From Ann Arbor to Sheffield : Around the World in 80 Years . I . William Graham Hoover, Ruby Valley Nevada [Thanks to Karl Travis and Fernando Bresme]

- 1. Ann Arbor to Washington D C for WW II
- 2. Washington D C to Ann Arbor for PhD
- 3. Ann Arbor to Livermore via Durham
- 4. Livermore in the 1960s
- 5. Livermore/Australia in the 1970s
- 6. Livermore/Austria in the 1980s
- 7. Some Recent Collaborations

1. Ann Arbor to Washington D C [1936 to 1953]





Edgar Malone Hoover Jr taught econometrics at the University of Michigan until World War II \rightarrow D C

Classroom Tools from the 1940s





To Washington (as well as Germany) Pittsburgh (the 1960s) → California

2. Washington D C to Ann Arbor*via* Oberlin Early Mentors [1953 to 1961]

Woodrow Wilson High School



← Louise Stull aka "Quiz Stull"



Oberlin College's Luke Steiner, also a fan of ``Pop Quizzes"



Harvard's Stuart Rice



3. Ann Arbor to Livermore via Durham (1958 – 1962)

Andy De Rocco



Doctoral Research on Virial Series involved working out 468 7-Body Mayers' Integrals, which were soon to be replaced by 171 Ree-Hoover Integrals. Using an IBM 704 with the Michigan Algorithmic Decoder.







Advice from Peter Debye → "Go to the Library. Read until you are puzzled. Then, pursue that Puzzle".

George Uhlenbeck's Advice : ← "That's a Standard Form !"



3. Ann Arbor to Livermore via Durham (1958 - 1962)

"Molecular Motions" 1959 Scientific American

"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 ."



Berni Alder



Tom Wainwright

4. Durham NC to Livermore CA (1961 – 2005) Molecular Dynamics and Monte Carlo for Hard Particles after a year of integral equations.



Postdoctoral Year at Duke University with Jacques Poirier The menthol smell of Salem cigarettes was pervasive. Continued work on cluster integrals and interviewed with Bill Wood at Los Alamos along with Berni and Tom at LRL. Lawrence Livermore was my choice, leading to work with Berni and Tom along with Eyring's student Francis Ree.



4. First West Coast Publication (1963) : Modeling 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 Correlated Motion of *rows* of disks. "Hexatic"? Approximate Partition Function [phase-space integral] gave :

Transition Pressure and Density correct to few % . van-der-Waals'-like loop for solid-fluid transition . Expansion of solid properties in powers of V/V_o - 1.



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

4. Hard-Disk Models at Livermore (1963 - 1968)

Correlated Cell Model for the Hard-Disk Solid and Hexatic Phases . Virial Series for the Fluid for disks and spheres 171 / 468 for B_7 . Clisby and McCoy used Ree-Hoover Diagrams, 4,980,756 / 9,743542 for B_{10} .



4. Solid + Hexatic + Fluid Phases for Hard Disks

Engel-Anderson-Glotzer-Isobe-Bernard-Krauth (2013 PRE)

Ronen Zangi + Stuart Rice





4. 1960s at the Livermore Laboratory :

NEMD

- Many joint papers with Berni, Tom, Francis, and David
- Two of the 18 "Studies in Molecular Dynamics" [1959-1980]
- 5.1970s: Transition to University Professor at DAS
- 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
- Interesting PhD projects with Ashurst, Moran, Kum, Castillo



5. Hard-Disk Free Volumes at Canberra Australia Sabbatical (1977 - 1978)



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Nathan Edgar Hoover and I and Kenton Hanson (UCB) found a percolation transition for disks at 1/4 the close-packed density.



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5. Molecular Dynamics - Ashurst, Holian, Ladd, Moran, and Straub



6. 1987: Galton Board with Bill Moran → Nonequilibrium Steady State

Time-Reversible Isokinetic Dynamics

→ Gives fractal distributions !

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



Clint Sprott (2015)





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



 $0 < \alpha < \pi$

6. Shuichi Nosé publishes two amazing papers in 1984 ! Canonical (isothermal) dynamics ← Hamiltonian (isoenergetic) mechanics .



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

Met Shuichi Nosé and Harald Posch → Two Sabbaticals in Japan (1989) & Wien (1985)





Notre Dame



6. Newton, Nosé, and Nosé-Hoover Nonergodic versions of p(q) for the One-Dimensional Harmonic Oscillator



(Posch, Vesely, Hoover, Physical Review A 1985 and 1986)

7. Ergodicity *can* be achieved by waiting 30 years and using "Weak Control" of $< p^2 > and < p^4 >$





Nosé-Hoover ($\zeta = 0$)



"0532 Model" ($\zeta = 0$)



Patra, Sprott, Hoovers: Molecular Physics+Molecular Simulation (2015-2016)

7. "The Invariant Tori of Knot Type and the Interlinked Invariant Tori in the Nosé-Hoover System" (2015) L Wang and X-S Yang, arXiv 1501.03375 and Chaos

Trefoil Knots *

Interlinked Tori or "Links"



7. Our Collaborations with Piotr Pieranski and Clint Sprott show amazing Complexity (as in Wang+Yang arXiv 2015)

Consider the relatively simple (qpζ) NH Knot type below. Note that this Knot is *not* the Ballantine UnKnot





7. Piotr Pieranski : Knot Specialist, an expert in Nosé-Hoover Topology





Tale of Three Tori :

The Yellow Torus Encircles the Red .

The Red Torus Encircles the Blue .