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
Toshio Kawai at Keio University

Lyapunov Spectrum
Strings of Springs
Harald Posch at University of Vienna

Evenings/Weekends

Taisuke Boku also at Keio
Sigeo Ihara at Hitachi

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

\[
\frac{\dot{f}}{f} = -\frac{\dot{\Omega}}{\Omega} = \dot{S}_{\text{ext}} / k = -\sum_k \lambda_k
\]

Nonequilibrium steady states:

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

Oscillator with \( T(q) = 1 + \varepsilon \tanh(q) \)

Negative Lyapunov sum → Dissipation

Irreversible Thermodynamics & Computational Fluid Dynamics

\[
\dot{s} = \left( \frac{\eta}{T} \right) \dot{\varepsilon}^2 + \kappa | \nabla \ln T |^2
\]

\[\mathcal{R} = gh^3 / \nu D_T\]
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!

\[ \frac{\partial \rho}{\partial t} \equiv -\nabla \cdot (\rho v) \]

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

We use fourth-order Runge-Kutta integration throughout.

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, $\tau$.

Internal Kinetic energy must be measured relative to the local velocity.

Four-fold expansion, Periodic boundaries, 128 x 128 grid for $\rho$ and $K$.

\[
\rho_g = \sum_j w_{gj} ; \quad P = \rho e = \rho T = \rho^2 / 2
\]
Convergence of the Free Expansion Entropy $N_k \ln(4)$

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

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

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

Upper curve – wrong!

Lower Curve - correct

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

$$0 < S/N_k < \ln 4 \quad \text{for} \quad N = \{2^8, 2^{10}, 2^{12}, 2^{14}, 2^{16}\}$$

$$0 < \text{time} < \tau/2$$
Rayleigh-Bénard Flow (Gravity & T gradient)  
Finite-Difference (left) & Smooth Particles (right)

Oyeon Kum

Velocity

density

Temperature

\[ \mathcal{R} = \frac{gh^3}{vD_T} = \left( \frac{40}{0.4} \right)^2 = 10,000; \quad \frac{\Delta T}{\langle T \rangle} = 1; \quad v = D_T \]

5000 smooth particles & field quantities computed on a grid
Rayleigh-Bénard Flows produce many types of Solutions

\[ \mathcal{R} = 6,400 \]

\[ \mathcal{R} = 40,000 \]

\[ \mathcal{R} = 200,000 \]

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

Temperature contours
Matching molecular dynamics & continuum mechanics \rightarrow thesis research

Steady-State Molecular Dynamics

Continuum Mechanics

Time delayed responses in continuum mechanics:

Time-delayed stress response to strain rate (Maxwell)

\[
\sigma + \tau_\sigma \dot{\sigma} = \eta \dot{\varepsilon}
\]

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

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.
$\phi^4$ Model for Chaotic Fourier Heat Conduction: Aoki & Kusnezov

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

$\phi^4$ 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.

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

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

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 $(6 \times 4)$, $(12 \times 4)$ and $(18 \times 4)$ $\phi^4$ models with 4 cold particles and 4 hot particles

**Instantaneous Gauss’ Principle**

\[
\dot{p} = F - \zeta p; \quad \zeta = \frac{\langle F \cdot p \rangle}{\langle p^2 \rangle} \quad \text{p}^2 \text{ control}
\]

\[
\dot{p} = F - \zeta p^3; \quad \zeta = \frac{\langle F \cdot p^3 \rangle}{\langle p^6 \rangle} \quad \text{p}^4 \text{ control}
\]

**Integral Feedback**

\[
\dot{p} = F - \zeta p; \quad \dot{\zeta} = \langle p^2 \rangle - 1 \quad \text{p}^2 \text{ control NH}
\]

\[
\dot{p} = F - \zeta p^3; \quad \dot{\zeta} = \langle p^4 \rangle - 3\langle p^2 \rangle \quad \text{cubic p}^4 \text{ control}
\]

\[
\dot{p} = F - \zeta p - \xi p^3; \quad \dot{\zeta} = \langle p^2 \rangle - 1 \quad \dot{\xi} = \langle p^4 \rangle - 3\langle p^2 \rangle \quad \text{p}^2 \text{ and p}^4 \text{ control HH}
\]

\[
\dot{p} = F - \zeta p; \quad \dot{\zeta} = \langle p^2 \rangle - 1 - \xi \dot{\xi} \quad \dot{\xi} = \langle \xi^2 \rangle - 1 \quad \text{chain control MKT}
\]

\[
\dot{p} = F - \zeta^3 p; \quad \dot{\zeta} = \langle p^2 \rangle - 1 \quad \text{cubic (} \zeta^3 \text{) p}^2 \text{ control}
\]

**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.

$\phi^4$ 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**: $kT_c = \langle F^2 \rangle / \langle \nabla^2 H \rangle$ likewise constrained
A single weak-control variable led to ergodicity in three phase-space dimensions \((q,p,\zeta)\). The “0532 Model” is a simple example that we discovered.

\[
\lambda(t)_{\text{min}} \leq \lambda(t) \leq \lambda(t)_{\text{max}}
\]

Nosé-Hoover thermostat

\[
\dot{q} = p; \quad \dot{p} = -q - \zeta p; \quad \dot{\zeta} = \frac{p^2}{T} - 1
\]

Weak control with the 0532 thermostat

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

\(\varepsilon = 0.5\)
2016 Ian Snook Prizes: Small System Ergodicity

Prizes to be awarded for the most interesting paper describing singly-thermostated 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.

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

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

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!

Old Faithful and the Baidurya Bhattacharyas

Clint Sprott
Puneet Patra