Yokohama to Ruby Valley Nevada :
Around the World in 80 Years . II .

[Thanks to Karl Travis and Fernando Bresme]

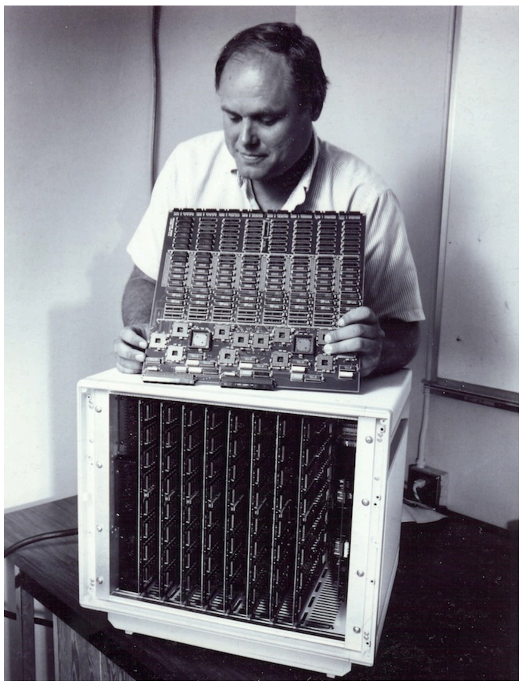
Carol G. Hoover & William G. Hoover
Ruby Valley Nevada

1. To Yokohama from Livermore
2. 15 years in Livermore & 10 years in Ruby Valley Nevada : Molecular Dynamics and Continuum Mechanics

1. Life in Japan at Keio University in Yokohama
Molecular Dynamics : 1989 – 1990 and beyond

Parallel Algorithms

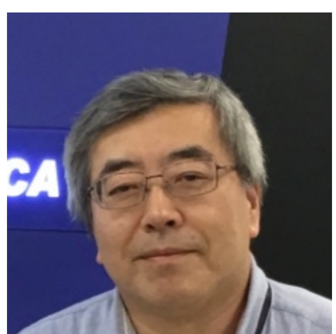
Tony De Groot
at LLNL



$30,000 SPRINT versus
$30,000,000
Cray Computers
1,036,800 particles !!

Toshio Kawai
at Keio University

Taisuke Boku
also at Keio

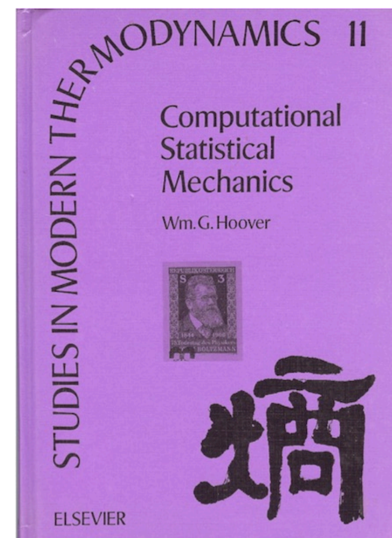


Sigeo Ihara
at Hitachi

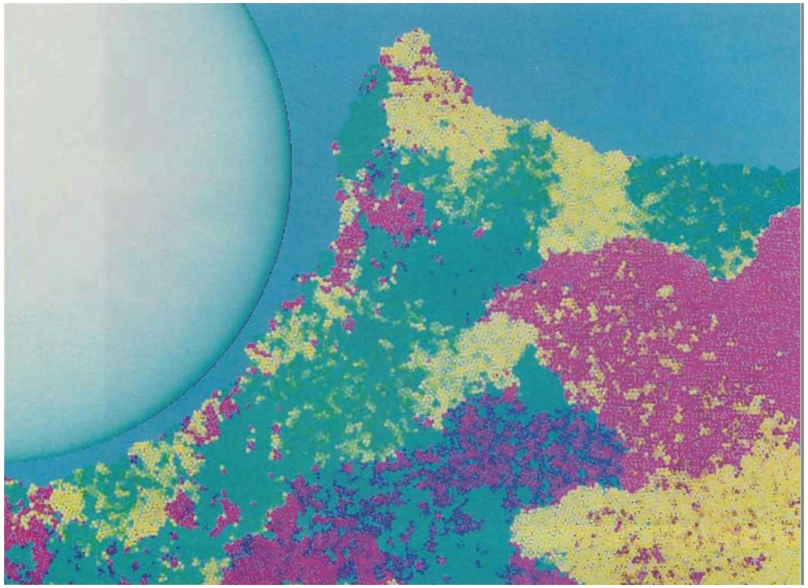
Lyapunov Spectrum

Strings of Springs
Harald Posch
at University of Vienna

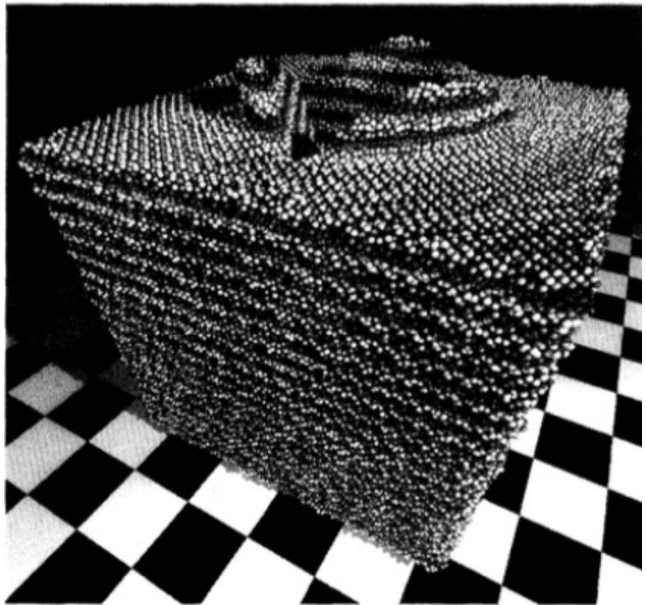
Evenings/Weekends



Two & Three-Dimensional Parallel Simulations of Indentation

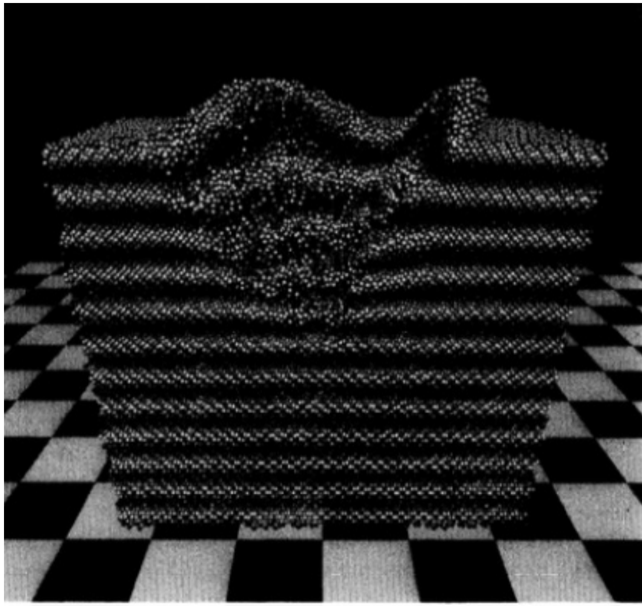


Nonequilibrium indentation for 720 x 1440 particles in two dimensions . Lennard-Jones with an embedded-atom potential models a granular solid representing metals such as copper or nickel . Molecular dynamics on Tony De Groot's SPRINT computer with message-passing processors .



Work of indentation → Surface + elastic energy Plastic yield strength.

Tetrahedral indentation : 72 x 72 x 72 silicon atoms with Stillinger-Weber ϕ



2. Past is Prologue : Research at LLNL (1990-2005)

Howard Hanley's 1982 Boulder Conference : "Nonlinear Fluid Behavior"

Nosé's two 1984 papers → Bill's 1985 Nosé-Hoover paper

Ciccotti & Hoover's 1985 Fermi School on Molecular Dynamics

How does reversible microscopic mechanics produce irreversible behavior ?

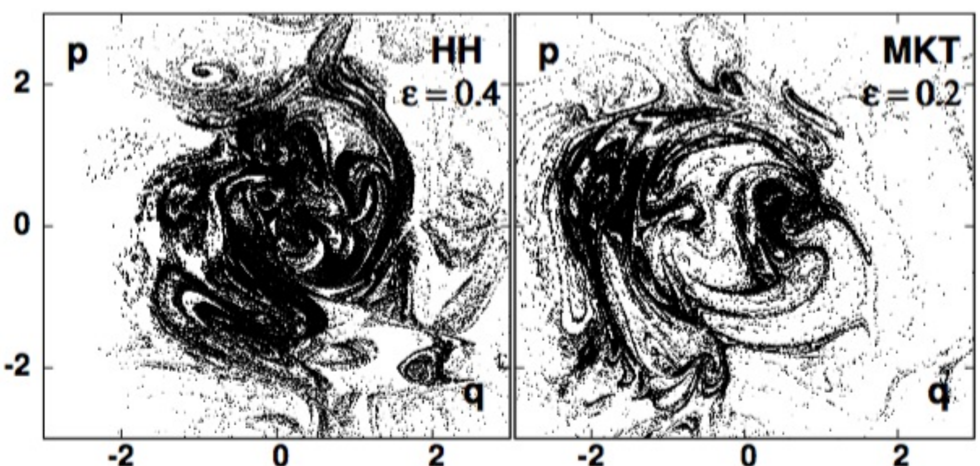
$$\dot{f}/f = -\dot{\otimes}/\otimes = \dot{S}_{ext}/k = -\sum_k \lambda_k$$

Nonequilibrium steady states :

At least one thermostat is needed for diffusion, shear, or heat flow.

Oscillator with T(q) = 1 + εtanh(q)

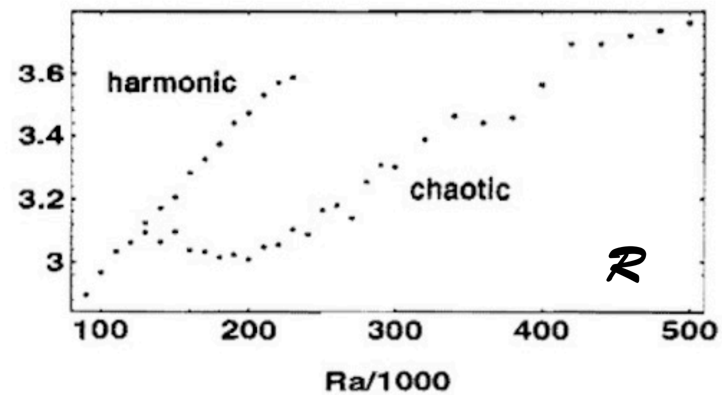
Negative Lyapunov sum → Dissipation



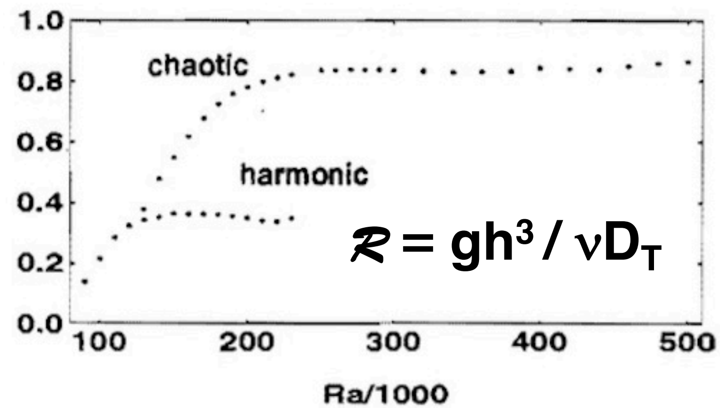
Irreversible Thermodynamics & Computational Fluid Dynamics

$$\dot{s} = (\eta/T)\,\dot{\epsilon}^2 + \kappa\,|\,\nabla \ln T\,|^2$$

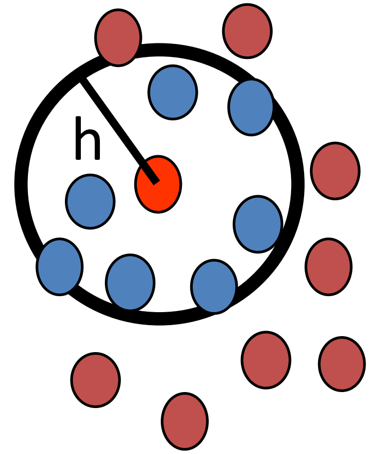
$\dot{S}$



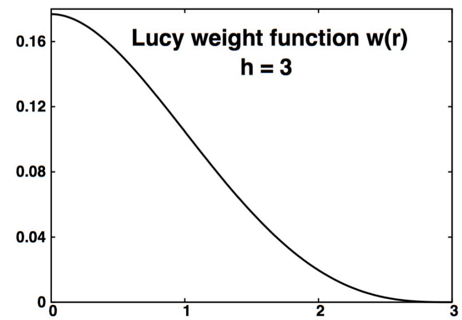
λ



Smooth Particle Applied Mechanics (SPAM)
Lucy & Monaghan 1977



“Particle density” from neighbors within a smoothing length, h



Continuum field variables are computed as weighted sums over all particles within the smoothing length h

$$\rho(r) = \sum w(r - r_i) \ ; \ \rho(r)u(r) = \sum w(r - r_i)\, v_i$$

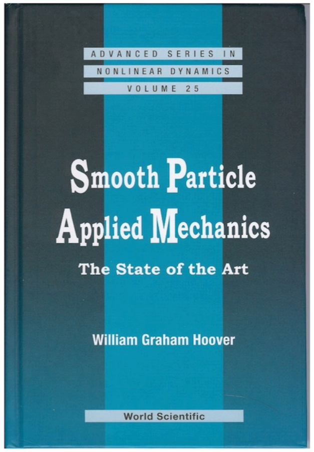
The continuity equation is automatically satisfied !

$$\partial\rho/\partial t \equiv -\nabla\cdot(\rho v)$$

$$\ddot{r}_i = \dot{v}_i = \sum_K \left[(P/\rho^2)_K + (P/\rho^2)_i \right] \nabla_K w_{iK}$$

We use fourth-order Runge-Kutta integration throughout .

Chapter 3 ;
Draft book online



williamhoover.info

Some applications of SPAM :
Free expansion of a gas, Rayleigh Bénard, fragmentation,
Smooth-particle averages of atomistic properties !

Free Expansion of SPAM Gas : Harald Posch

Difficult for finite-element algorithms because of severe shear deformation

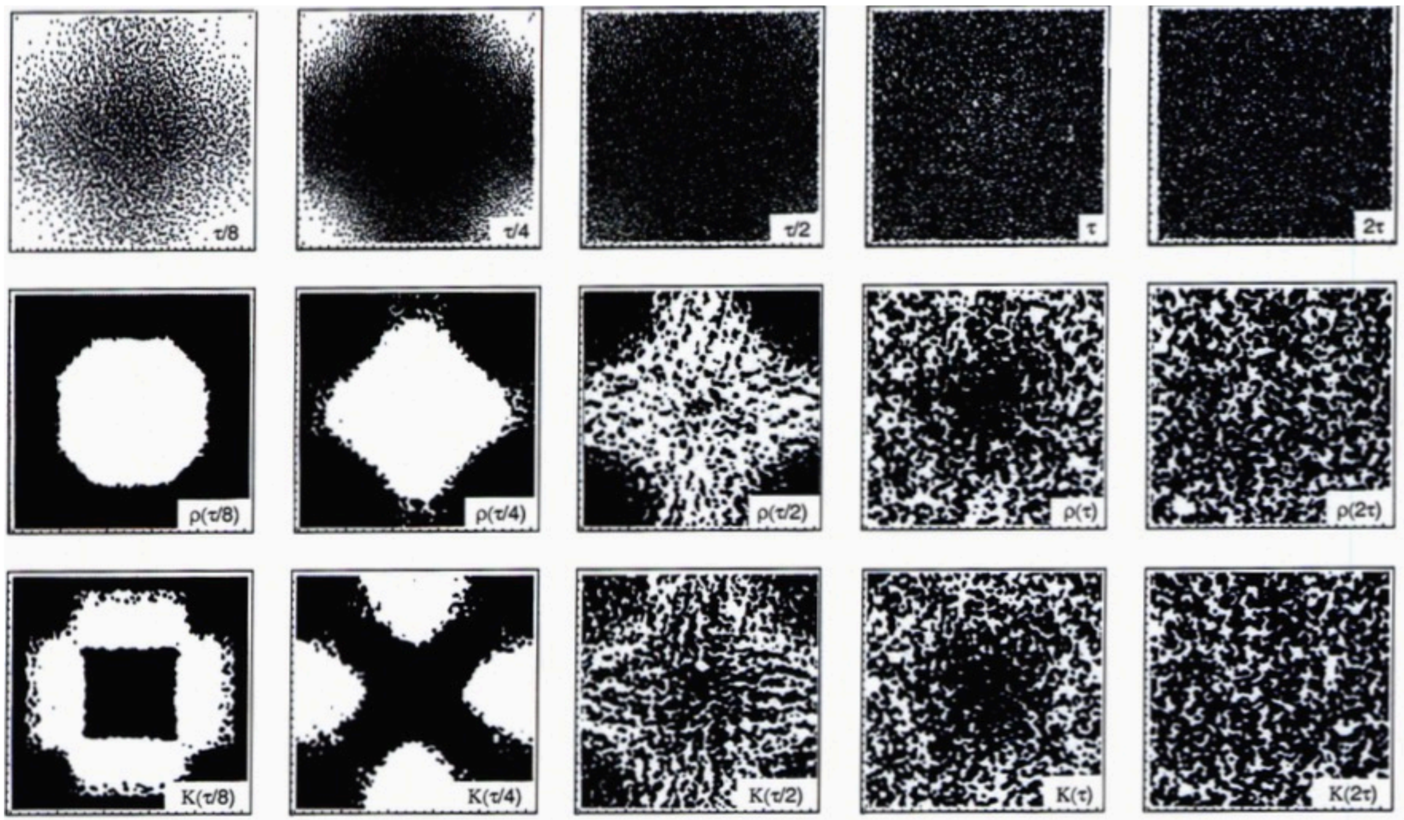
Equilibration is fast , and occurs in one or two sound traversal times , τ

Internal Kinetic energy must be measured relative to the local velocity

r

ρ

K



$\tau/8$ $\tau/4$ $\tau/2$ τ 2τ

Four-fold expansion, Periodic boundaries , 128 x 128 grid for ρ and K

$$\rho_g = \sum_j w_{gj} \;;\; P = \rho e = \rho T = \rho^2/2$$

Convergence of the Free Expansion Entropy Nk ln(4)

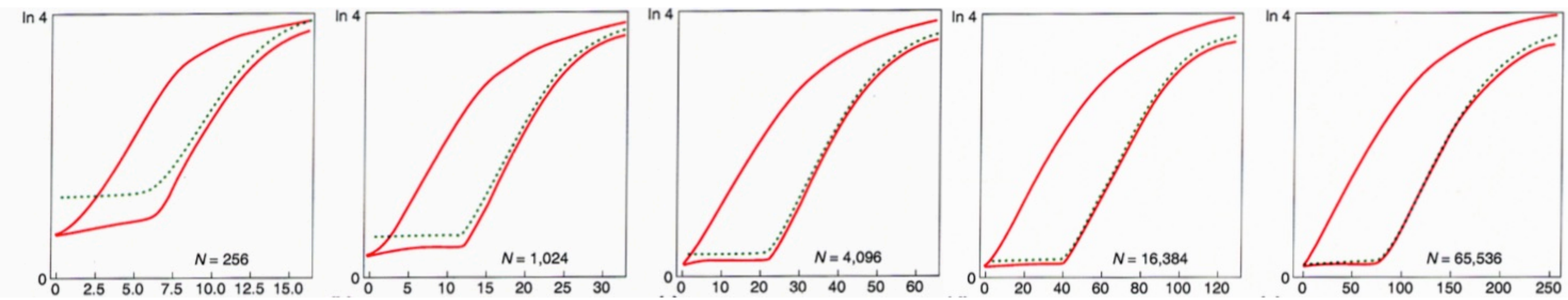
$$S_{Gibbs} = Nk\ln(e/\rho) \;\rightarrow \text{constant}$$

$$S_{Laboratory} = k\sum_L\left[\ln\left(e_{Lab} + v_{Lab}^2/2\right)/\rho_{Lab}\right]$$ Upper curve – wrong !

$$S_{Lagrangian} = k\sum_L\left[\ln\left(e_{Lag} + \left(v_{Lag} - \langle v\rangle\right)^2/2\right)/\rho_{Lag}\right]$$ Lower Curve - correct

Fluctuations in motion are kinetic energy . The equilibration is rapid ~ L / c rather than L^2 / D as would be expected for viscous or heat-conductive dissipation .

0 < S/Nk < ln 4 for N = { 2^8 , 2^{10} , 2^{12} , 2^{14} , 2^{16} }



0 < time < τ / 2

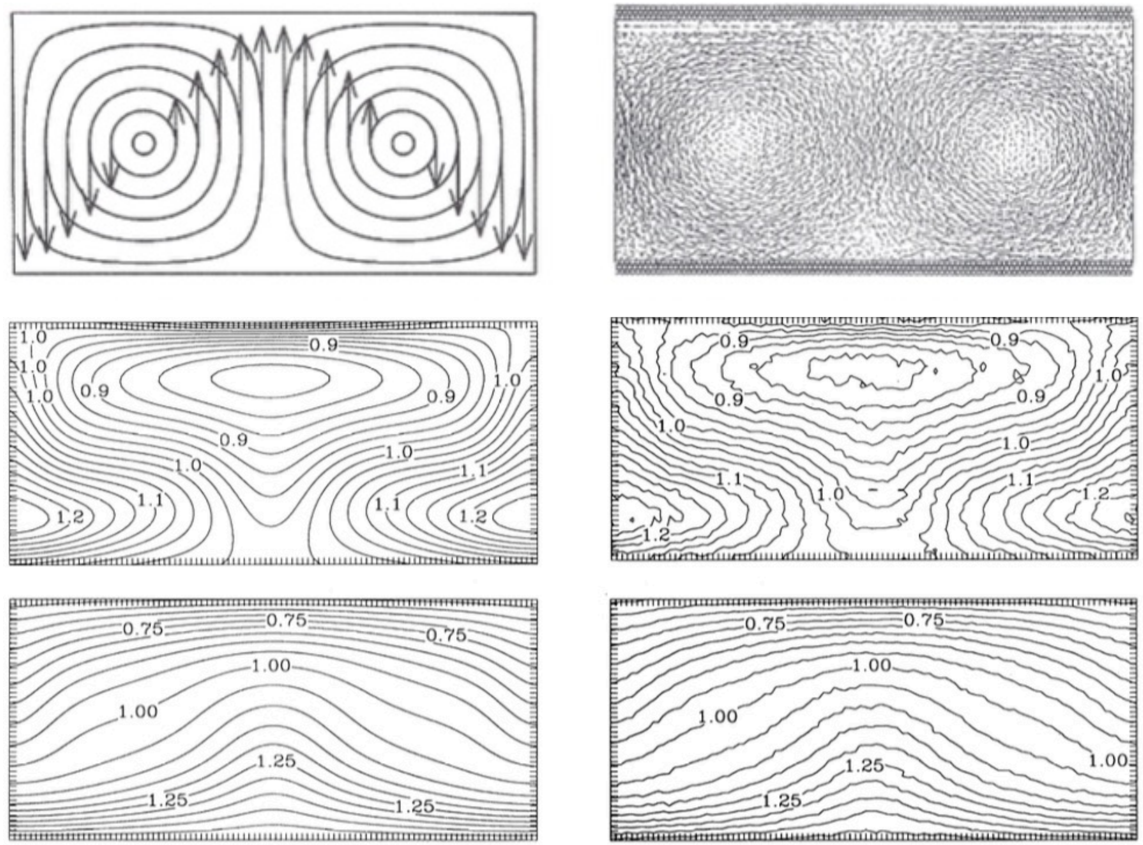
Rayleigh-Bénard Flow (Gravity & T gradient)
Finite-Difference (left) & Smooth Particles (right)

Oyeon Kum

Velocity

Density

Temperature



Gravity

T = 0.5

T = 1.5

$$\mathcal{R} = \frac{gh^3}{(\upsilon D_T)} = \left(\frac{40}{0.4}\right)^2 = 10,000\ ;\ \frac{\Delta T}{\langle T \rangle} = 1\ ;\ \upsilon = D_T$$

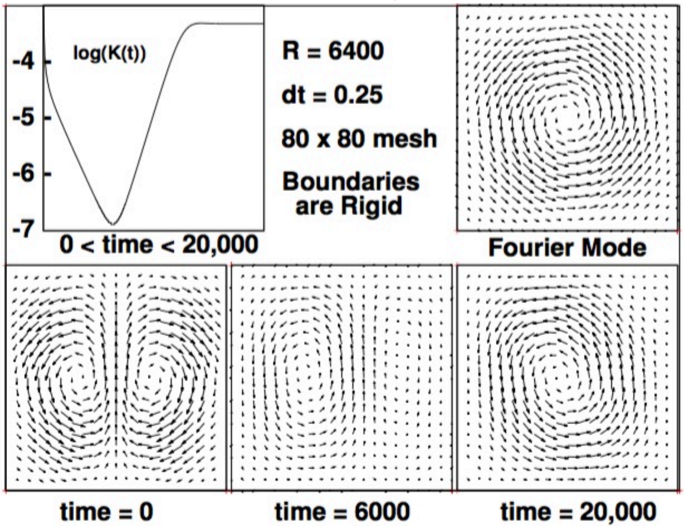
5000 smooth particles & field quantities computed on a grid

Rayleigh-Bénard Flows produce many types of Solutions

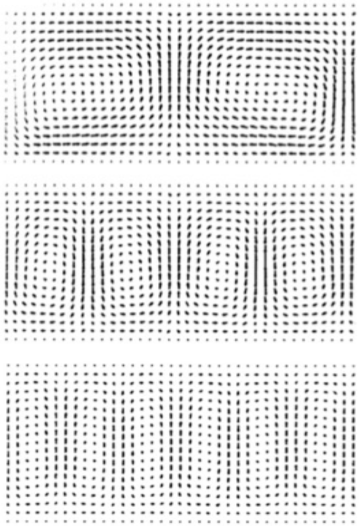
Vic Castillo

(1996)

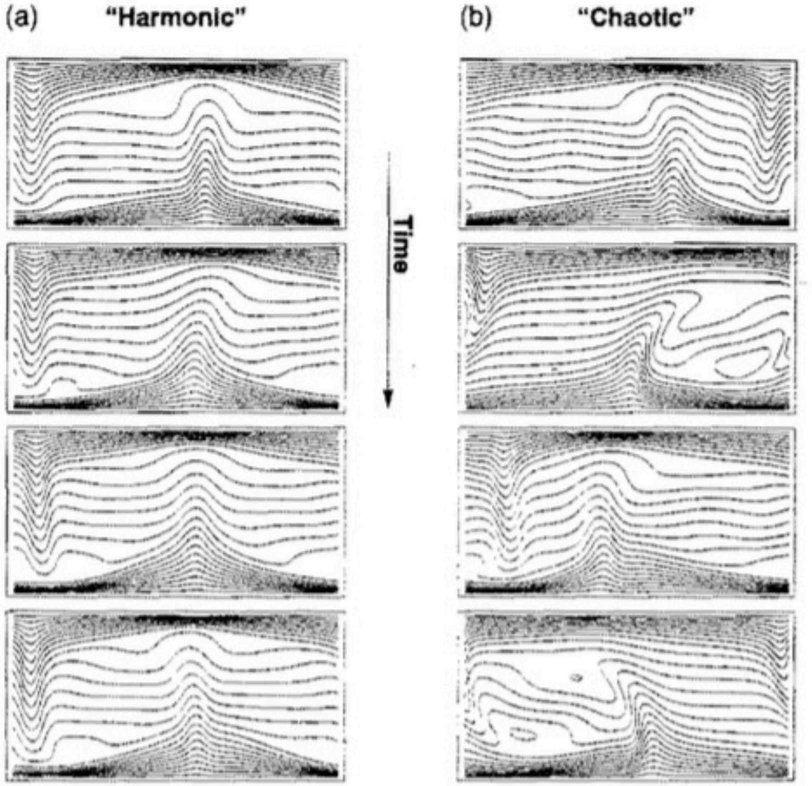
$\mathcal{R} = 6{,}400$



$\mathcal{R} = 40{,}000$

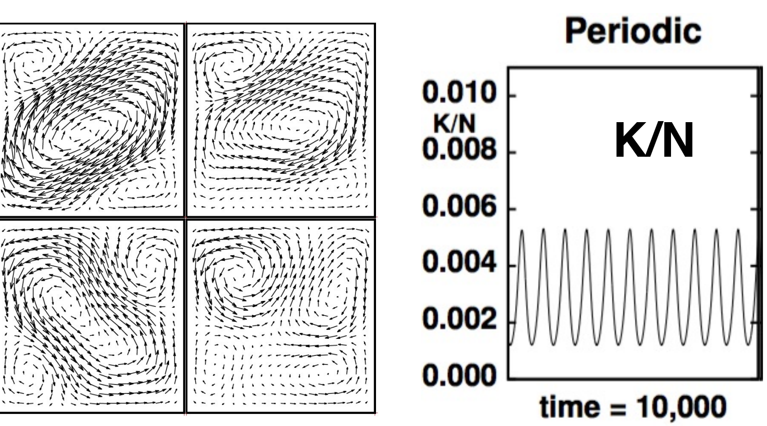


$\mathcal{R} = 200{,}000$



Temperature contours

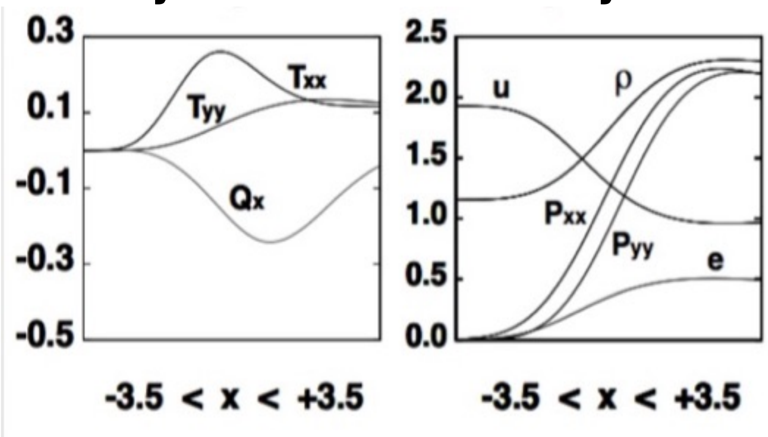
$\mathcal{R} = 160{,}000$ 80x80 zones



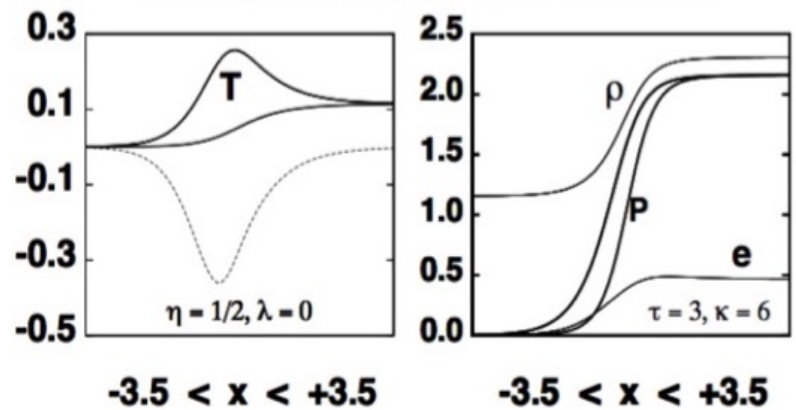
Shockwaves Revisited : Tensor Temperature, Time Delay, Work & Heat Division (2012)

Matching molecular dynamics & continuum mechanics → thesis research

Steady-State Molecular Dynamics



Continuum Mechanics



Time delayed responses in continuum mechanics :

Time-delayed stress response to strain rate (Maxwell)

$$\sigma + \tau_\sigma \dot{\sigma} = \eta \dot{\epsilon}$$

Time-delayed heat flux response to a thermal gradient (Cattaneo)

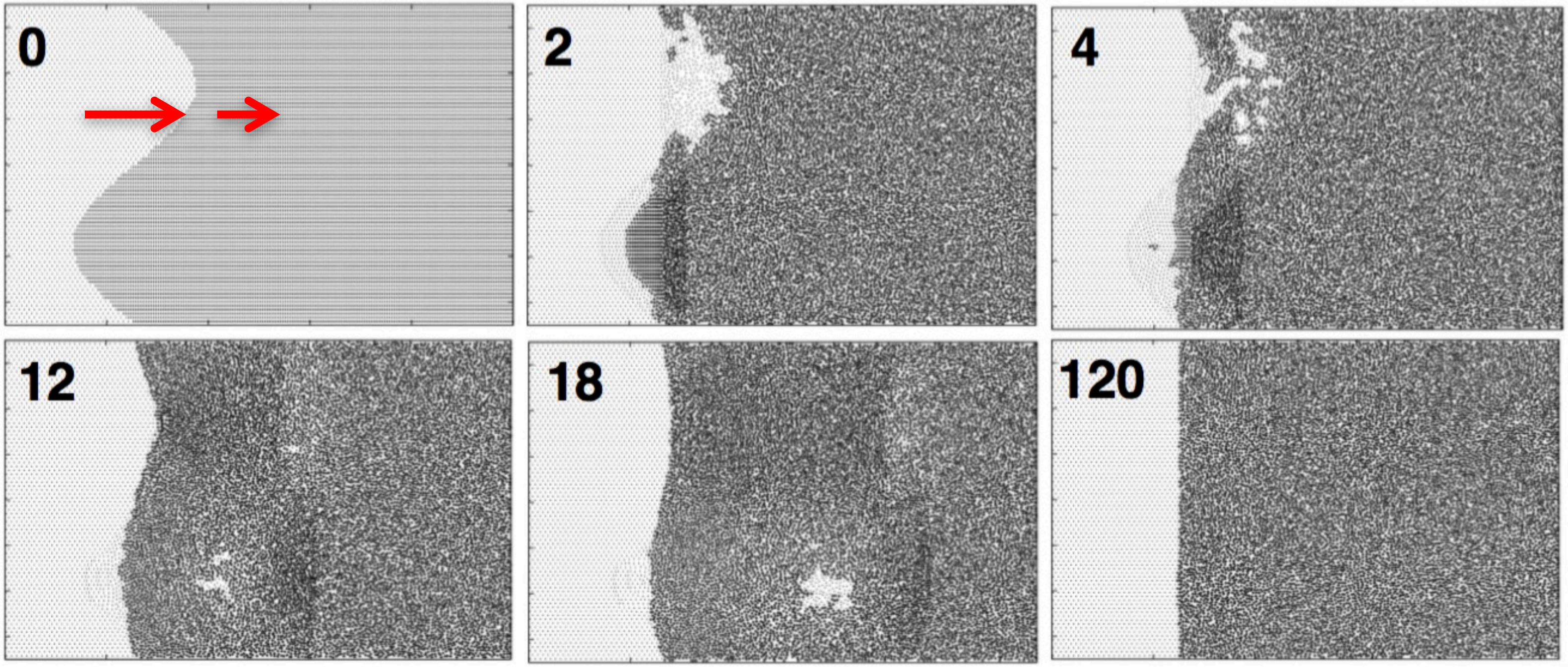
$$Q + \tau_Q \dot{Q} = -\kappa \nabla T$$

Division of heat and work into longitudinal and transverse components

Paco Uribe

Stability analysis for shockwaves with time delays

Shockwave Stability with Twofold Compression

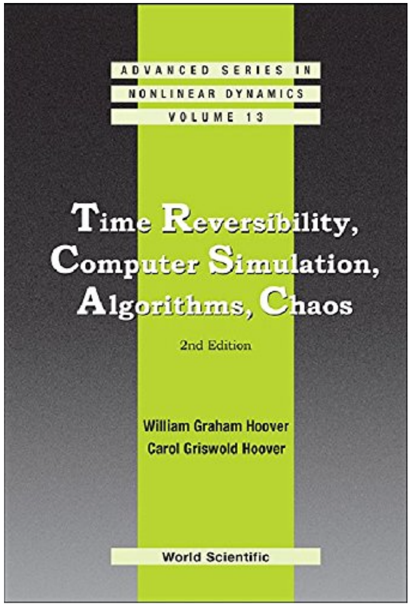


Lagrangian flow with shock fixed in location

Initial cold material is a triangular lattice . Hot material is an unstable square lattice at twice the cold material's density . The top = bottom boundaries are periodic .

[Notice the tensile waves that appear in the third, fourth, and fifth snapshots]

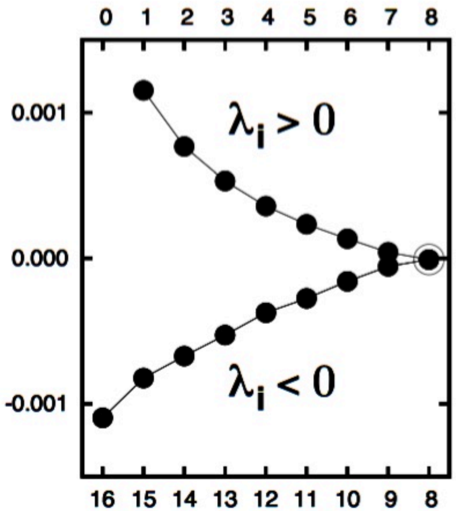
Most recent results are in Chapter 6

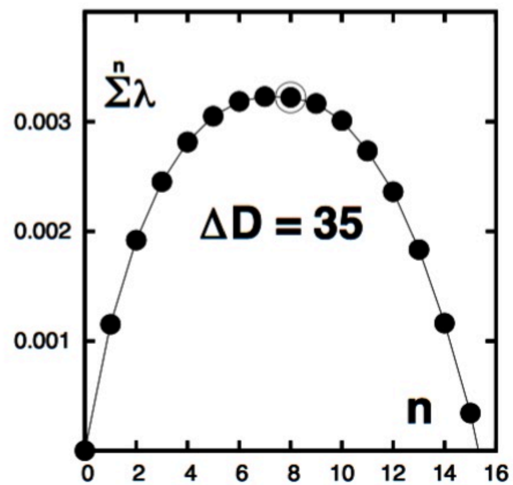


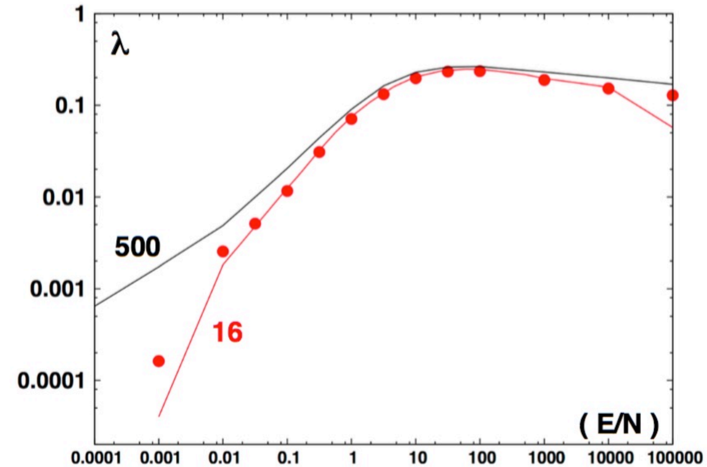
ϕ^4 Model for Chaotic Fourier Heat Conduction : Aoki & Kusnezov

$$\mathcal{H} = \sum \frac{p^2}{2} + \sum_{\text{pairs}} \frac{(q_{ij})^2}{2} + \sum \frac{q^4}{4}$$

ϕ^4 is a useful model with Fourier heat conduction



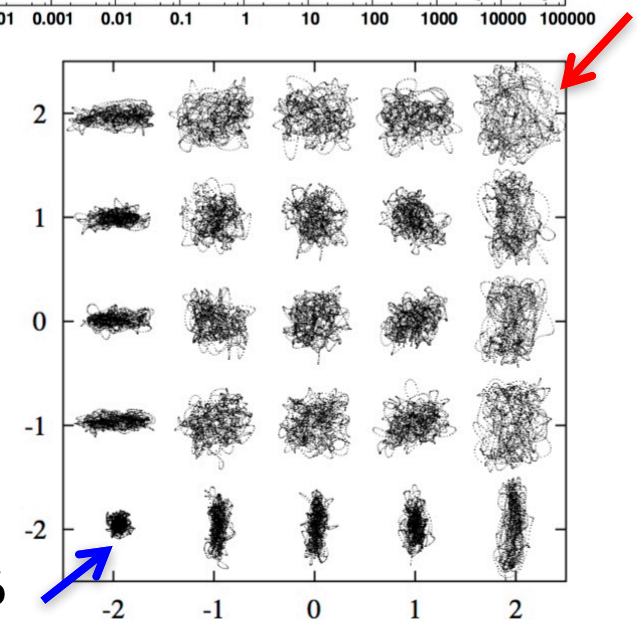




24 particle chain ; 50 dimensional phase space ;
Cold particle at 0.003 ; Hot particle at 0.027 .

$$\sum_{i=1}^{15} \lambda_i > 0 \; ; \; \sum_{i=1}^{16} \lambda_i < 0 \longrightarrow \Delta D = 35$$

102 dimensional phase space ;
1 cold particle, 1 hot particle



$\Delta D = 21.6$

Time-Reversible Deterministic Thermostats (Dresden 2002)

Measured heat transfer rate $\dot{Q}$ with seven thermostats using (6 x 4) (12 x 4) and (18 x 4) ϕ^4 models with 4 cold particles and 4 hot particles

Instantaneous Gauss' Principle

$$\dot{p} = F - \zeta p \ ; \ \zeta = \frac{\langle F \cdot p \rangle}{\langle p^2 \rangle}$$ p² control

$$\dot{p} = F - \zeta p^3 \ ; \ \zeta = \frac{\langle F \cdot p^3 \rangle}{\langle p^6 \rangle}$$ p⁴ control

CONCLUSIONS

$\dot{Q}$ & temperatures similar for two of the integral feedback thermostats : NH & HH

NH with one control variable is the simpler and is also easiest to use .

Integral Feedback

$$\dot{p} = F - \zeta p \ ; \ \dot{\zeta} = \langle p^2 \rangle - 1$$ p² control NH

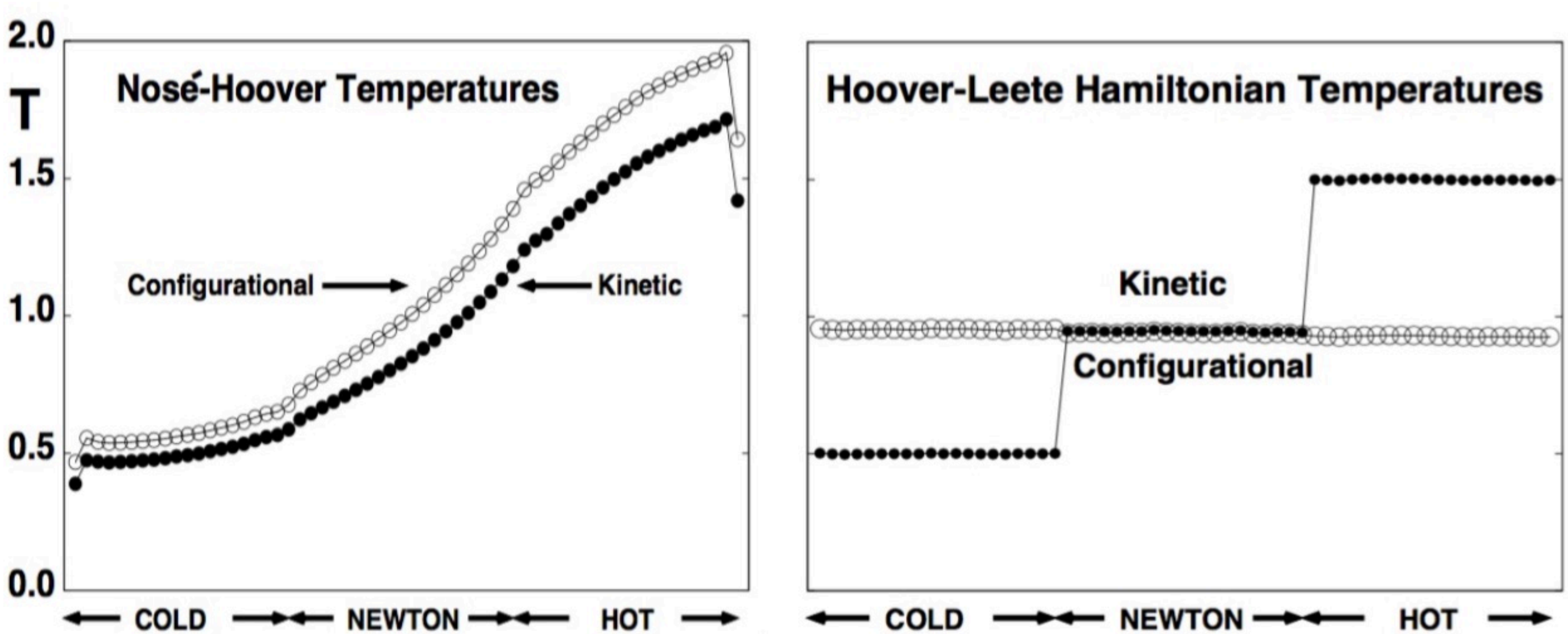
$$\dot{p} = F - \zeta p^3 \ ; \ \dot{\zeta} = \langle p^4 \rangle - 3\langle p^2 \rangle$$ cubic p⁴ control

$$\dot{p} = F - \zeta p - \xi p^3 \ ; \ \dot{\zeta} = \langle p^2 \rangle - 1 \quad \dot{\xi} = \langle p^4 \rangle - 3\langle p^2 \rangle$$ p² and p⁴ control HH

$$\dot{p} = F - \zeta p \ ; \ \dot{\zeta} = \langle p^2 \rangle - 1 - \zeta \xi \ ; \ \dot{\xi} = \langle \zeta^2 \rangle - 1$$ chain control MKT

$$\dot{p} = F - \zeta^3 p \ ; \ \dot{\zeta} = \langle p^2 \rangle - 1$$ cubic (ζ^3) p² control

Hamiltonian Thermostats Do Not Promote Heat Flow (2013)



ϕ^4 chain with 20 cold particles , 20 Newtonian particles , 20 hot particles

Nosé-Hoover mechanics for the two reservoir temperatures is not Hamiltonian-based and consequently can support heat flow .
Three Hamiltonian-based thermostats fail the test for heat flow :

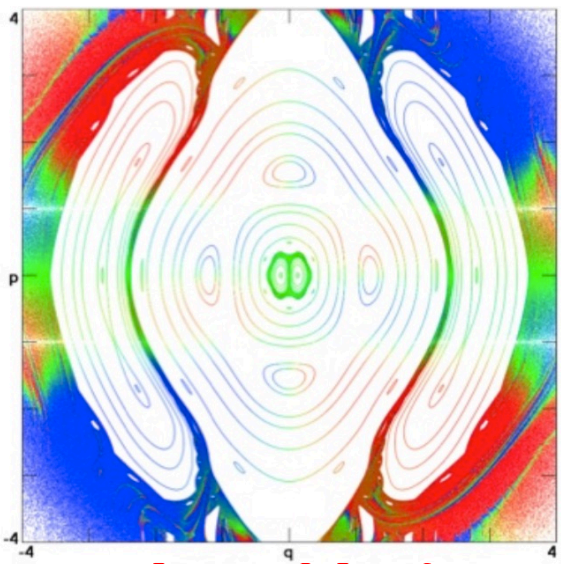
- **Nosé : T constrained by an additional degree of freedom, { s, p_s }**
- **Hoover-Leete isokinetic : $K(\dot{q})$ constrained by Lagrange multiplier**
- **Travis-Braga thermostat : $kT_c = \langle F^2 \rangle / \langle \nabla^2 \mathcal{H} \rangle$ likewise constrained**

Small System Ergodicity : Heat Conducting Oscillator (2015)

A single weak-control variable led to ergodicity in three phase-space dimensions (q,p,ζ) . The “0532 Model” is a simple example that we discovered .

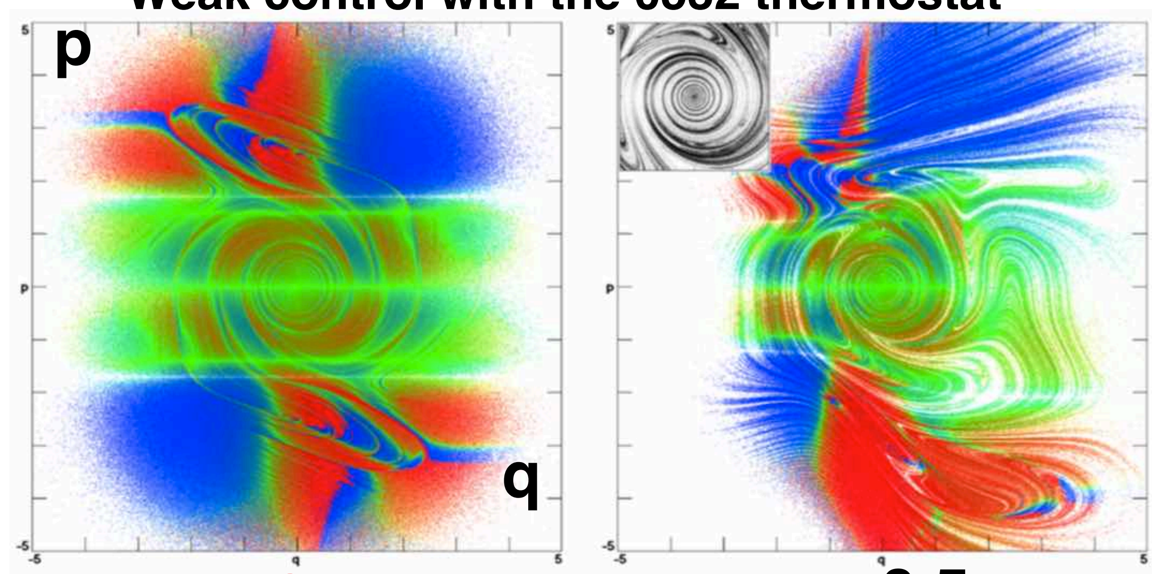
$$\lambda(t)_{min} \leq \lambda(t) \leq \lambda(t)_{max}$$

Nosé-Hoover thermostat



NOT ERGODIC !

Weak control with the 0532 thermostat



ERGODIC !

ε = 0.5

$$\dot{q} = p \,;\, \dot{p} = -q - \zeta p \,;$$

$$\dot{\zeta} = \frac{p^2}{T} - 1$$

$$\dot{q} = p \,;\; \dot{p} = -q - \zeta\left[0.05p + 0.32\left(\frac{p^3}{T}\right)\right] \;;$$

$$\dot{\zeta} = 0.05\left[\left(\frac{p^2}{T}\right) - 1\right] + 0.32\left[\left(\frac{p^4}{T^2}\right) - 3\left(\frac{p^2}{T}\right)\right]$$

2016 Ian Snook Prizes : Small System Ergodicity

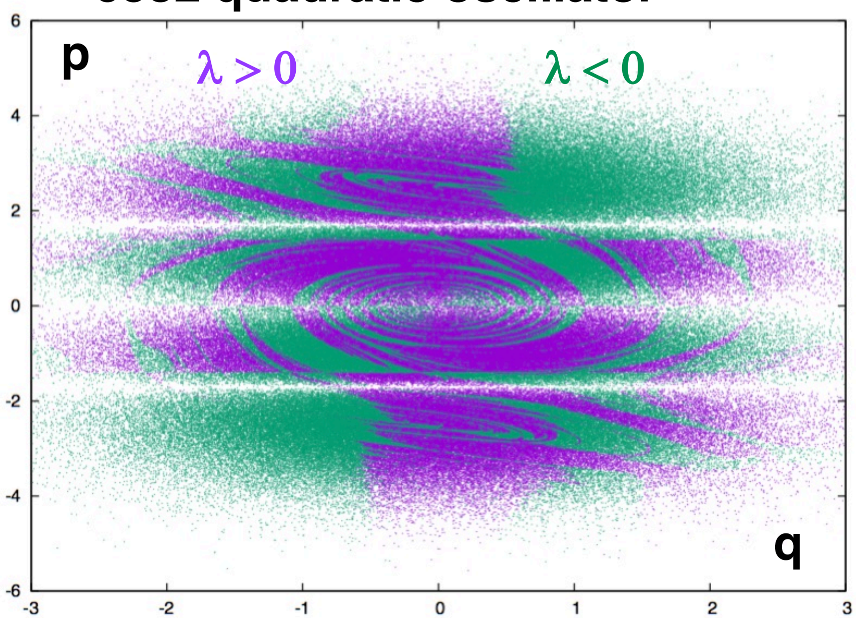
Prizes to be awarded for the most interesting paper describing <u>singly-thermostated</u> canonical systems . $500 from Bill and Carol Hoover and $500 from the Poznan Supercomputing & Networking Center as described in the arXiv and at cmst.eu .

$$\dot{q} = p \; ; \; \dot{p} = \underline{-q} - \zeta\left[0.05p + 0.32\left(\frac{p^3}{T}\right)\right] \qquad \dot{q} = p \; ; \; \dot{p} = \underline{-q^3} - \zeta\left[0.05p + 0.32\left(\frac{p^3}{T}\right)\right]$$

Weak control : $\dot{\zeta} = 0.05\left[\left(\frac{p^2}{T}\right) - 1\right] + 0.32\left[\left(\frac{p^4}{T^2}\right) - 3\left(\frac{p^2}{T}\right)\right]$

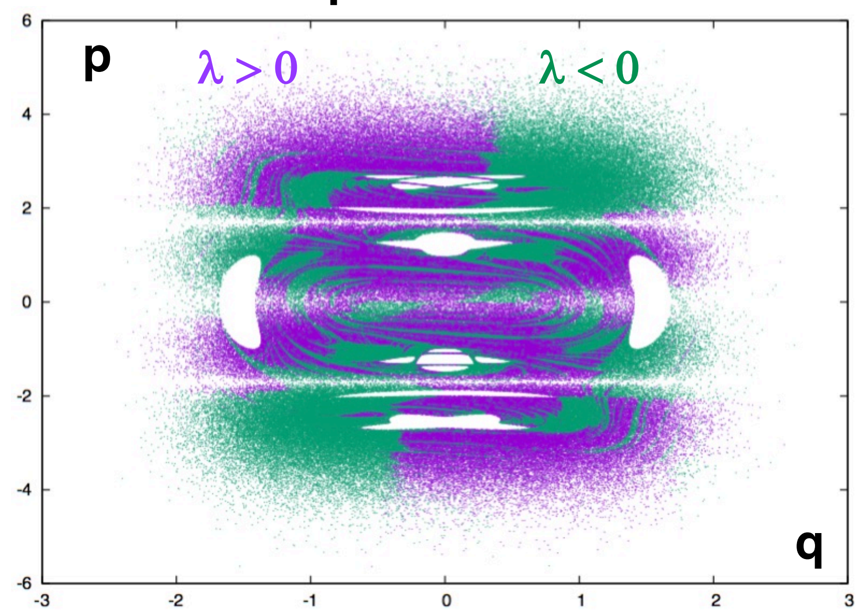
Ergodic

0532 quadratic oscillator

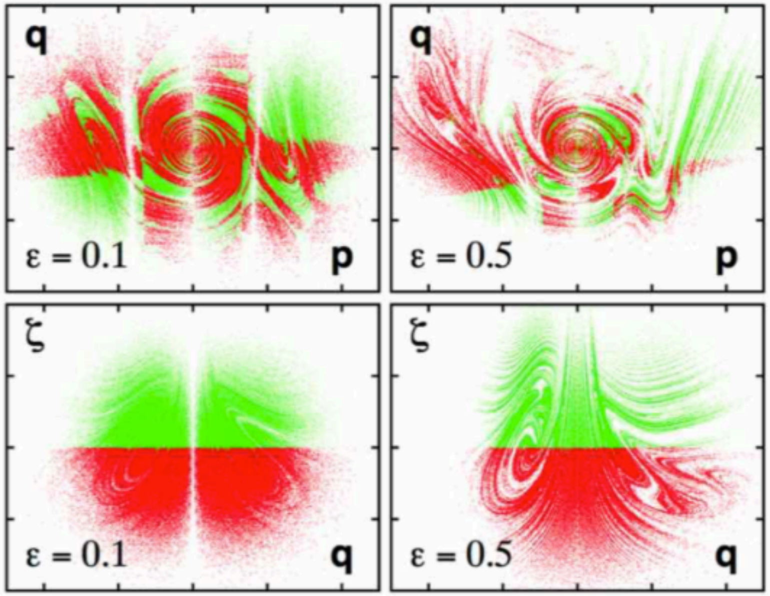


Nonergodic

0532 quartic oscillator



Collaborations : Are a **Good Thing !**



Clint Sprott

Old Faithful and the Baidurya Bhattacharyas

Puneet Patra