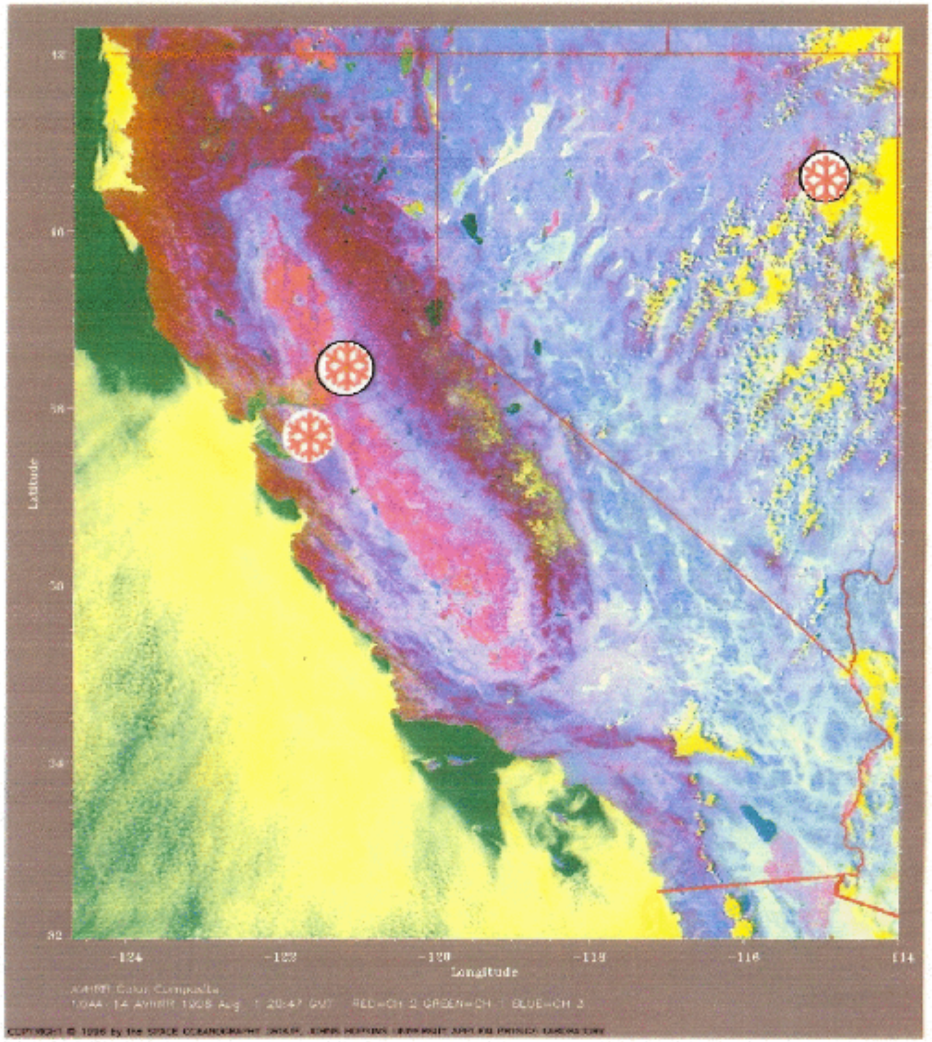
Ruby Valley, Nevada, USA

Saint Petersburg
3 July 2012

Overview of California and Nevada

Davis

Livermore



Ruby Valley

Our Neighbors' Llamas enjoy Ruby Valley

Local Ruby Valley Industry

MICRO-BREWED IN NEVADA'S HIGH COUNTRY

RUBY MOUNTAIN

BREWING COMPANY

VIENNA STYLE

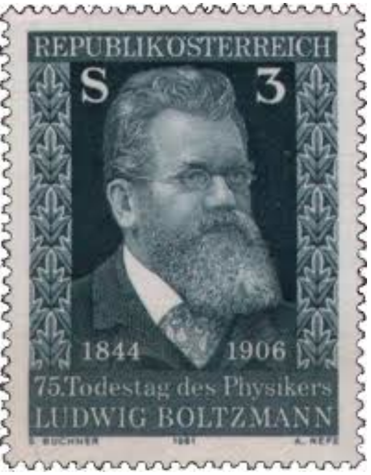
LAGER

Rudolf Clausius’ 1865 Version of the

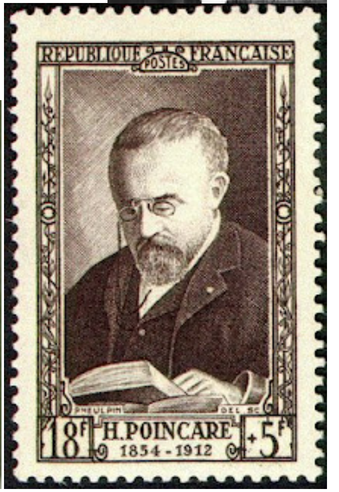
Second Law of Thermodynamics :

The Entropy of the Universe [or Any Closed System] Tends to a Maximum .

Time Dependence of Entropy ?



Entropy Increases
(df/dt →H Theorem)
(1872 : Second Law)



1896 : Entropy Recurs
(Zermélo-Poincaré)

Entropy Reverses
(Loschmidt, 1876)

Reversibility and Irreversibility Today

1. Thermodynamic Quantities from Particle Mechanics
2. Defining Temperature using Gibbs' Statistical Mechanics
3. Implementing Computational Thermostats into { F = ma }
4. Irreversibility from Thermostats : Successes of Nosé-Hoover Mechanics
5. Fractal Phase-space Distributions for Nonequilibrium Steady States
6. Irreversibility from Thermostats : Failures of Hamiltonian Mechanics
7. Irreversibility from Lyapunov Instability of Standard Hamiltonian Chaos
8. Summary

Relating { E, P, T, Q, . . . } to { q,p }

Energy is Simple : $E = \Sigma e_i = \Phi(q) + K(p)$; $K = \Sigma(p^2/2m)_i$

Pressure : Virial Theorem or Gibbs : $PV = \Sigma(rF)_{ij} + \Sigma(pp/m)_i$

(notice that reversing the time has no effect on P)

Heat Flux or Heat Theorem : $QV = \Sigma\, r_{ij} \bullet (pF/m)_{ij} + \Sigma(pe/m)_i$

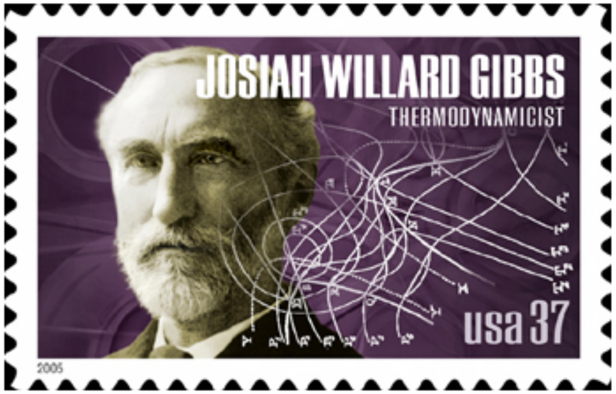
(notice that reversing the time changes the sign of Q)

Notice that the { Q , P } definitions Contradict Newton-Fourier :

$P_{xy} = -\eta\, [\, (du_x/dy) + (du_y/dx)\,]$; $Q_x = -\kappa\, (dT/dx)$

$\{ P,Q \}_{micro} \neq \{ P,Q \}_{MACRO}$

"Temperature" is Ambiguous



Gibbs' Statistical Mechanics .

Besides $T = (\partial E/\partial S)_V$, we have :

"Kinetic Temperature(s)" :

$$kT\int(\partial^2H/\partial p^2)e^{-H/kT}dp = \int(\partial H/\partial p)^2e^{-H/kT}dp$$

$$kT = < p^2/m > = < (\partial H/\partial p)^2 >/< (\partial^2H/\partial p^2) >$$

Similarly $kT = < p^4 >/ [3m < p^2 >]$

"Configurational Temperature(s)" :

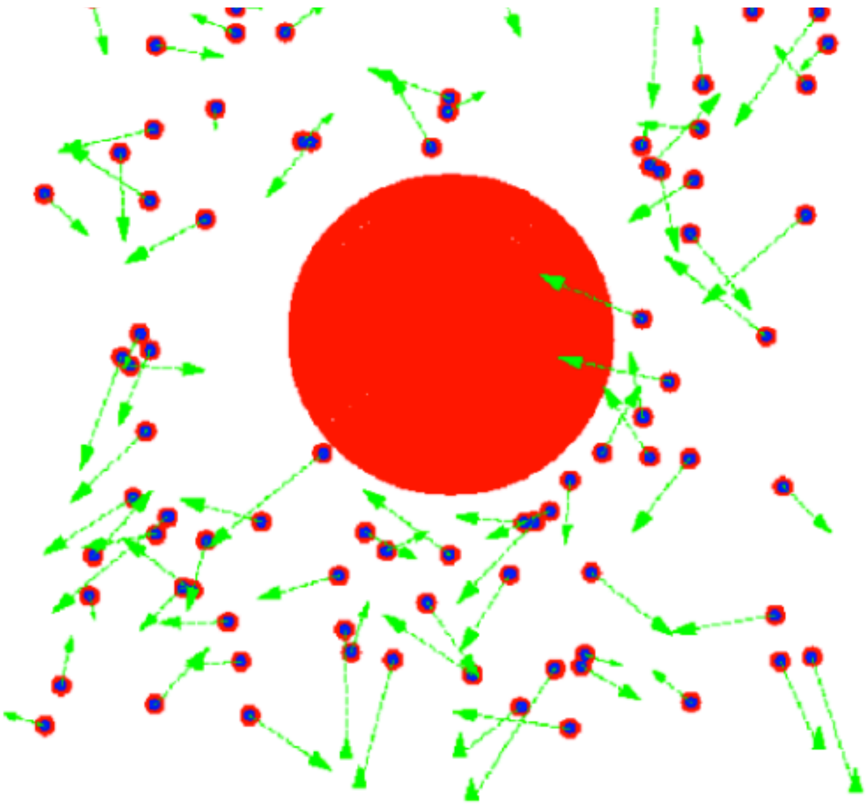
$$kT\int(\partial^2H/\partial q^2)e^{-H/kT}dq = \int(\partial H/\partial q)^2e^{-H/kT}dq$$

$$kT = < (\partial H/\partial q)^2 >/< (\partial^2H/\partial q^2) >$$

Analysis from Kinetic Theory

Ideal Gas Thermometer

$$< p^2/m > = kT = PV/N$$



Temperature is just the *comoving* Kinetic Energy .

Computing Macroscopic Spatially-averaged Field Variables from Molecular Dynamics { q,p } data using Lucy's Normalized and *Very-Smooth* Weight Function

$$\rho(r_0) = \Sigma_j w(|r_j - r_0|) \text{ with}$$

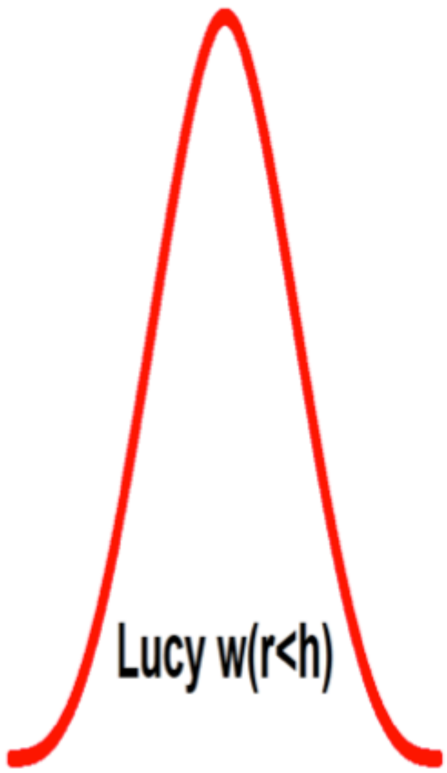
$$w_{1D} = C[1 - (r/h)]^3[1 + 3(r/h)]$$

$$C_{1D} = (5/4h)$$

$$C_{2D} = (5/\pi h^2)$$

$$C_{3D} = (105/16\pi h^3)$$

h = 3 is a good choice!



Extracting { E, P, T, Q, . . . } from { q,p }

Field Variables are defined using *"Smooth-Particle"* averages :

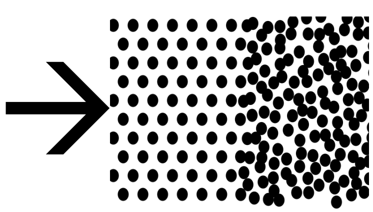
$\rho(r,t) = \Sigma m_i w(r-r_i)$; $\rho u(r,t) = \Sigma m_i v_i w(r-r_i)$; $\rho e(r,t) = \Sigma m_i e_i w(r-r_i)$.

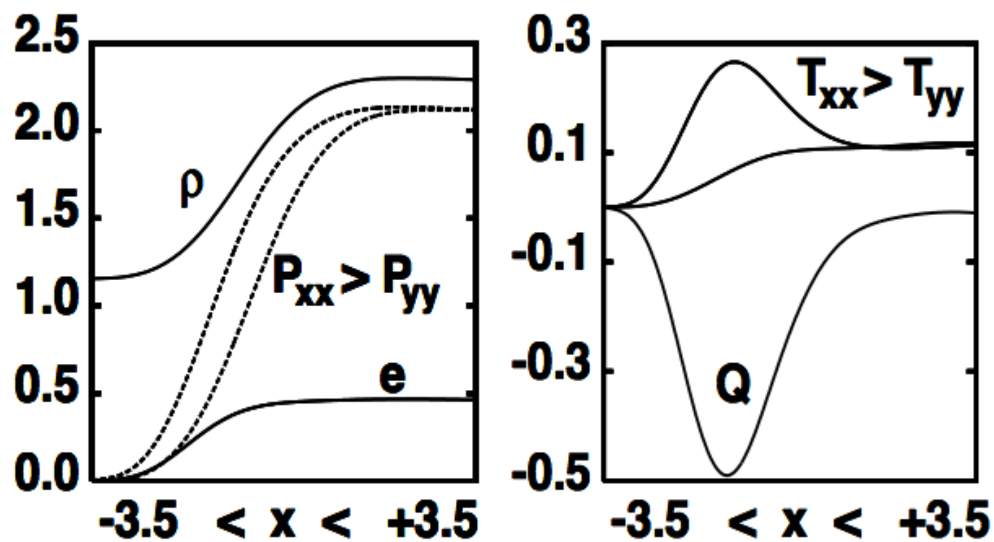
(the Continuity Equation is *exactly* satisfied by these definitions) .

These averages are computed using Lucy's weight function :

$w(r<h) = (5/\pi h^2)[\, 1 + 3(r/h)\,][\, 1 – (r/h)\,]^3$ is *very* smooth !

Typical Profiles from a Strong Shockwave Simulation based on Molecular Dynamics





Mechanical Thermal

1 & 2. Thermodynamics & Temperature

- ✪ Density, Velocity, Energy, Pressure, Temperature, and Heat Flux can be formulated in terms of { q,p } .
- ✪ Local instantaneous values of $\rho(r,t)$, $u(r,t)$, $e(r,t)$, $P(r,t)$, $T(r,t)$, and $Q(r,t)$ can be formulated using smooth-particle weighting functions with two continuous derivatives .
- ✪ Nosé-Hoover-Gauss thermostats reproduce hot and cold temperatures and give fractal distributions .

3. Implementing Thermostats is easy

- ✪ Thermostated degrees of Freedom typically obey a modified equation of motion : { $(dp/dt) = F - \zeta p$ } .

Particle Mechanics

$$F = ma$$

Imposing Constraints

$$\mathcal{L}(q,\dot{q}) \rightarrow \mathcal{H}(q,p)$$

Kinetic Temperature

$$\dot{q} = (p/m)\;;\;\dot{p} = F - \zeta p\;;$$

$$\dot{\zeta} = [\,(K/K_o) - 1\,]/\tau^2$$

Keio University 1989-1990

Shūichi Nosé 1951-2005

Gary Morriss & Carl Dettmann

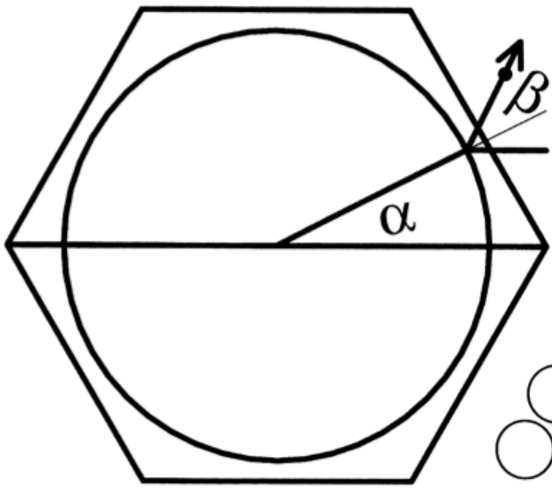
1996

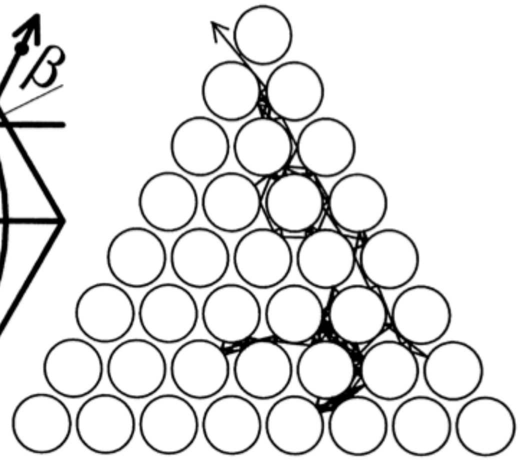
A "Hamiltonian" which can generate Gibbs' Canonical Ensemble :

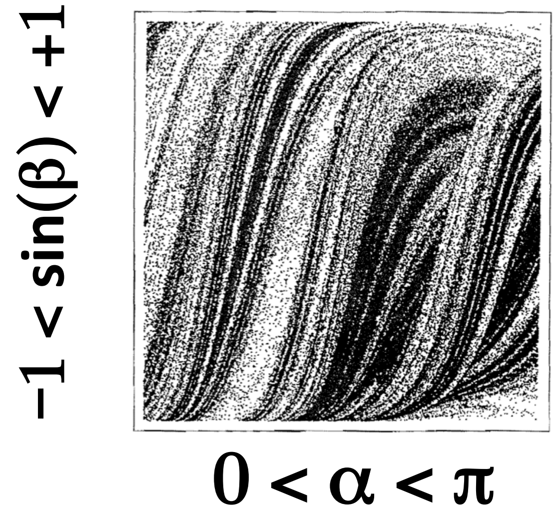
$$\mathcal{H} = \sum (p^2/2ms) + s[\ \Phi(q) + NkT \ln s + (P_s^2/2M)\ ] = 0\ !$$

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

Simplest Thermostated System : Galton Board







[Yes, there IS a ``Hamiltonian” which will generate this motion !]

Motion Equations between Collisions :

$$\dot{p}_x = E - \zeta p_x \ ; \ \dot{p}_y = -\zeta p_y \ ; \ \zeta = E p_x$$

“isokinetic” so that $p_x^2 + p_y^2 = 1$ and

$$p_x \dot{p}_x + p_y \dot{p}_y = 0 \ .$$

Evolution of a "Hamiltonian" Fractal

[Wm. G. Hoover, B. Moran, C. G. Hoover, W. J. Evans (1988)]

Volume 133, number 3 PHYSICS LETTERS A 7 November 1988

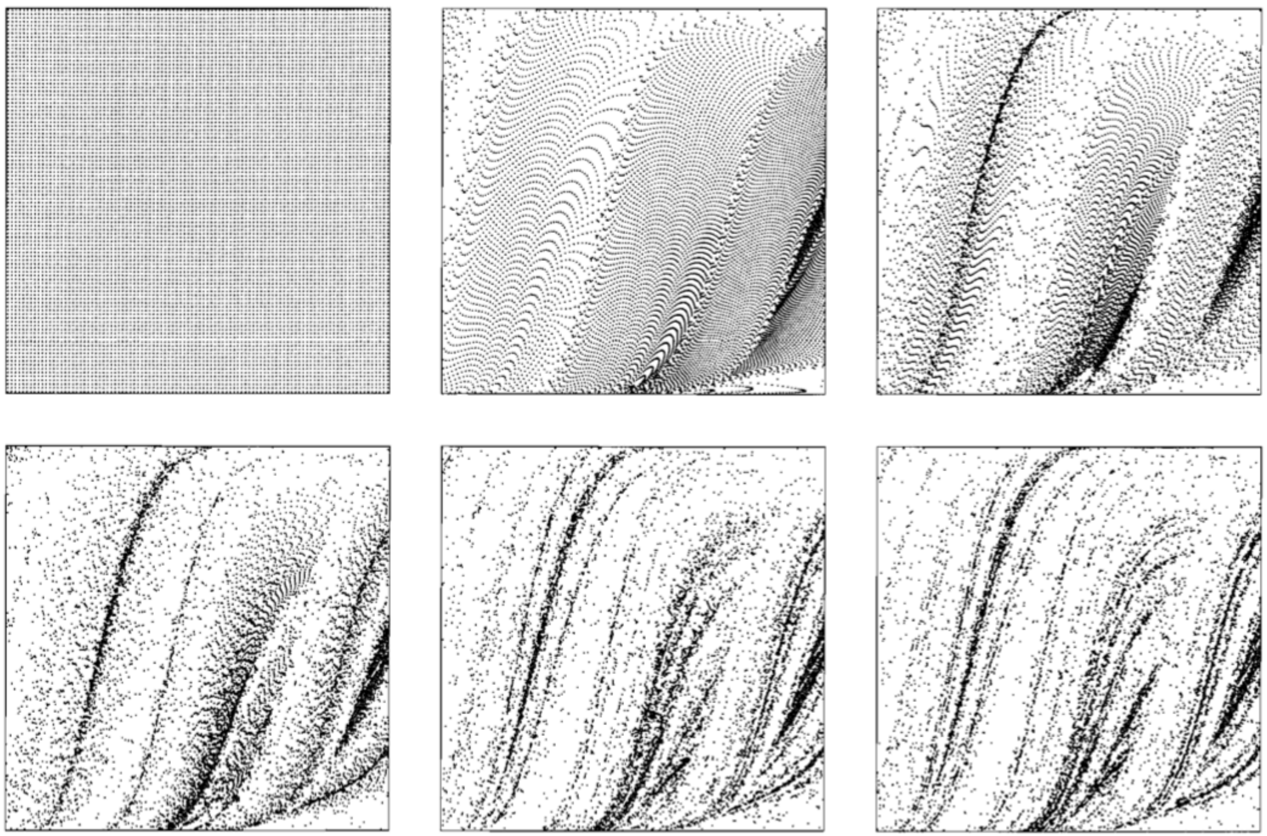
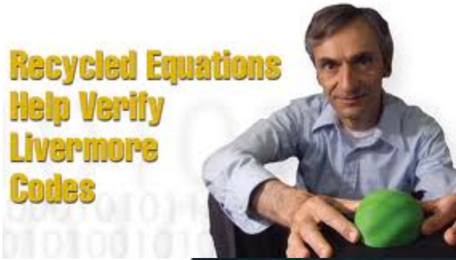
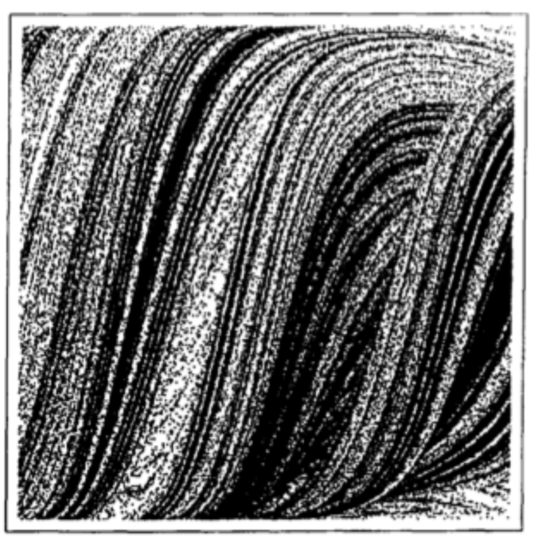


Fig. 2. Time development of 10000 Galton board trajectories for a field $E=3p^2/m\sigma$ indicating the convergence of phase-space volume to a strange attractor. The ordinate is the sine of the angle, relative to the normal, made by the velocity after collision. The abscissa is the angle at which the collision occurs relative to the field direction. Thus a head-on collision at the "top" of a scatterer corresponds to a point at the middle of the right-hand boundary of these phase-space sections. The Poincaré-section views shown correspond to 10000 phase-space states occupied after 0, 1, 2, 3, 5, and 10 collisions.

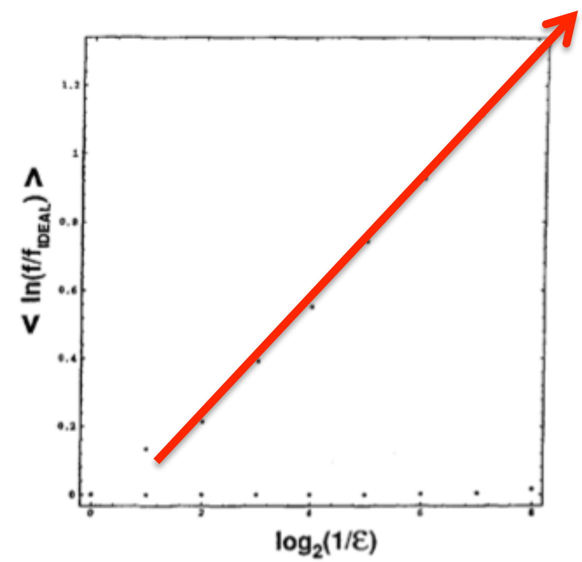


Typical MultiFractal Phase-Space Distribution for the Galton Board Collision Problem :

- A mass point falls through a triangular lattice of scatterers .
- The mass point's speed is constrained by Gauss' thermostat .
- 300,000 successive collisions are collected, with each of them described by its location and its velocity direction (two angles) .



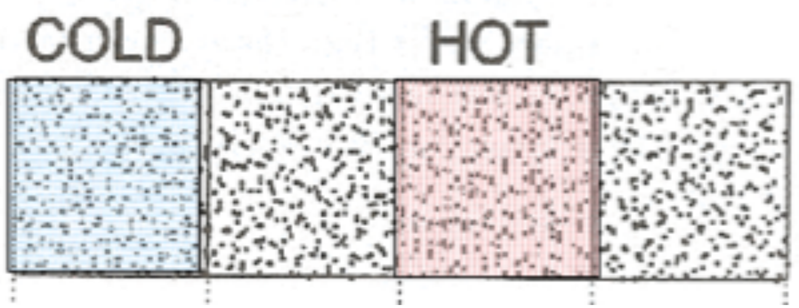
Fractal Divergence of the Coarse-Grained Entropy $-S(1/\varepsilon)/k$ →



Heat Flow with 7 *non*Hamiltonian and 3 Hamiltonian Thermostats *

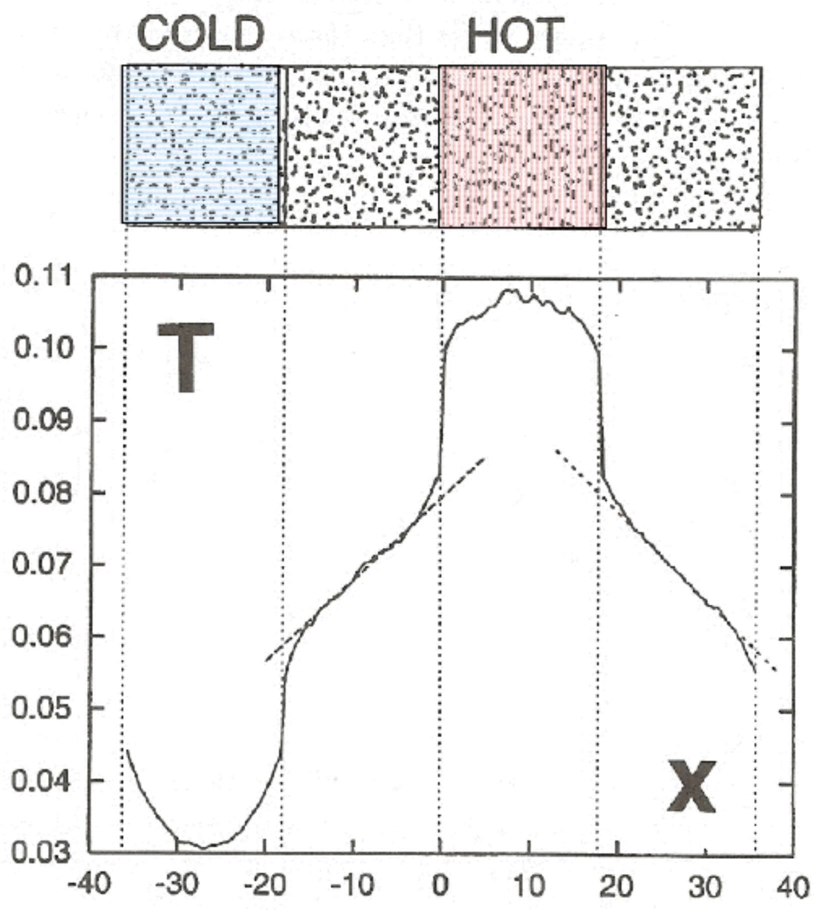
``Sandwich" Simulations , with a HOT Region , a COLD Region , and two Hamiltonian Regions .

Only the *nonHamiltonian* Simulations Obey Fourier's Law : $Q_x = -\kappa(dT/dx)$.



* Dresden 2004

Four Chamber Periodic Problem

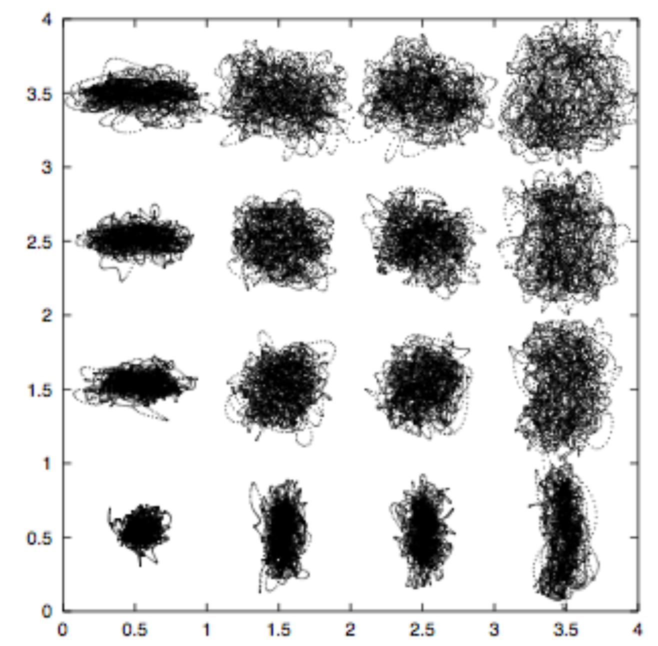


ϕ^4 : An Excellent Model for Fourier Heat Conduction

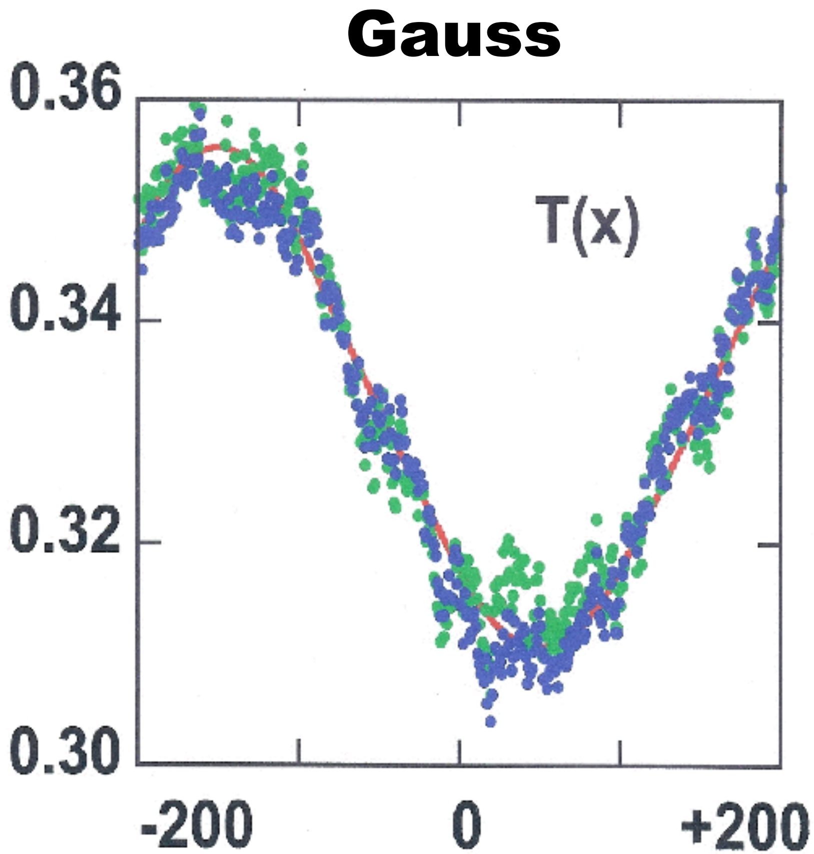
Tether Particles with δ^4 and add Nearest-Neighbor Hooke's Law ; Solve with 4^{th}-order Runge-Kutta and Observe Fourier Heat Flow .

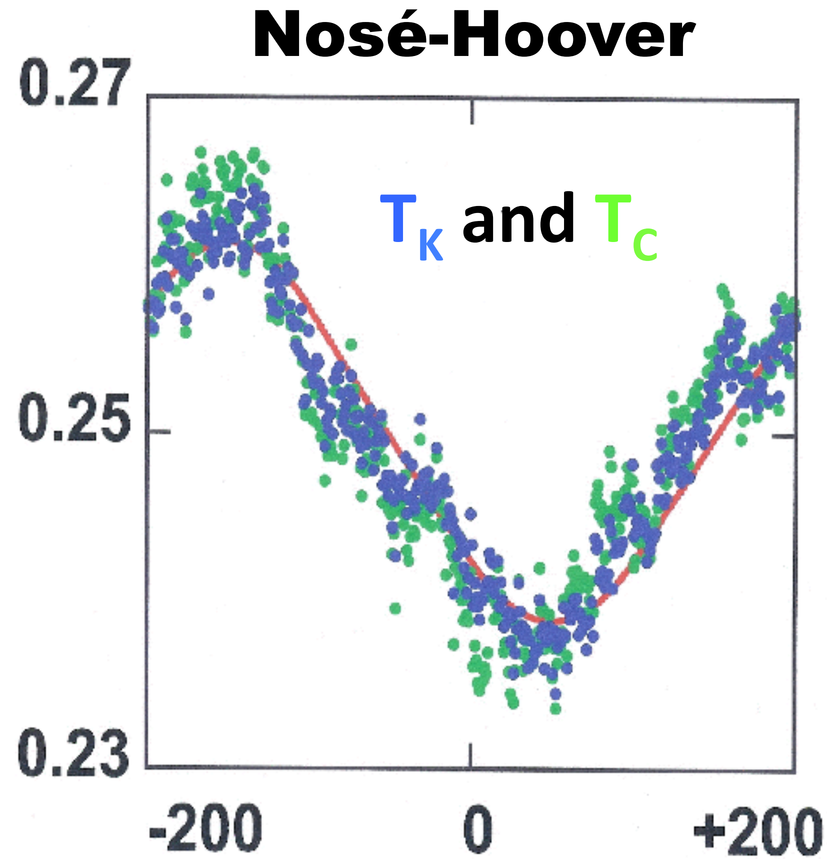

Ken Aoki & Dimitri Kusnezov

From ϕ^4 Lyapunov Spectrum the limiting large-system Dimensionality Loss $\Delta D \sim 43$ with one HOT Particle and one COLD Particle .



Gauss & Nosé-Hoover Profiles : Kinetic & Configurational T(x)





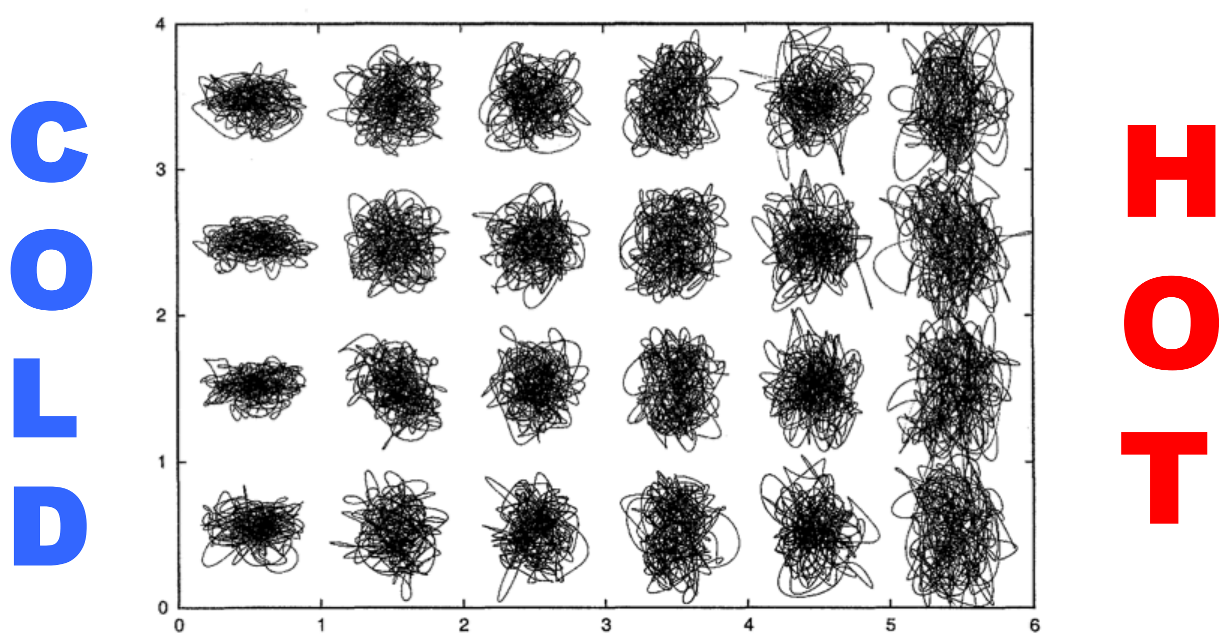
4. Irreversibility from Thermostats

Seven Successes of Nosé-Hoover-Gauss . . . mechanics :

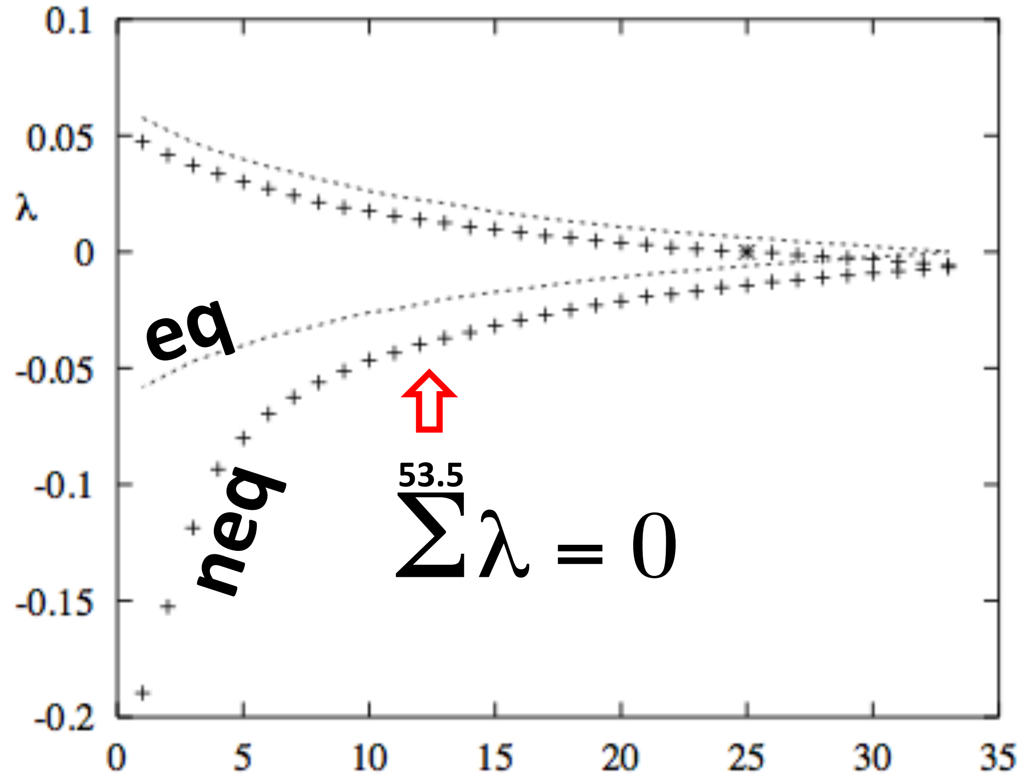
Differential and Integral Feedback control of < p^2 > and < p^4 > .

System Lengths of 4+2 , 8+2 , and 16+2 Columns of Particles

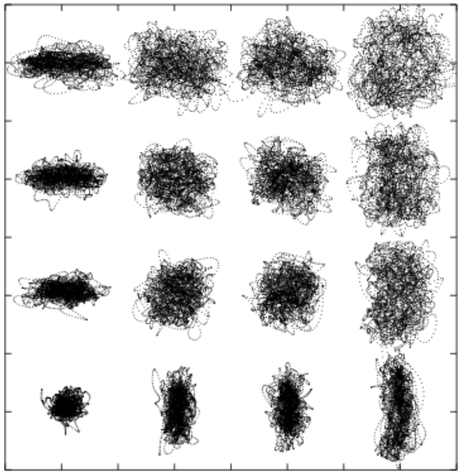
***All* give similar estimates for the ϕ^4 model's heat conductivity .**



5. ϕ^4 Model Lyapunov Spectra (2002)



D = 53.5



Phase-Space Dimensionality Loss ΔD is 12.5 .

Thermostat Dimensions = 2 x 5 = 10 ;

Hamiltonian Dimensions = 4 x 14 = 56 ;

$T_1 = 0.001$ and $T_{16} = 0.009$.

5. Fractal Nonequilibrium Steady States

Suppose that Work is converted into Heat :

For instance , $-(dW/dt) = -P_{xy}(du_x/dy)V$.

$\{ (dp/dt) = F_{usual} - \zeta p \}$

→ $\zeta = -(du_x/dy)P_{xy}V/NkT$.

→ Liouville's Theorem : $(d \ln f/dt) = -(\ / \ ) = N\zeta$.

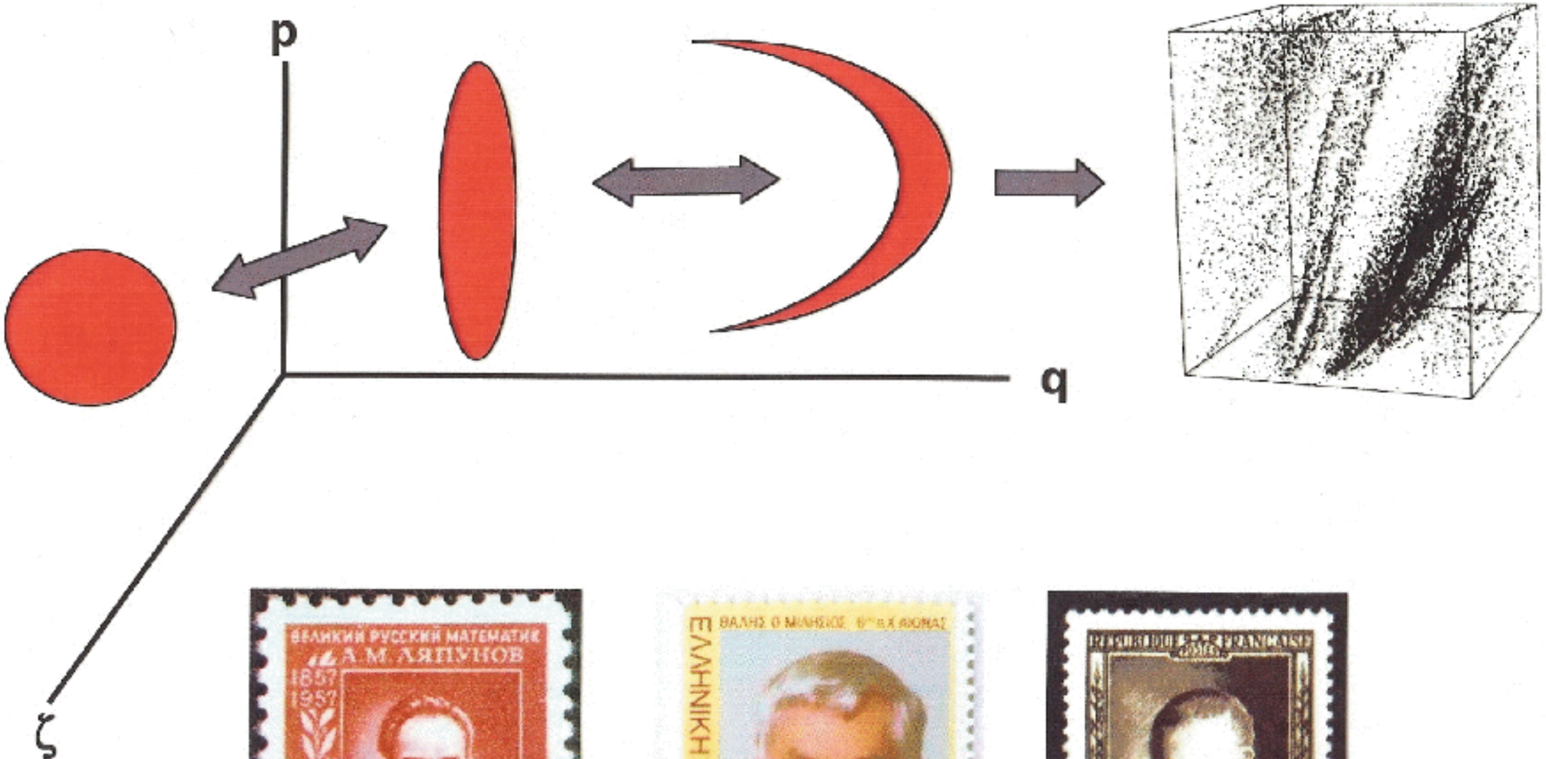
→ $\Sigma' \lambda_i = 0$ → $\Delta D = N\zeta/\lambda_1$.

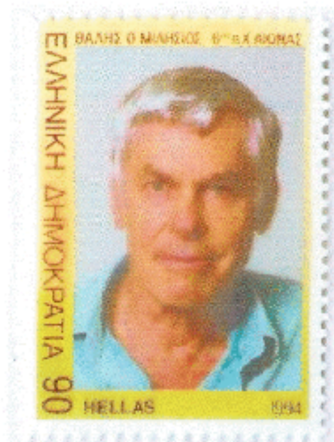
→ Suppose that Heat Flows from Hot to Cold :

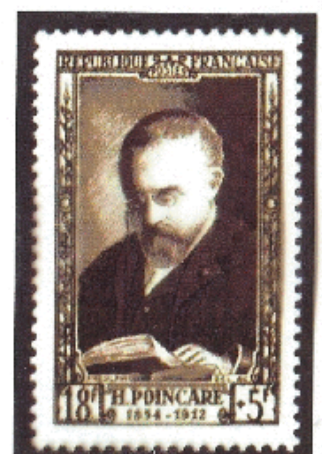
→ $(d \ln f/dt) = -(\ / \ ) = \Sigma\zeta$.

→ and again , $\Delta D = \Sigma\zeta/\lambda_1$.

Generic Nonequilibrium Phase Space Flow







MultiFractal Attractor Lessons from Time-Reversible Motion Equations

- Nonequilibrium States are very Rare .
- Comoving phase volume vanishes .
- Distributions' Dimensionality Reduced .
- Distributions are Singular everywhere .
- Gibbs' Entropy diverges to $-\infty$.
- Forward Stability > Backward Stability .

6. Hamiltonian Thermostats : 3 Types which Fail :

$$kT = \langle (\nabla \mathcal{H})^2 \rangle / \langle \nabla^2 \mathcal{H} \rangle$$

Tom Leete ↘

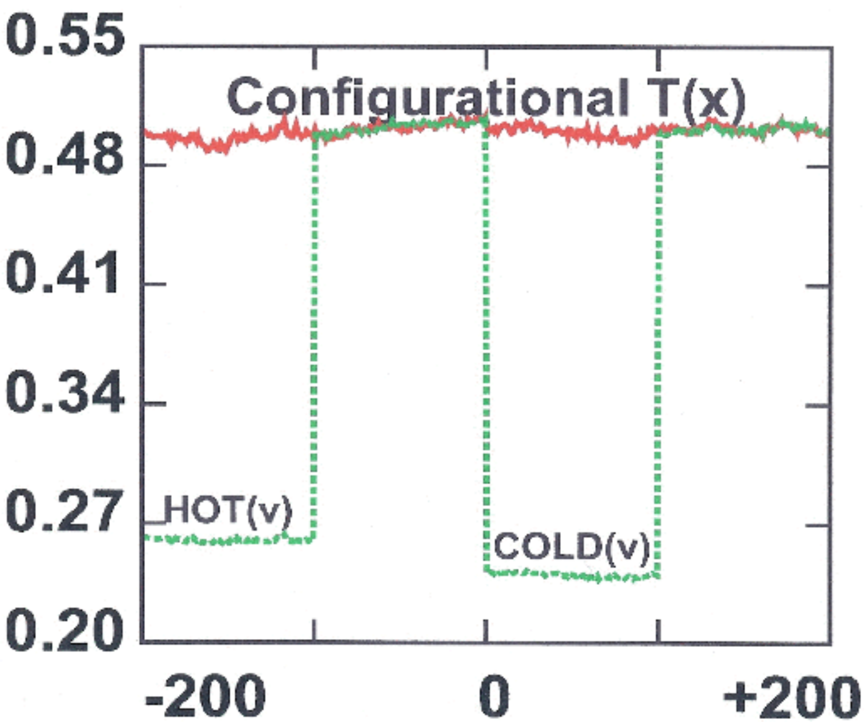
West Virginia University 1976

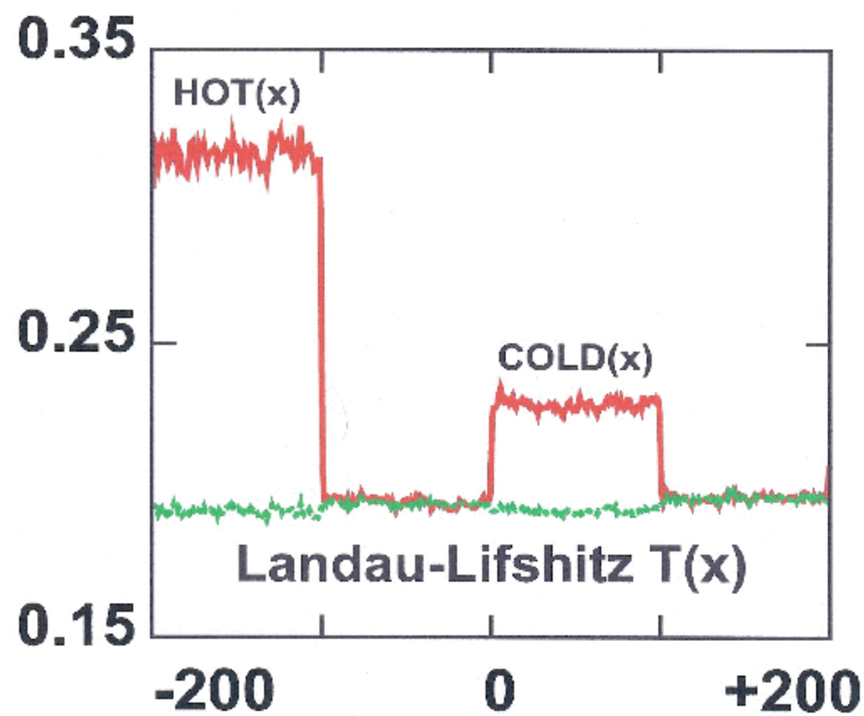
$$\mathcal{H} = [\,4K(p)K_0\,]^{1/2} + \Phi - K_0$$

← 2012 !

$$\mathcal{H}_{\ln} = kT \ln(|q|) + (p^2/2m) \rightarrow e^{-\mathcal{H}/kT}$$

Hoover-Leete & Landau-Lifshitz Kinetic & Configurational T(x) .*





* JCP 2007

Why are Hamiltonian Thermostats Failures ? *

At present, there are three types which have been tried :

- Landau-Lifshitz controls Configurational Temperature .
- Hoover-Leete controls the Kinetic Temperature .
- A Log-thermostat yields Gibbs' Canonical Distribution .

Four Reasons why all such Hamiltonian Thermostats Fail :

- Specifying Energy, Temperature, and Density is Too Much !
- Hamiltonian Thermostats don't generate a Heat Flux .
- Hamiltonian Thermostats fail to give the right Temperatures .
- Hamiltonian Thermostats cannot generate Fractals .

* See five recent arXiv contributions -- two by Campisi , Zhan , Talkner , and Hänggi [they promote the Log-Thermostat] as well as three other contributions , by Meléndez , by Hoover , and by Meléndez and Hoover [pointing out the four defects of these three types of Hamiltonian thermostats] .

7. Irreversibility ← Hamiltonian Mechanics ?

Consider the Reversal of Strong Shockwaves Created by the Collision of Two Blocks :

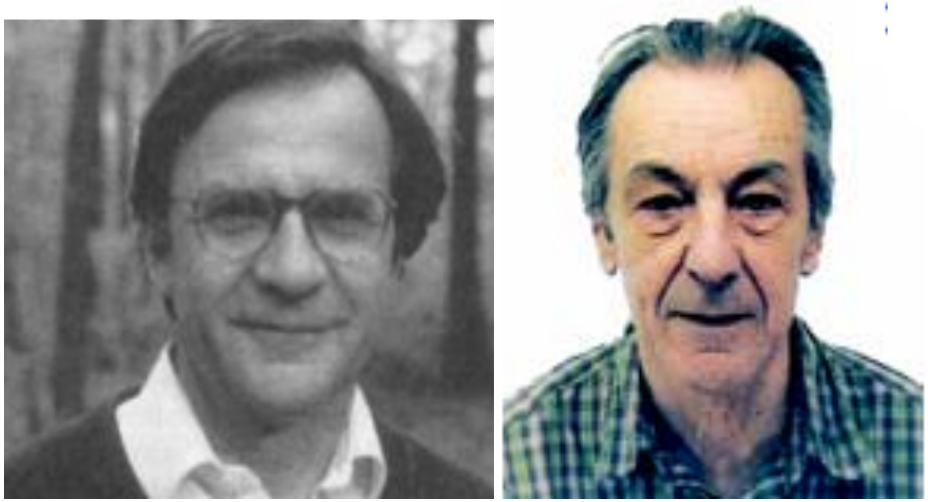
→  ←

Examine **Lyapunov Instability** **Near the Trajectory , Finding the Particles Most Important to Stability .**

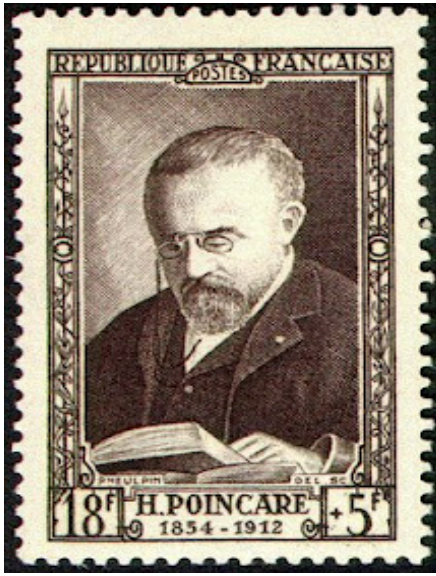
Irreversibility from a Bit-Reversible Version of Newtonian Mechanics ?

Solve { F(q) = ma } with "Integer Leapfrog" , A Centered-Difference Highly-Stable Algorithm :

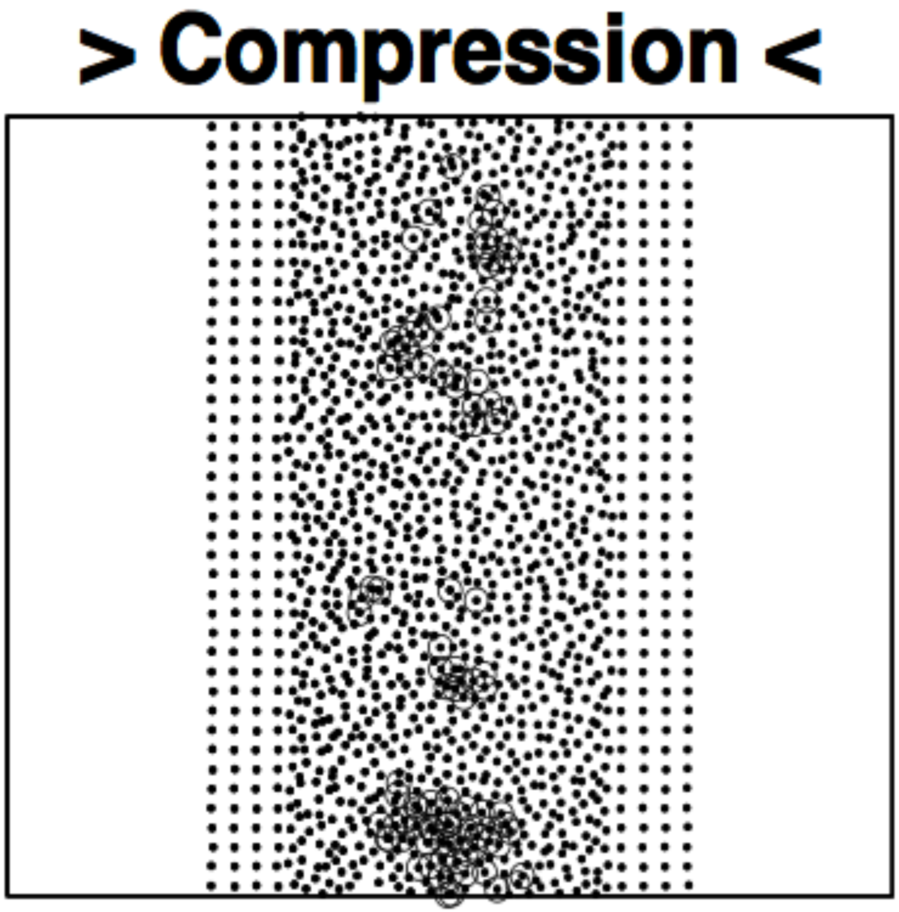
$$\{\ q_+ - 2q_0 + q_- = [\ (F(\ q_0\ )/m)(dt)^2\ ]_{\text{Integer}}\ \}$$

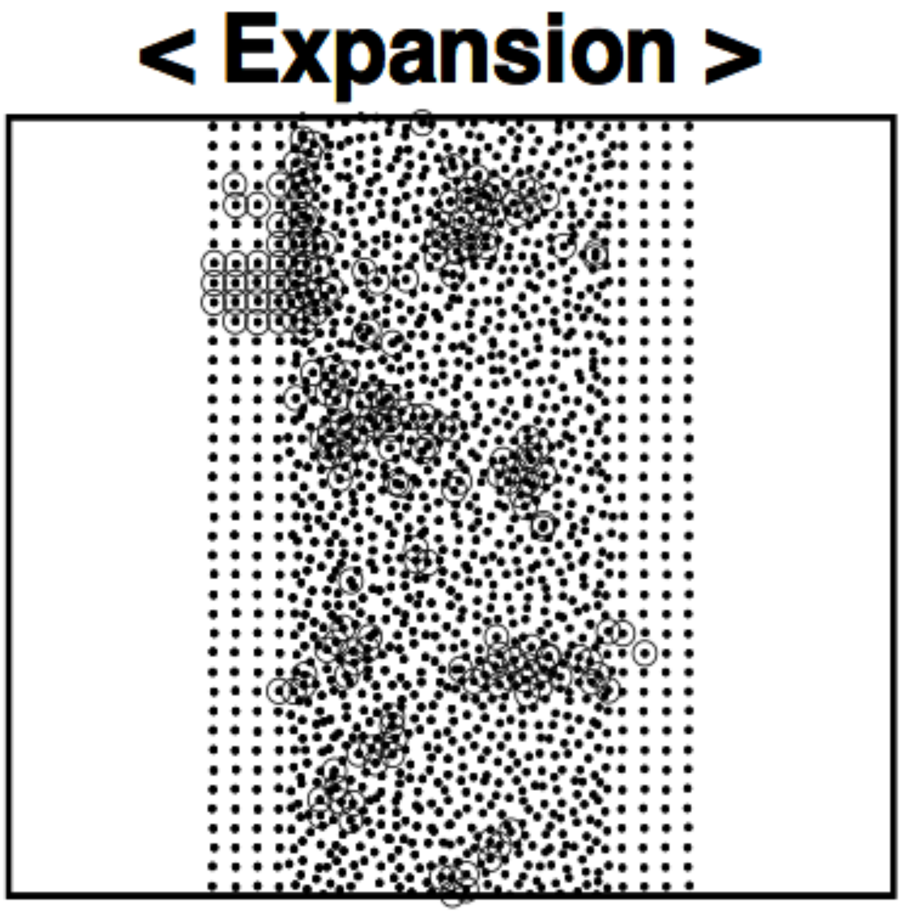


Dominique Levesque and Loup Verlet



7. Precisely Time-Reversible Hamiltonian Shockwave Simulation Two-Fold Compression-Expansion of N = 800 Colliding Cold Blocks





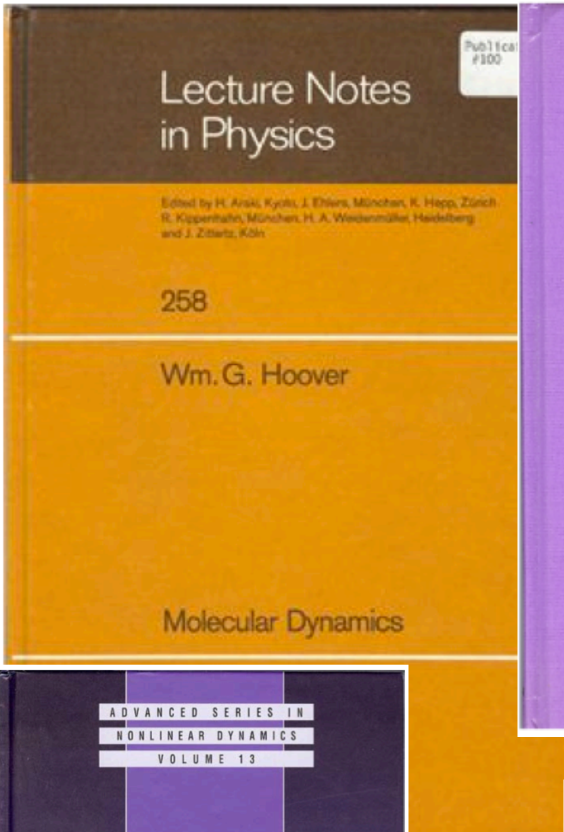
101 Important Particles

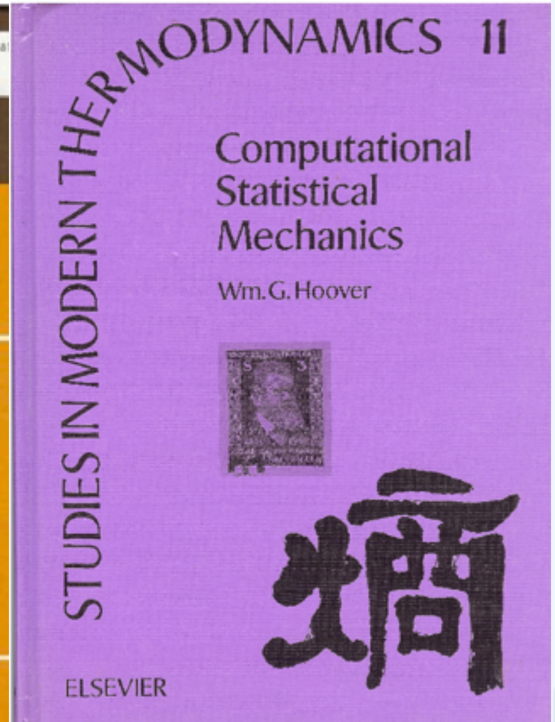
212 Important Particles

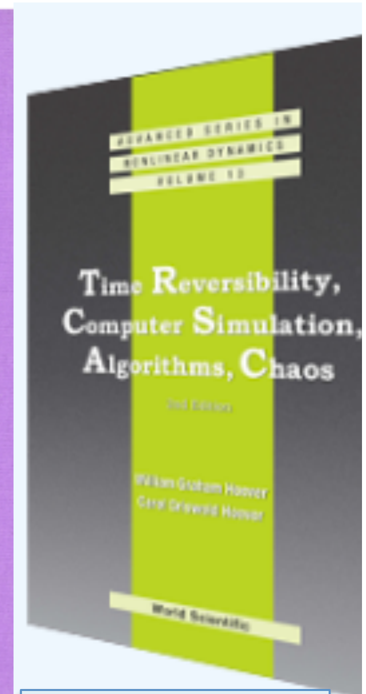
8. Summary : Status of the Irreversibility Paradox in 2012

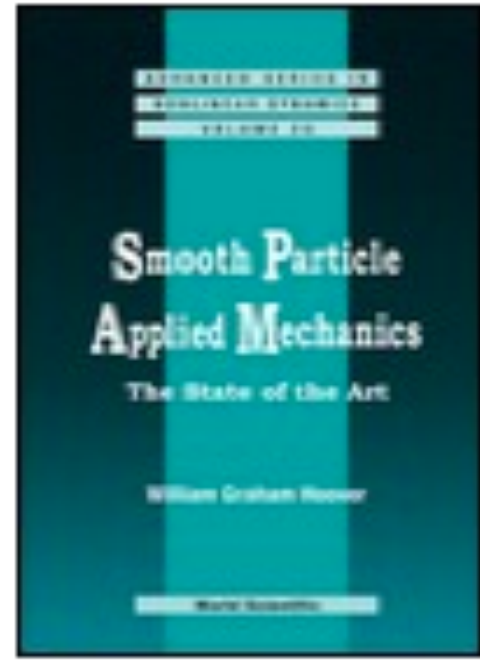
- Nonequilibrium Simulations Require NonHamiltonian Mechanics
- Thermostated Systems + Chaos → Fractals and the Second Law
- Phase Space Dimensionality is Reduced , Time Symmetry Broken
- Fractals explain the Success of Nosé-Hoover/Gauss Thermostats
- Liouville's Theorem explains Failure of Hamiltonian Thermostats
- Fractals likewise explain the Failure of Hamiltonian Thermostats
- Isolated Hamiltonian Systems + Chaos also Break Time Symmetry
- There is Plenty of Work to do Investigating Lyapunov Instability

References in Addition to http://williamhoover.info

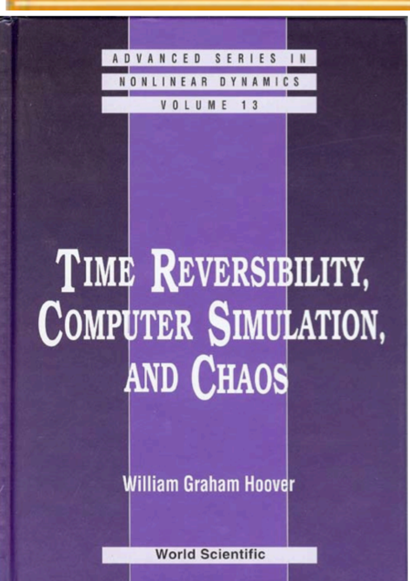








New ↑



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Acknowledgments

Peter Hänggi

Michele Campisi

Harald Posch

Marc Meléndez

Carl Dettmann

Rainer Klages