An Appreciation of Berni Julien Alder

by William Graham Hoover, Ruby Valley Nevada

1. PreHistory at Ann Arbor and Durham
2. Los Alamos *versus* Livermore
3. Berni → Francis Ree, Dave Young, Brad Holian
4. Teller Tech Prof → Bill Ashurst, NEMD
5. Shuichi Nosé → Carol and Thermostats
6. Symmetry Breaking → Posch and Sprott
7. 2015 Snook Prize
8. Berni's Ongoing Legacy

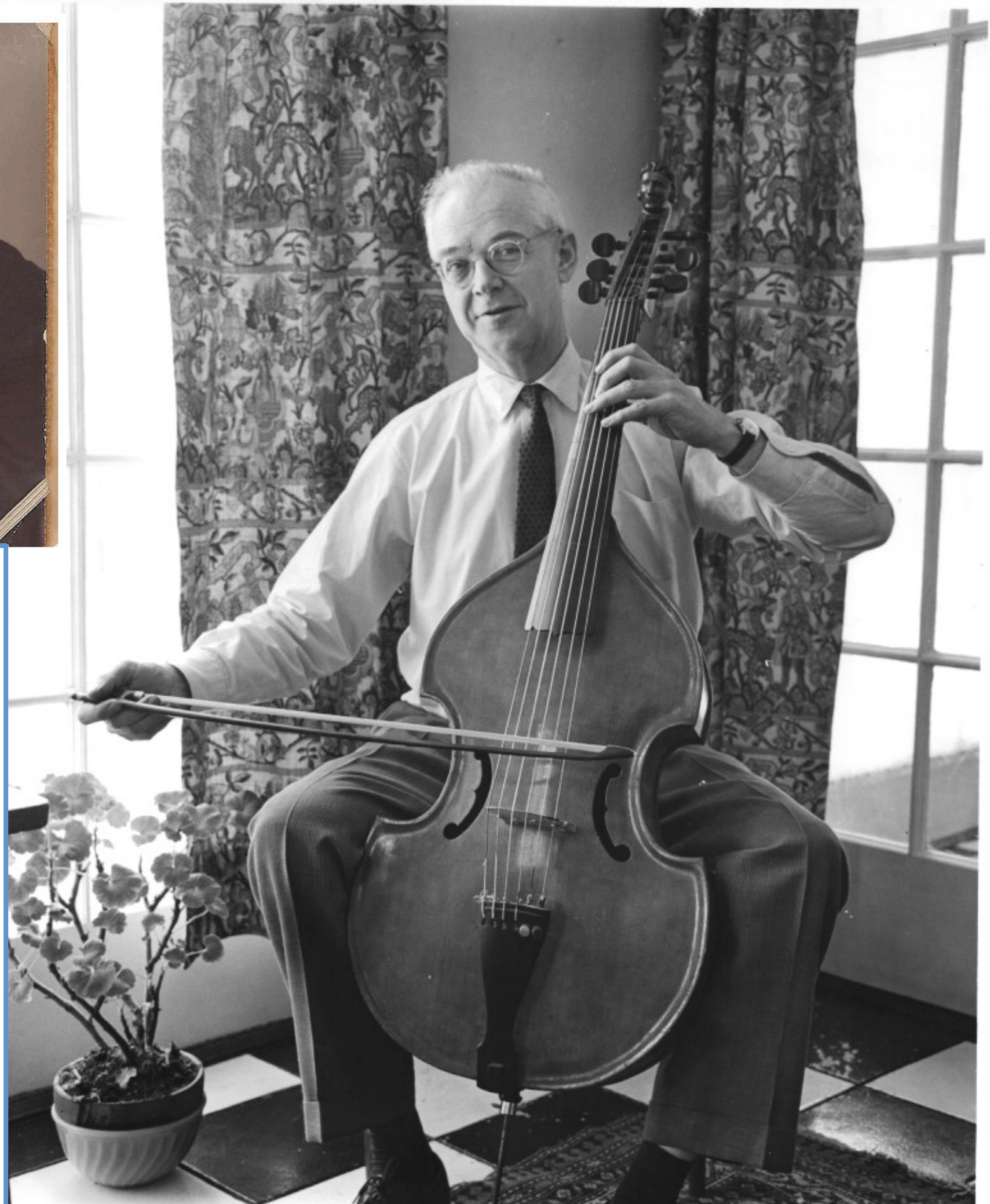
Washington DC 1944

Mary Frances Wolfe Hoover
Radcliffe '29

Edgar Malone Hoover Junior
Harvard '28

To Ann Arbor MI in 1936

Pittsburgh PA 1960-1972 →

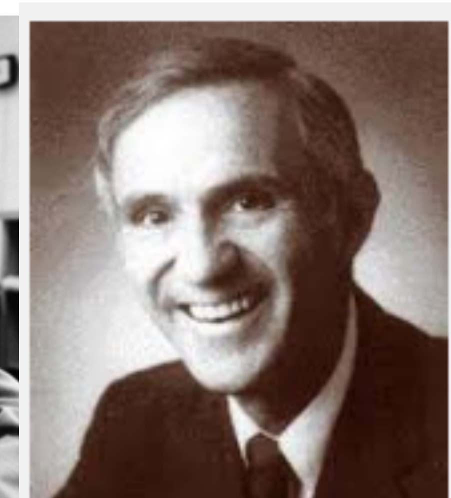


#1: PreHistory at Ann Arbor and Durham

EMH [OPA, Navy, OSS, CIA, Council of Economic Advisors]

WGH [Oberlin ’58 ; UMichigan PhD ’61]

George Uhlenbeck Kinetic Theory
Andrew De Rocco Statistical Mechanics
FORTRAN : three-hour evening lecture
IBM 704 + Michigan Algorithmic Decoder



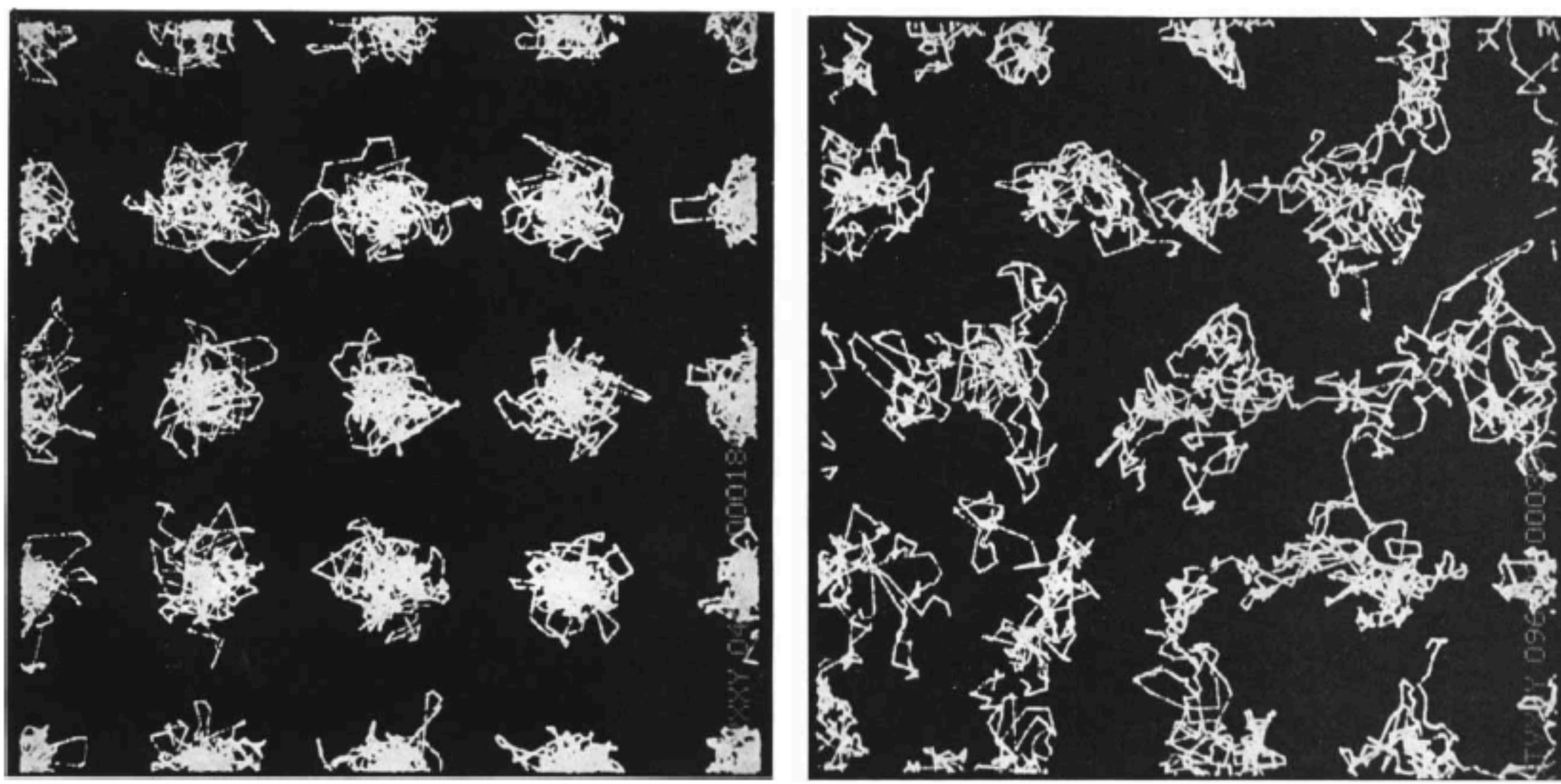
Line printer output following a MAD compiler error on an IBM 704 computer at the University of Michigan, c. 1960

MM →

Molecular Motions

Berni Alder and Tom Wainwright Scientific American 1959

One of the aims of molecular physics is to account for the bulk properties of matter in terms of the behavior of its particles. High-speed computers are helping physicists realize this goal



PostDoctoral Year at Duke University with Jacques Poirier ,

Leading to Interviews with Bill Wood (LANL) and Berni (LRL)

#2: $1100/month @ LANL versus $1300/month @ LRL
Easy decision, using what our neighbors call "Cowboy Math"
At LRL I met and worked with David Young and Francis Ree

First West Coast Publication, explaining the melting of hard disks :

PHYSICAL REVIEW LETTERS

VOLUME 11 | 15 SEPTEMBER 1963 | NUMBER 6

COOPERATIVE MOTION OF HARD DISKS LEADING TO MELTING

B. J. Alder, W. G. Hoover, and T. E. Wainwright
Lawrence Radiation Laboratory, University of California, Livermore, California

Movies of Melting Hard Disks showed Cooperative Motion of *rows* of disks. Using the corresponding Partition Function [phase-space integral] gave :

Transition Pressure and Density correct to few % .
van der Waals' loop for solid-fluid transition .
Expansion of solid properties in powers of v_f .

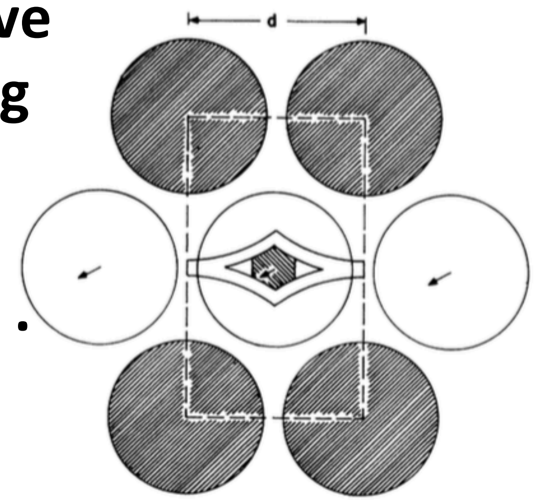


FIG. 1. Configurations of the cell of elastic disks. The shaded particles are fixed. Free areas available to the central wanderer are shown.

#3: LRL : Tom Wainwright, Francis Ree, Brad Holian, David Young, Hugh DeWitt, Harry Sahlin, Alan Hindmarsh, . . .

1960s :

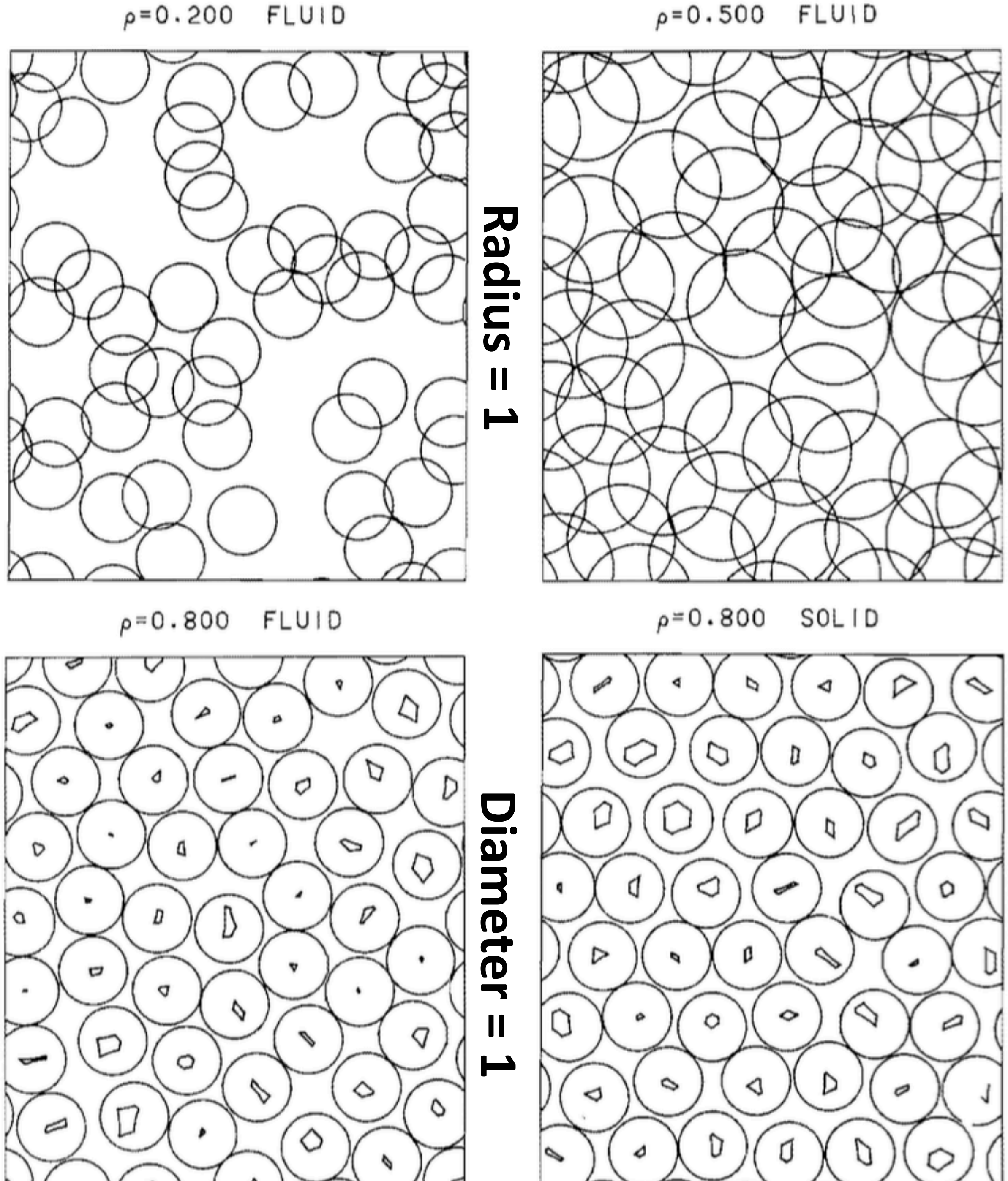
- Many joint papers with Berni, Tom, Francis, and David
- Two of the 18 “Studies in Molecular Dynamics” [1959-1980]
- Yin Yin abalone plus more melting of hard disks and hard spheres

#4: Transition to University Professor at DAS

1970s :

- In 1971 Berni → Professorship at Dept of Applied Science !
- Teaching, research contracts, sabbaticals, students (Carol !)
- West Coast Statistical Mechanics meetings with colleagues
- Gordon Conferences → Bob Watts : Australia 1977-1978

OZ: Nathan Edgar Hoover and Kenton Hanson (UCB) we found A **percolation transition** for disks At 1/4 the close-packed density .



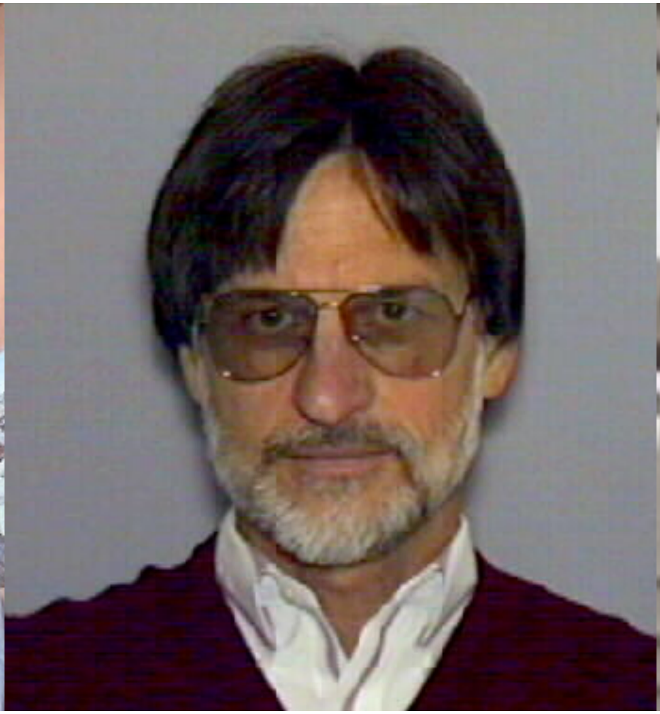
#4: Physics in the Department of Applied Science :

Bill Ashurst (NEMD → transport coefficients and fracture)

Bill Moran (fracture, continuum mechanics, dynamical systems)

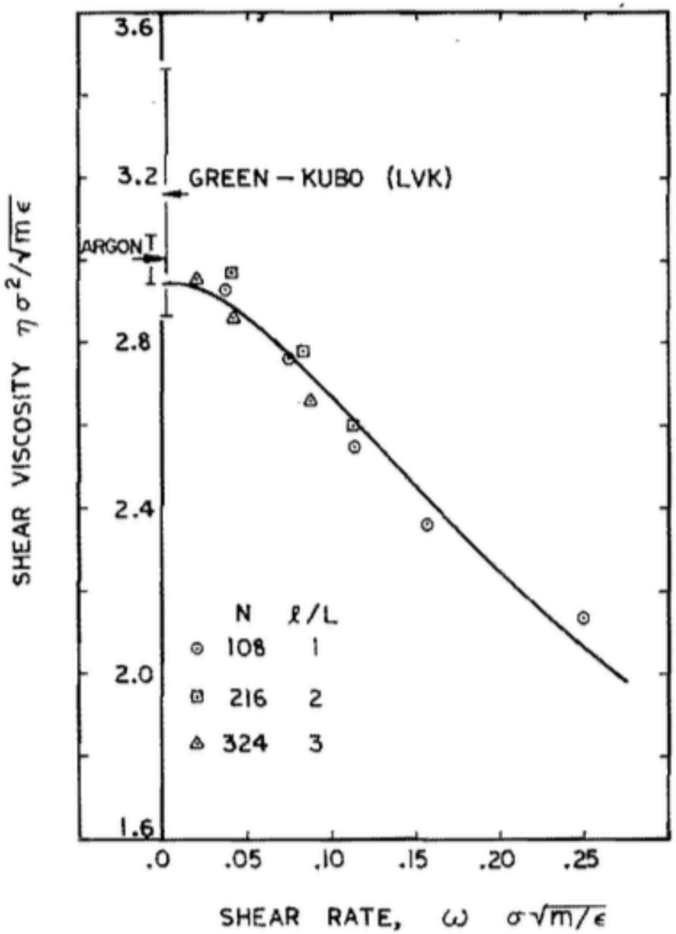
Brad Holian (shockwaves and dynamical systems)

Brad Holian   Bill Ashurst   Bill Moran

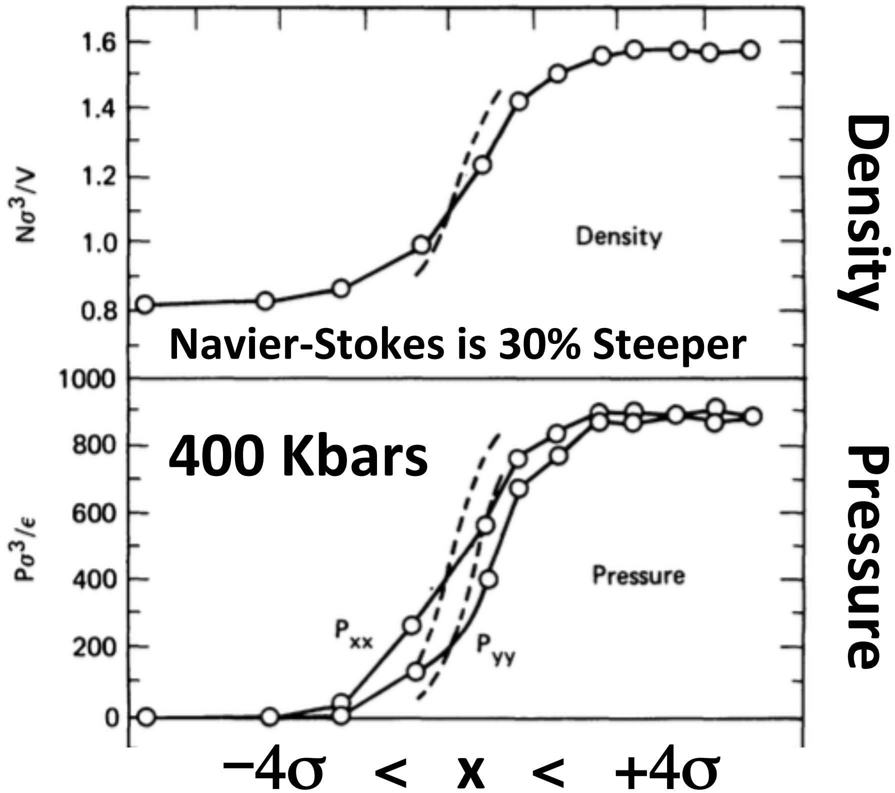


#4: Molecular Dynamics with Ashurst, Holian, Straub

Molecular Dynamics with Periodic Isothermal shear
→ "Shear-Thinning"



Molecular Dynamics with Steady-State Shockwave
→ "Shear-Thickening"



1984 →

#5: Shuichi Nosé publishes 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

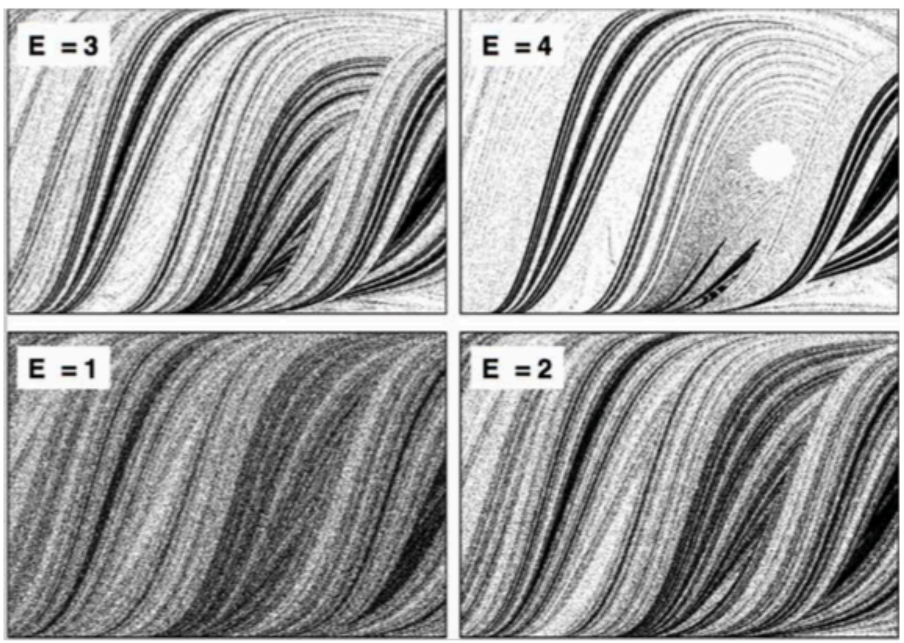
1987: Galton Board with Bill Moran
→ Nonequilibrium Steady State

Time-Reversible Isokinetic Dynamics
→ Gives fractal distributions !

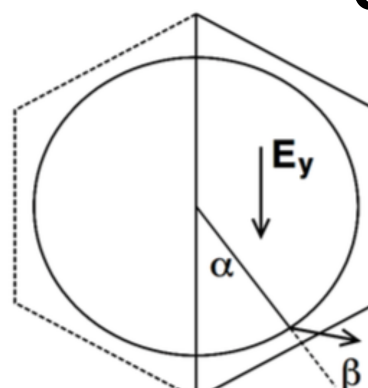
$$dx/dt = u \; ; \quad du/dt = -\zeta u \; ;$$
$$dy/dt = v \; ; \; dv/dt = -E - \zeta v$$

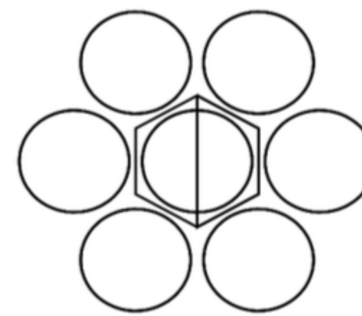
Clint Sprott

$-1 < \sin(\beta) < +1$



$0 < \alpha < \pi$





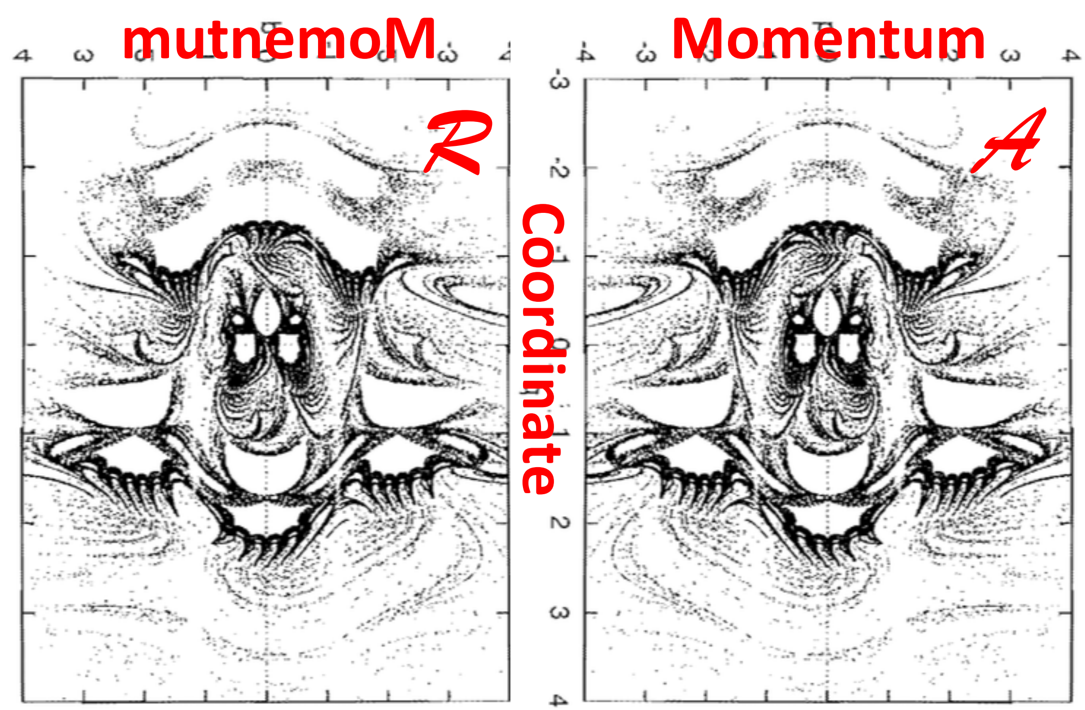
#6: Nosé's thermostat → Repellor-to-Attractor Flows

Dissipation ← Time-Reversible Deterministic Mechanics

Simplest Case : Oscillator with a Temperature Gradient :

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

Obeys Second Law and generates very nice fractals

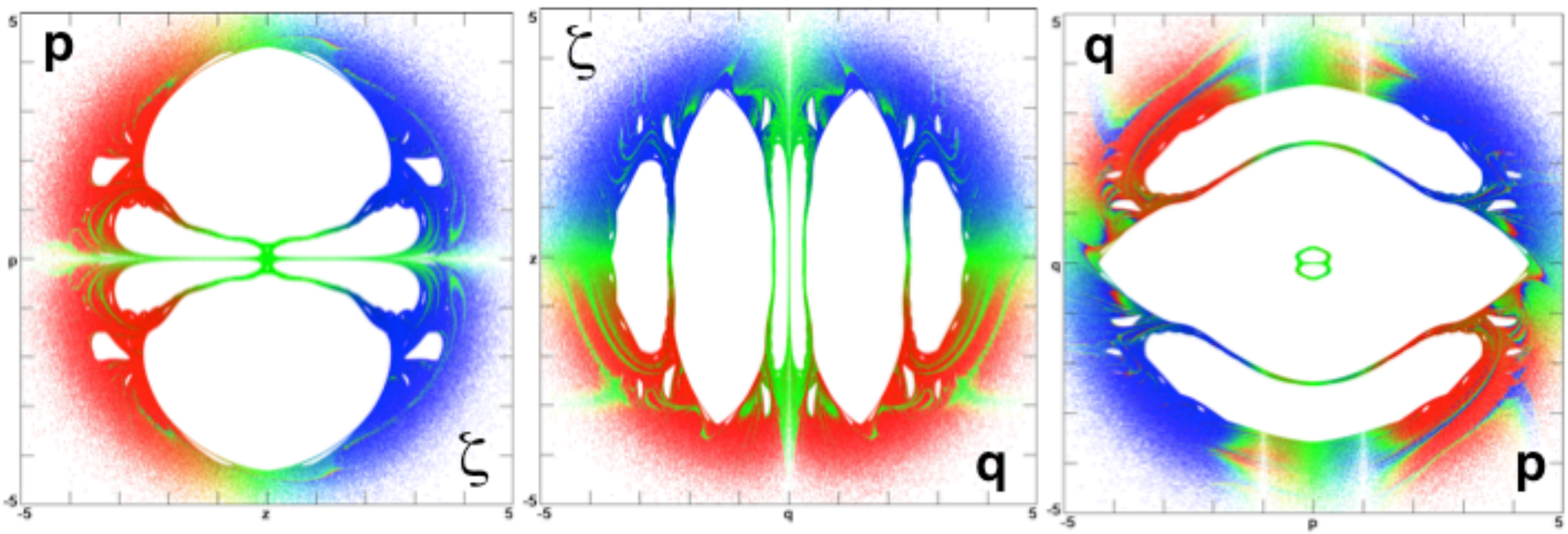


Harald Posch's 65^{th} Birthday -- Wien 2007

#6: Back to the Ergodic Oscillator Problem in the Silver State

Nosé-Hoover dynamics is consistent with $e^{-E/kT}$, but . . .

$$dq/dt = p \; ; \; dp/dt = -q - \zeta p \; ; \; d\zeta/dt = [(p^2/mkT) - 1] :$$



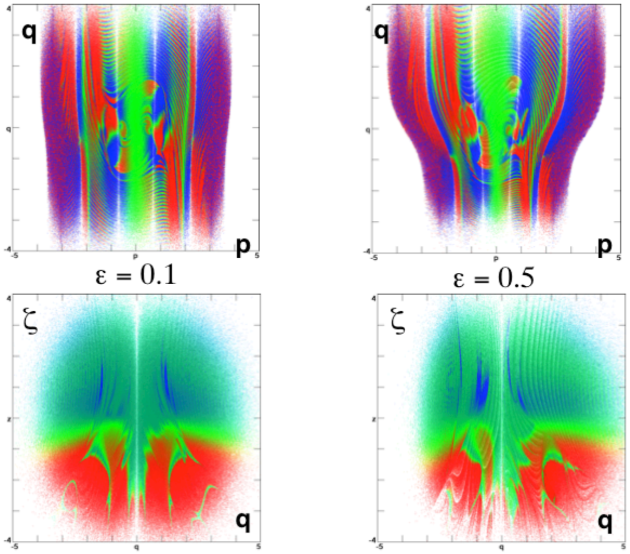
"Weak" cubic control of *two* moments → ergodicity :

$$dq/dt = p \; ; \; dp/dt = - q - \zeta [Ap + B(p^3/T)] \; ;$$

$$d\zeta/dt = A[(p^2/T) - 1] + B[(p^4/T^2) - 3(p^2/T)]$$

and still consistent with $e^{-E/kT}$!

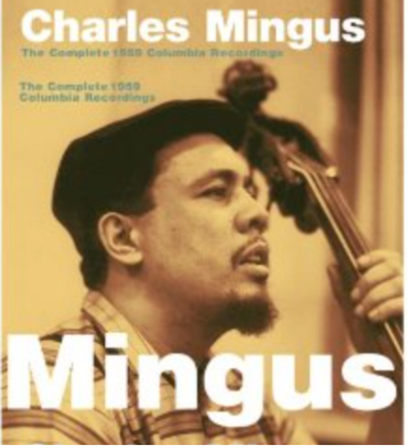
Collaborations : Are a Good Thing !



Old Faithful and the Baidurya Bhattacharyas

Clint Sprott

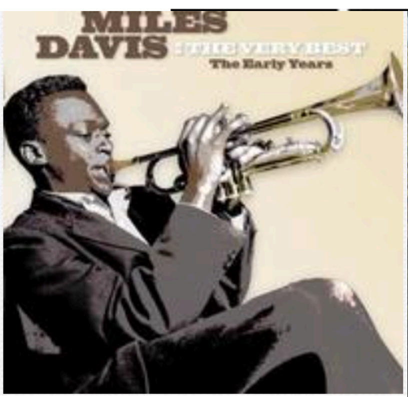
Puneet Patra



#7: 2015 Ian Snook Prize :

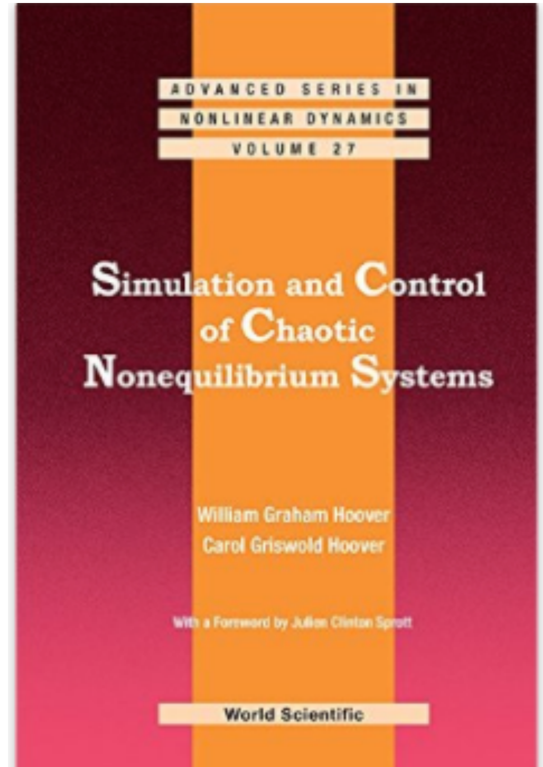
$1000 US for the most interesting Ergodic Time-Reversible Map Of Unit Square Into Itself

← 1996 **Computational Methods in Science and Technology 21 , to appear (2015)**



2007 with Ian & Marie →

#8: Berni's Ongoing Legacy as a Reliable Guide :



1. Identify an Interesting Problem ,

2. Make a "Horseback Guess" .

3. Carry out simulations to validate the Guess ,

4. Describe the Results in intuitive terms ,

using Words rather than equations .

Thank you Berni ! Happy Birthday #90 !