Two-Temperature Time-Delayed Dense-Fluid Shockwaves with Molecular Dynamics and Continuum Mechanics

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For more details see our preprint at the Website: http://williamhoover.info

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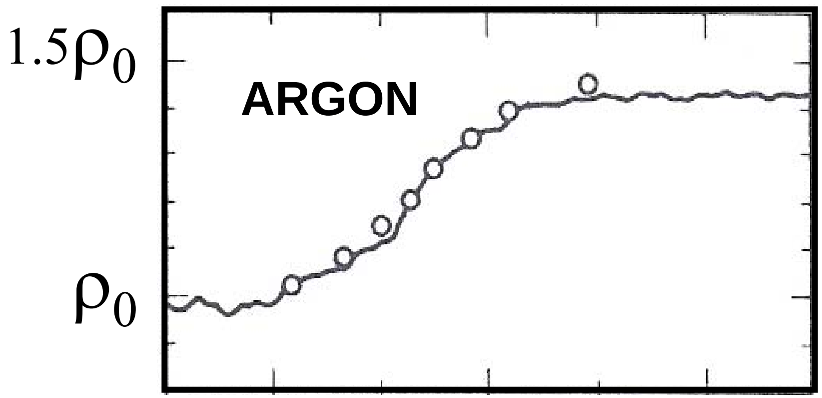
1. Shockwaves -- What, Why, and How?
2. [Reversible] Molecular Dynamics
3. [Irreversible] Continuum Mechanics
4. Solutions of Navier-Stokes → T(x)
5. Molecular Dynamics → T_{xx} and T_{yy}
6. New Model, with Solutions, Analysis
7. Reversibility and Stability in Shocks

1.1 What is a Shockwave?

Near-Discontinuity in { ρ, u, e, σ, T } :
Density, Velocity, Energy, Stress, and Temperature all Jump in a few Free Paths .



Phys Rev Letts
1979

Shockwaves provide a Simple Laboratory for studying nonlinear Transport . The boundary conditions are equilibrium . Curve is K&D MD .

1.2 Why are Shockwaves Useful?

Momentum Conservation → Pressure

Energy Conservation → E(P,V)

$$(P + \rho u^2)_{COLD} = (P + \rho u^2)_{HOT}$$

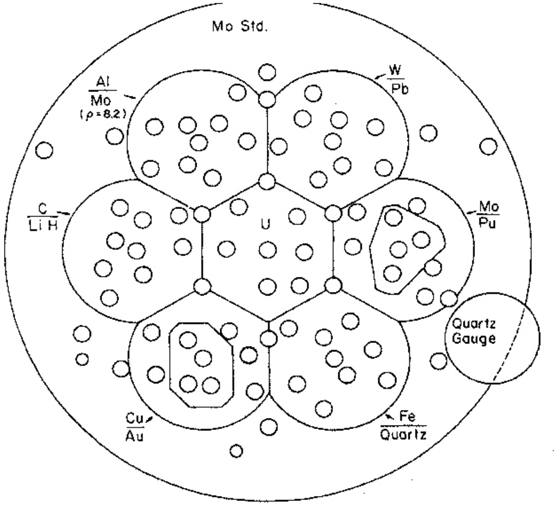
Inelastic Stagnation Results :

$$\rho_0 u_p^2 = P_{HOT}$$

$$\Delta e = \tfrac{1}{2}(u_p^2) = (PV)_{HOT}$$

1.3 How are Real Shocks Generated ? Explosives → Threefold Compression

12-60 Megabars: Al, C, Fe, LiH, SiO_2, U …



PHYSICAL REVIEW A VOLUME 29, NUMBER 3 MARCH 1984

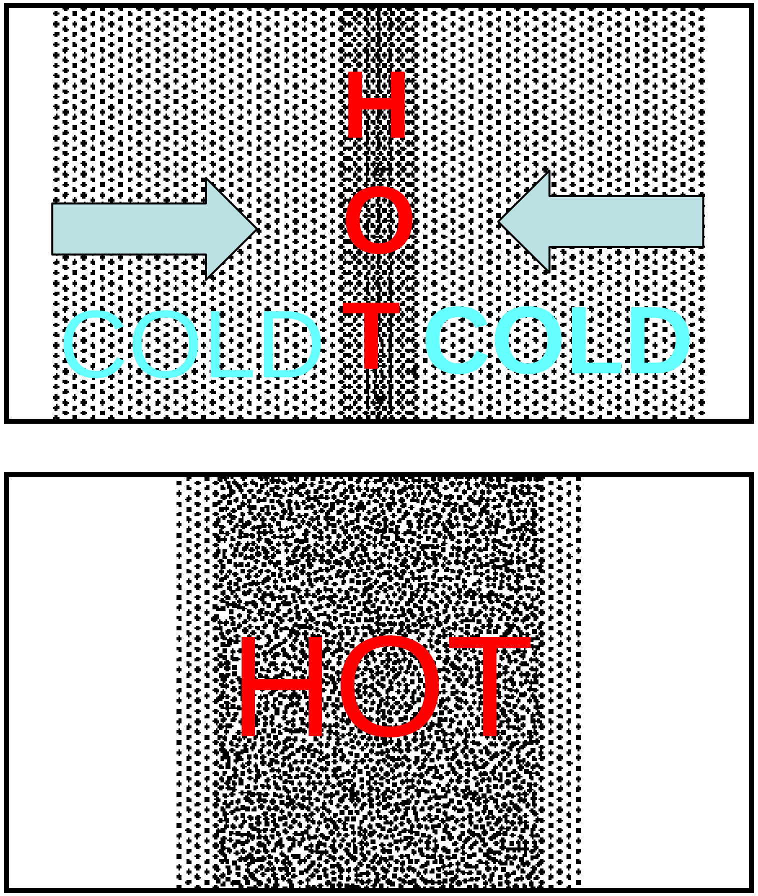
Shock-wave experiments at threefold compression

Charles E. Ragan III
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 3 June 1983)

2.1 Molecular Dynamics Techniques: Collision of Two Cold Blocks

$$u_p^2 / 2 \Rightarrow \Delta e$$

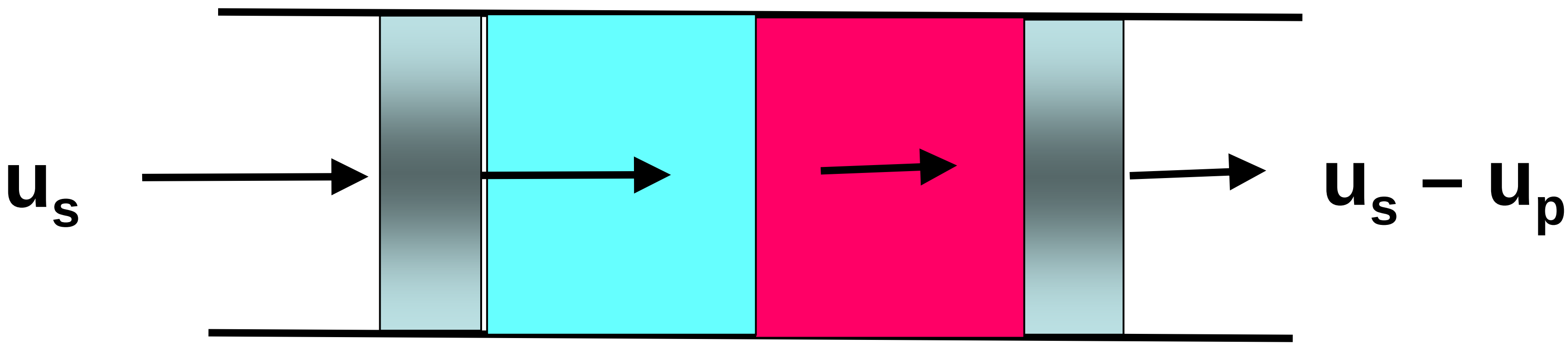
Conversion of
Kinetic Energy to
Internal Energy
[Heat]



2.2 Molecular Dynamics Techniques

1. Collision of two zero-pressure blocks

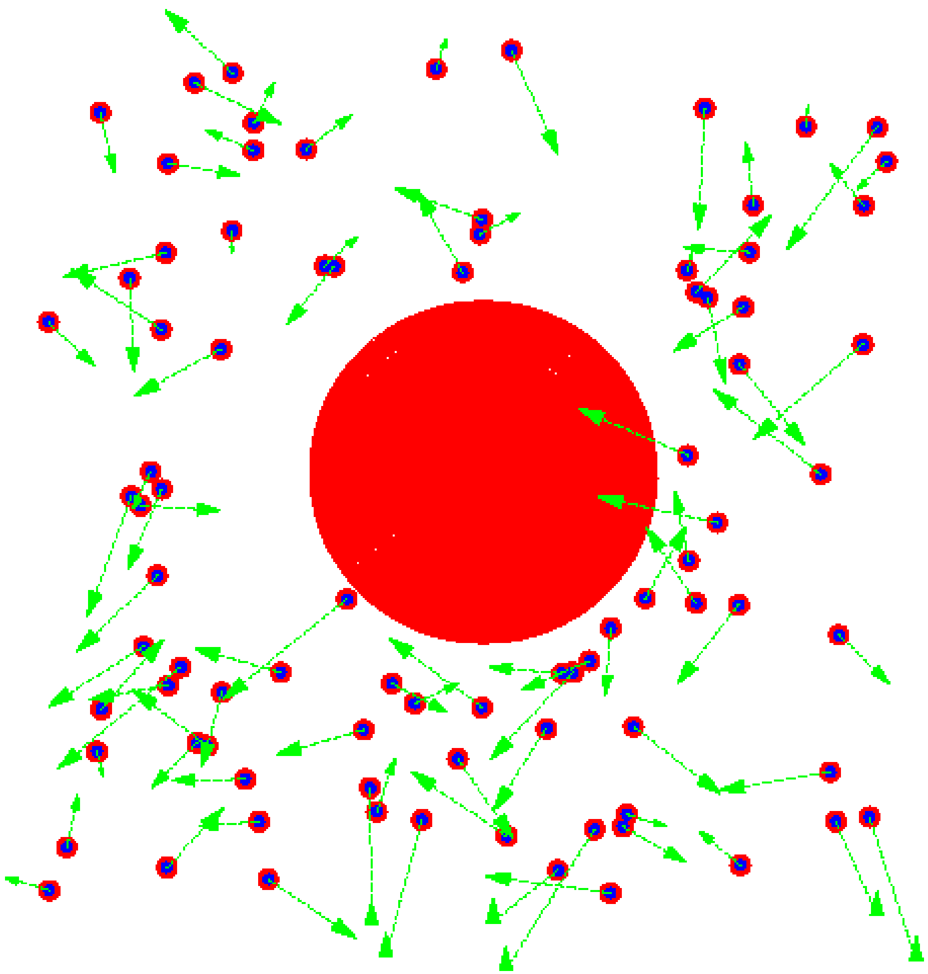
2. Two Treadmills @ u_s and [$u_s - u_p$] .



Use F = ma with 4th-order Runge-Kutta .

2.3 Analysis from Kinetic Theory & Statistical Mechanics

Ideal Gas Thermometer



Temperature is just the *comoving* Kinetic Energy .

2.4 T, P, and Q from Dynamics

$kT = \langle (p^2/m)_I \rangle$ **[Comoving p]**

$PV = \Sigma(pp/m)_I + \Sigma(rF)_{IJ}$

$QV = \Sigma(pe/m)_I + \Sigma(rF \cdot p/m)_{IJ}$

$\{ m[r(t+dt) - 2r(t) + r(t-dt)] = F(t)(dt)^2 \}$

Evidently the dynamics is time-reversible and can even be made *bit-reversible* .

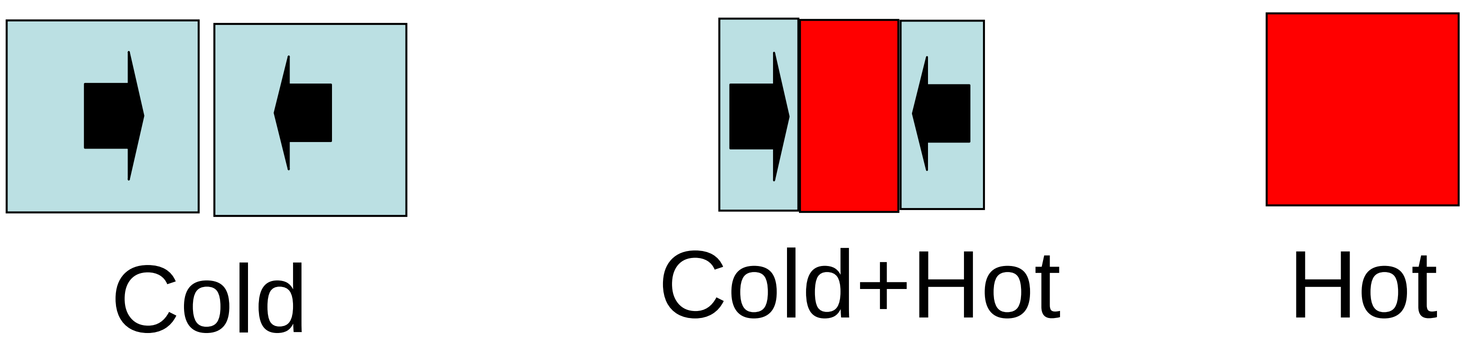
Runge-Kutta → 6 digits for 24,000 steps .

2.5 Molecular Dynamics Techniques

- **Use fourth-order Runge-Kutta integrator with double precision to solve dynamical equations of motion with a pair potential :**

$$\phi(r > 1) = (10/\pi)(1 - r)^3 \, .$$

- **Use periodic Boundaries in y direction.**
- **Use Treadmill or Collision of Blocks in x .**



2.6 Spatially-averaged Profiles in One, Two, or Three Dimensions with Compact Weight Functions

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

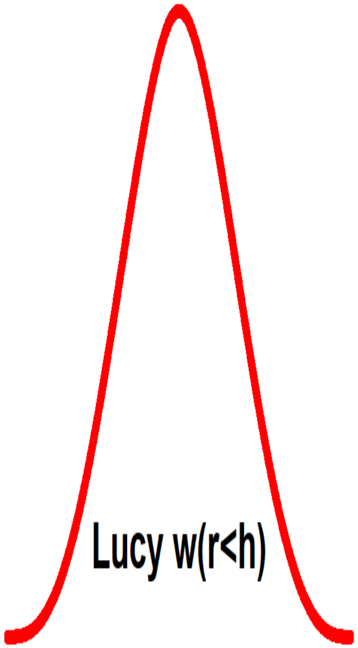
$$w_{1D} = C[1 - (r/h)]^3[1 + 3(r/h)]$$

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

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

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

h = 3 is a good choice!



3.1 [Irreversible] Continuum Mechanics

$$\dot{\rho} = -\rho\nabla \bullet u \text{ and } \rho\dot{u} = -\nabla \bullet P \text{ and}$$

$$\rho\dot{e} = -\nabla u : P - \nabla \bullet Q \text{ with}$$

$$P = P_{eq} - \eta[\nabla u + \nabla u^t] \text{ and } Q = -\kappa\nabla T$$

The continuum equations are irreversible because they incorporate Newtonian viscosity in the Pressure and Fourier heat conduction in the Heat Flux .

3.2 Fourier's Heat Conduction and Newton's Viscosity

$$Q = -\kappa \nabla T$$

$$P = [P_{eq} - \lambda \nabla \bullet u]I - \eta [\nabla u + \nabla u^t]$$

3.3 Irreversibility in Continuum Mechanics

$$\sigma = \eta \dot{\varepsilon} \;\text{ and }\; Q = -\kappa \nabla T$$

If the motion is reversed (by playing a movie backwards) the shear stress σ changes sign but the heat flux does not.

In molecular dynamics the exact opposite occurs, with stress invariant while the heat flux vector Q changes sign !

The Comoving Fluxes are Constant ; from the Continuity, Motion, and Energy Equations there are 3 Constant Fluxes :

$$\rho u,$$

$$P_{xx} + \rho u^2,$$

$$\rho u[e + (P_{xx}/\rho) + (u^2/2)] + Q_x$$

Irreversible, Entropy increases !

3.5 Solving the Continuum Equations

1. Compute density ρ at cell centers .

2. Compute u, e, T, P, σ, Q at the nodes .

3. Use *second-order* space differencing and *Fourth-order* Runge-Kutta time integration of (d/dt){ ρ, u, e, T, P, σ, Q } to evolve a solution .

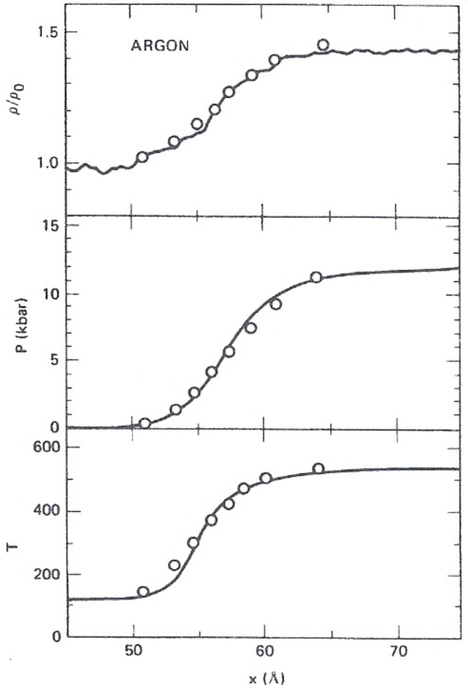
4. This algorithm shows that shockwaves are stable and reveals their detailed structure .

3.6 Solutions for Weak Shockwaves are a good start

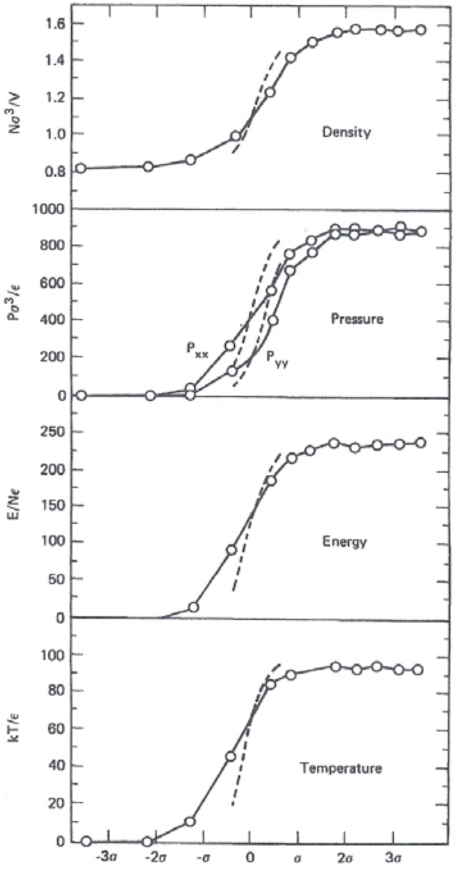
Landau and Lifshitz' Fluid Mechanics solves this for constant η and κ. The profiles all have exponential forms.

$$\rho = \frac{\rho_{COLD} e^{-x/\lambda} + \rho_{HOT} e^{+x/\lambda}}{e^{-x/\lambda} + e^{+x/\lambda}}$$


3.7 Navier-Stokes *vs* Molecular Dynamics



Navier-Stokes Shockwidths are *too Narrow* for Strong Shocks (Linear) transport Coefficients are *too Small* ! →



Weak Shocks are the same .

50 kb & 400 kb

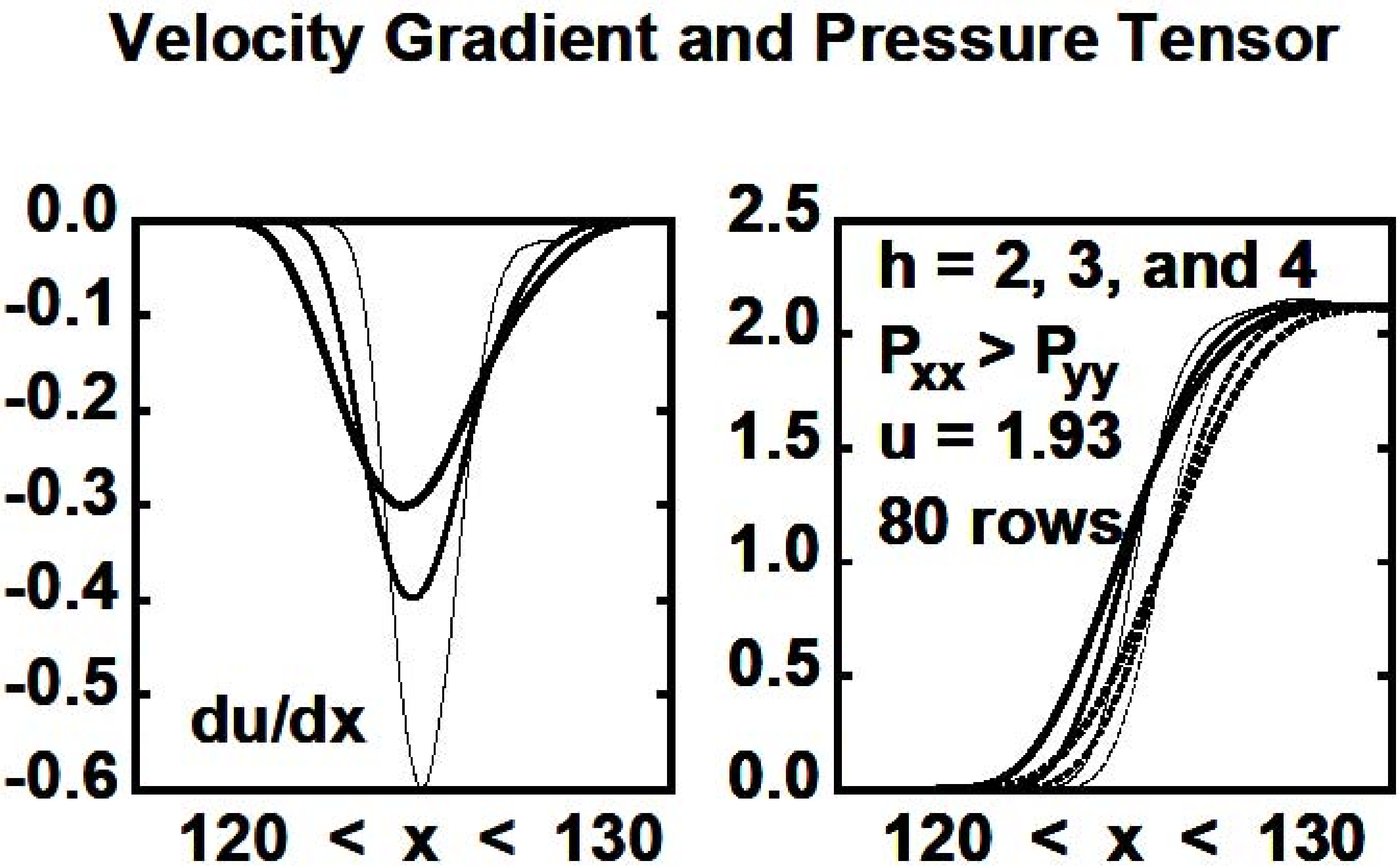
4.1 Some “Well-Known” Results

1. Shockwaves are “narrow”, with a width about equal to the mean free path .

2. Equilibrium boundary conditions (if any) are easy to implement .

3. *The details of the profiles depend upon how the averages are computed* .

4.2 Averages of Molecular Dynamics Data



Results from Garcia-Colin Festschrift

5.2 Some Newer Results

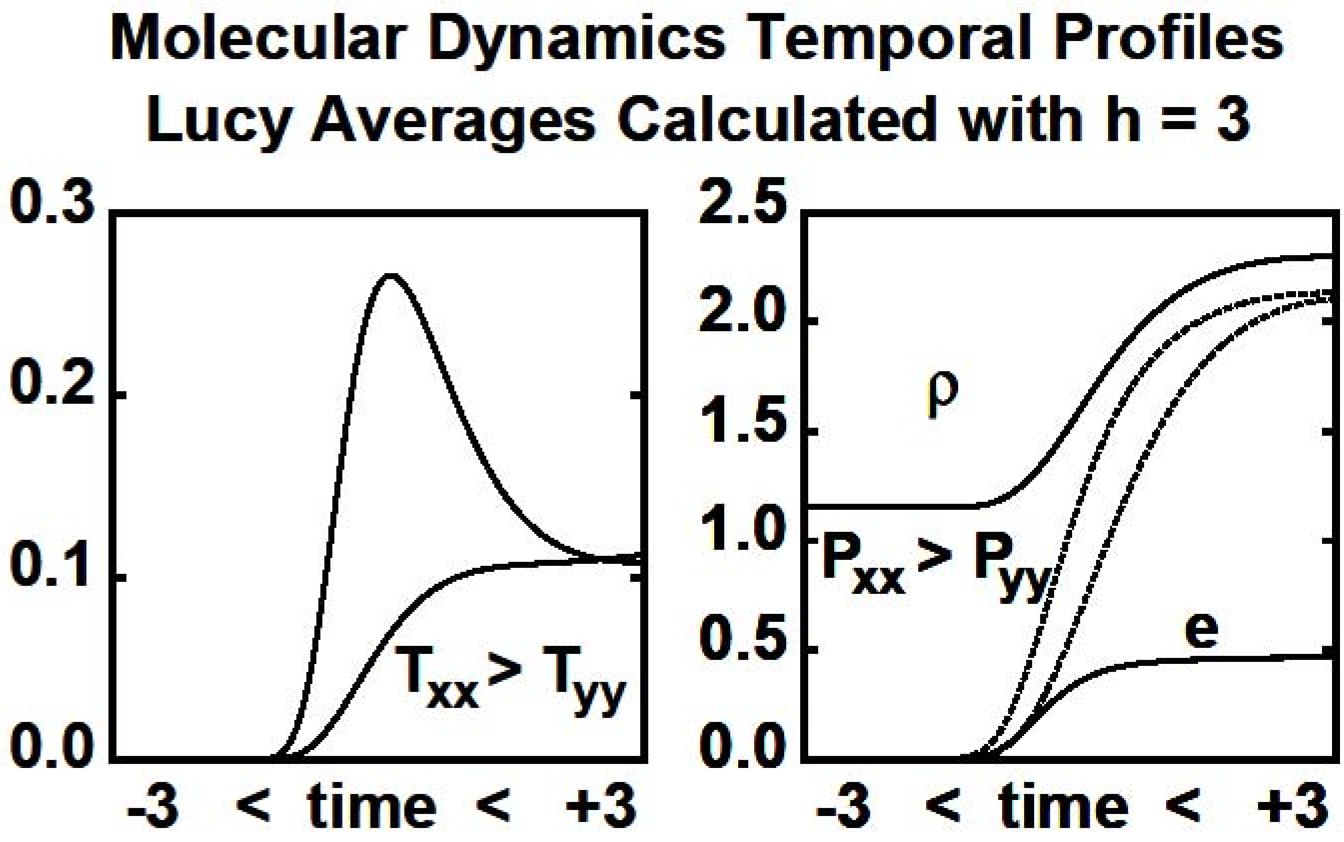
1. T_{xx} and T_{yy} are very different .

2. Fluxes delayed, non Navier-Stokes .

3. Sinewave shocks rapidly become planar, simplifying the analysis and demonstrating shock stability .

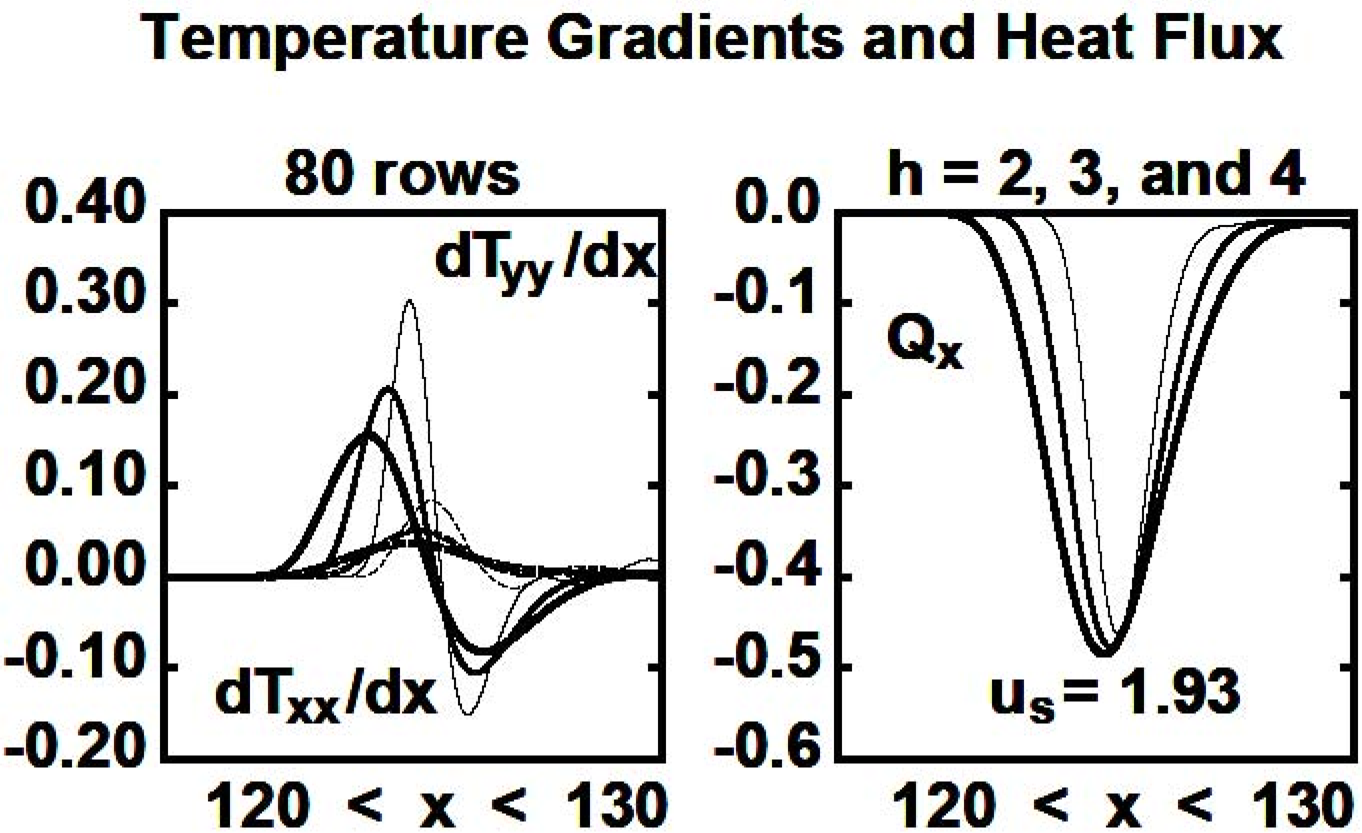
4. Instabilities { λ , Λ } & Time Symmetry .

5.3 Temperature is a Tensor!



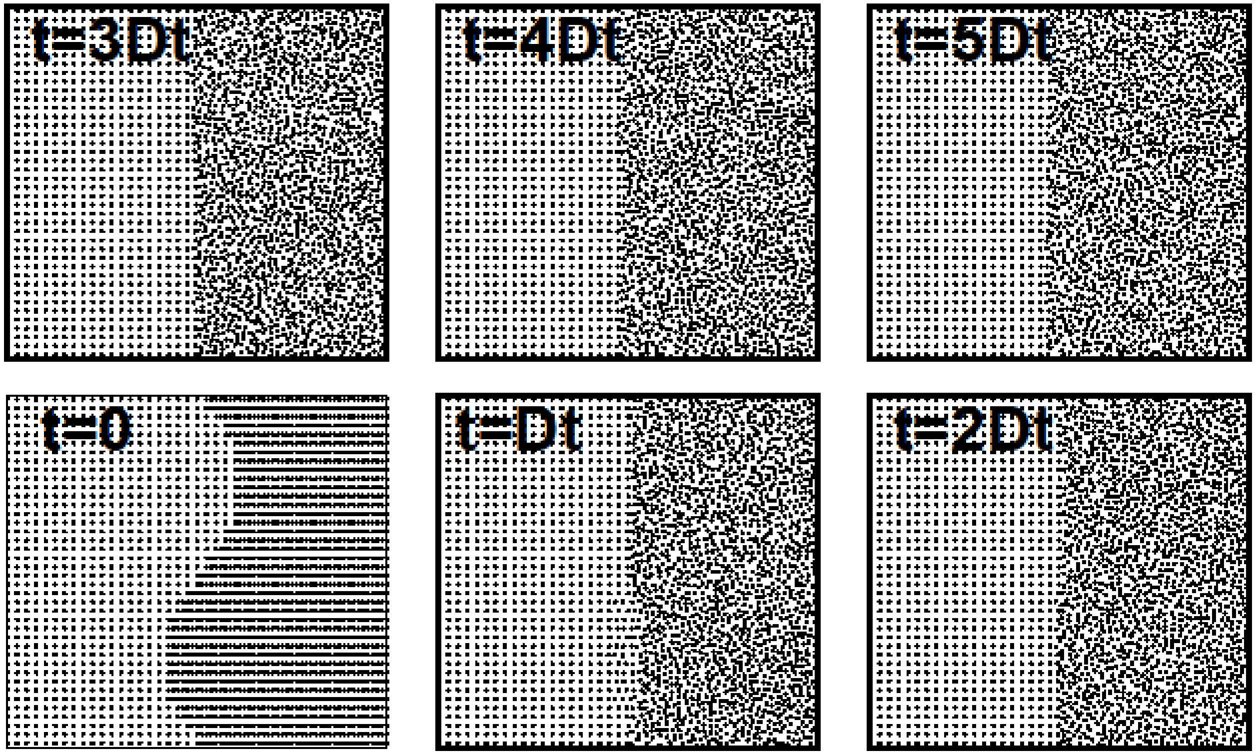
Physical Review E 81 (2010)

5.4 T_{xx} and T_{yy} are very Different and the Heat Flux Response is Late



Results from Garcia-Colin Festschrift

5.5 Planar Shocks are Stable!



Sinusoidal Initial Condition Decays .

Physical Review E (2009)

6.1 Grüneisen Model with T_{xx} & T_{yy}

- **$e = e_{COLD} + ck(T_{xx} + T_{yy})/2$**

- **$P_{EQUILIBRIUM} = P_{COLD} + \gamma\rho ckT$**

- **Q depends on (dT_{xx}/dx) and (dT_{yy}/dx) .**

- **Work and Heat likewise contribute differently to (dT_{xx}/dt) and (dT_{yy}/dt) .**

6.2 Temperature Tensor in Continuum Mechanics

1. Gradients contribute separately to Q_x .

$$Q_x = -\kappa_{xx} \nabla T_{xx} - \kappa_{yy} \nabla T_{yy}$$

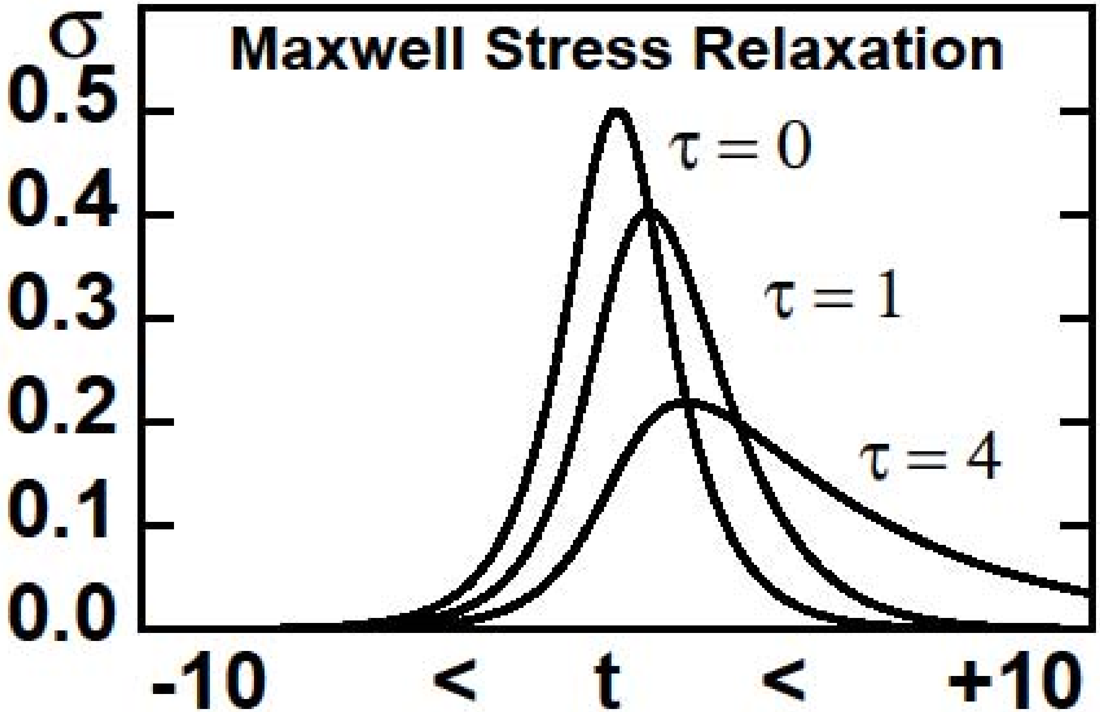
2. Work and Heat contribute separately To T_{xx} and T_{yy} with the sums correct .

$$\rho c k \dot{T}_{xx} = -\alpha \nabla v : P^{THERMAL} - \beta \nabla \bullet Q$$

$$\rho c k \dot{T}_{yy} = -(1-\alpha) \nabla v : P^{THERMAL} - (1-\beta) \nabla \bullet Q$$

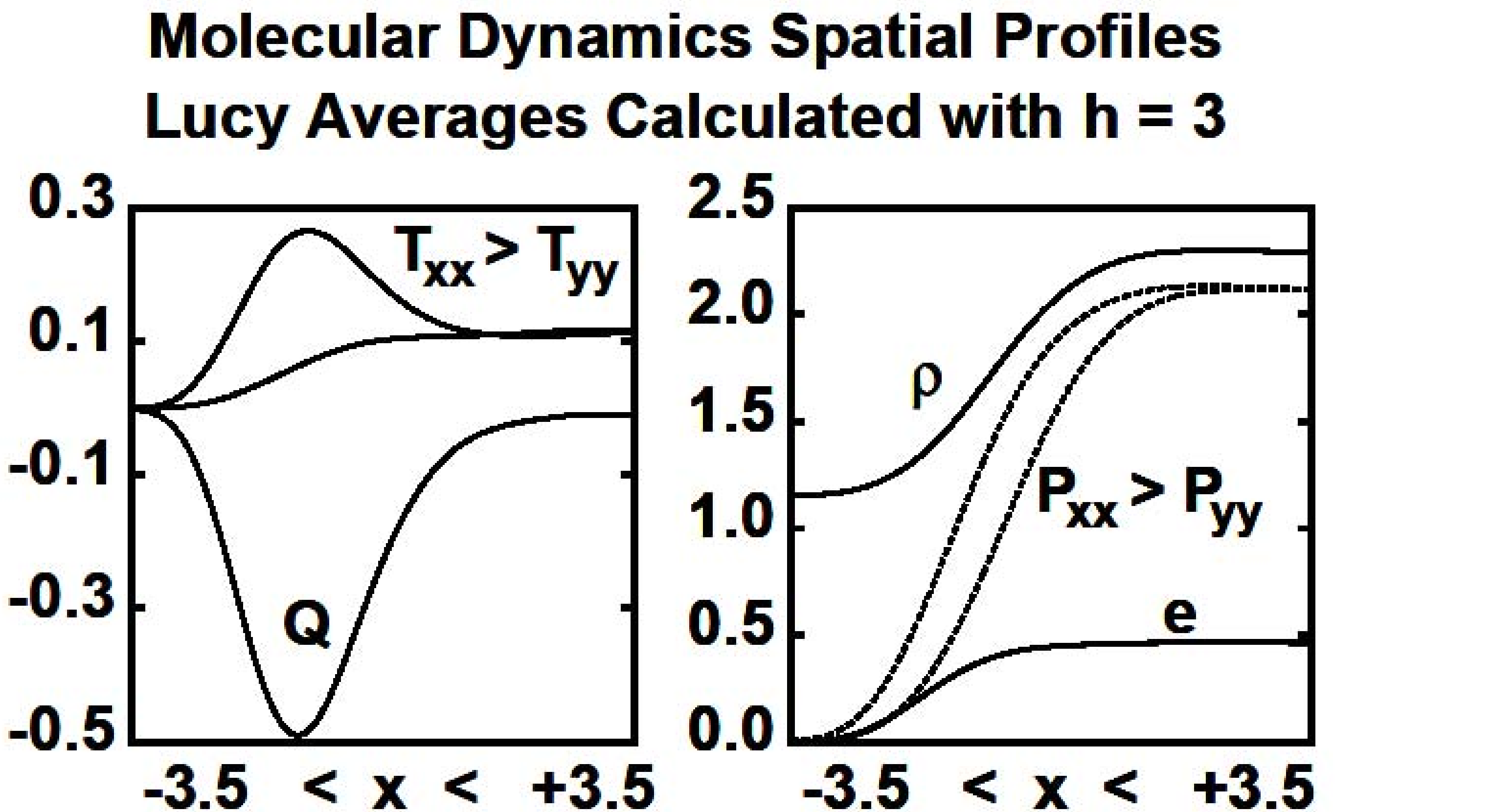
6.3 Delaying Stress & Heat Flux
Viscoelastic or Cattaneo Equation

$$\sigma + \tau(d\sigma/dt) = \eta(du/dx)$$



$$(du/dx) = 1/[\, e^{-t} + e^{+t} \,]$$

6.4 Typical Molecular Dynamics



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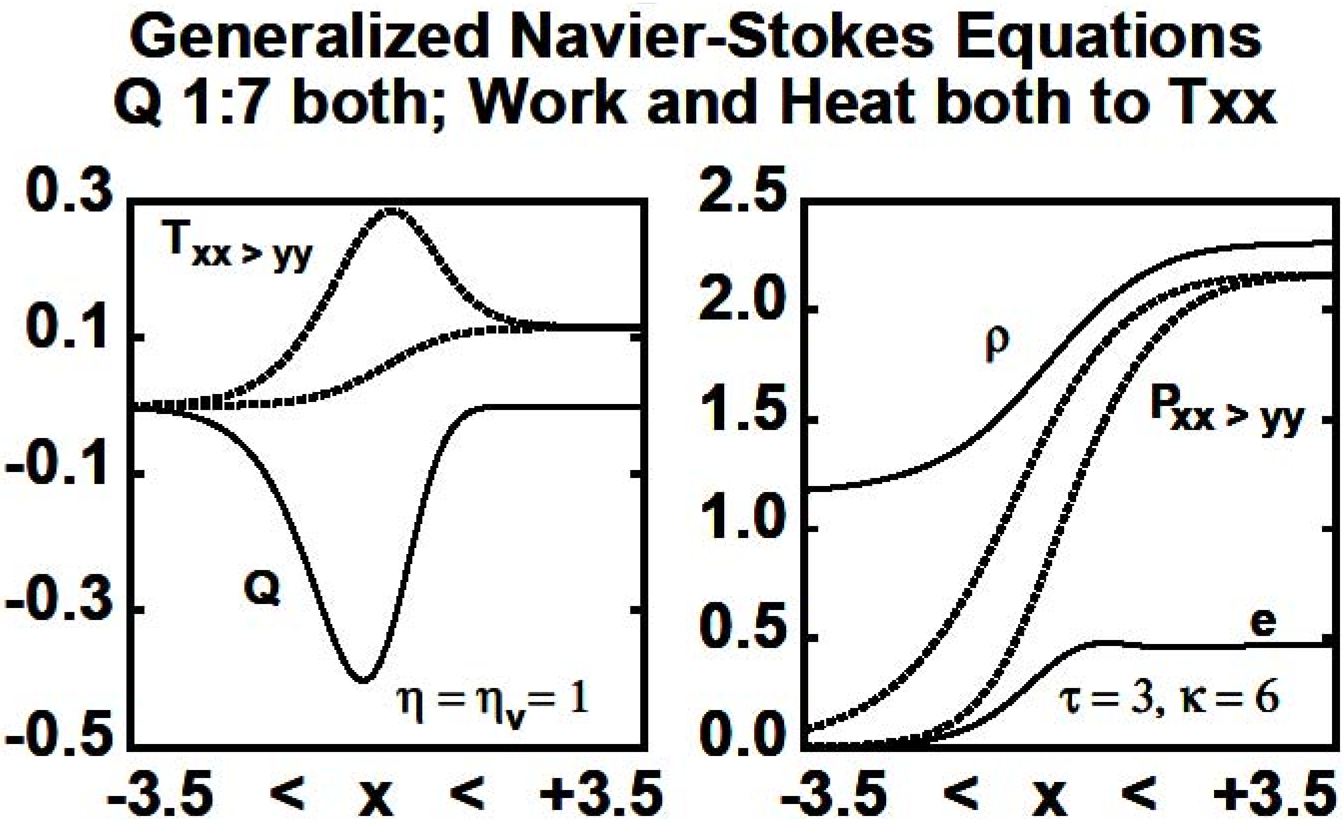
6.5 Typical Continuum Mechanics



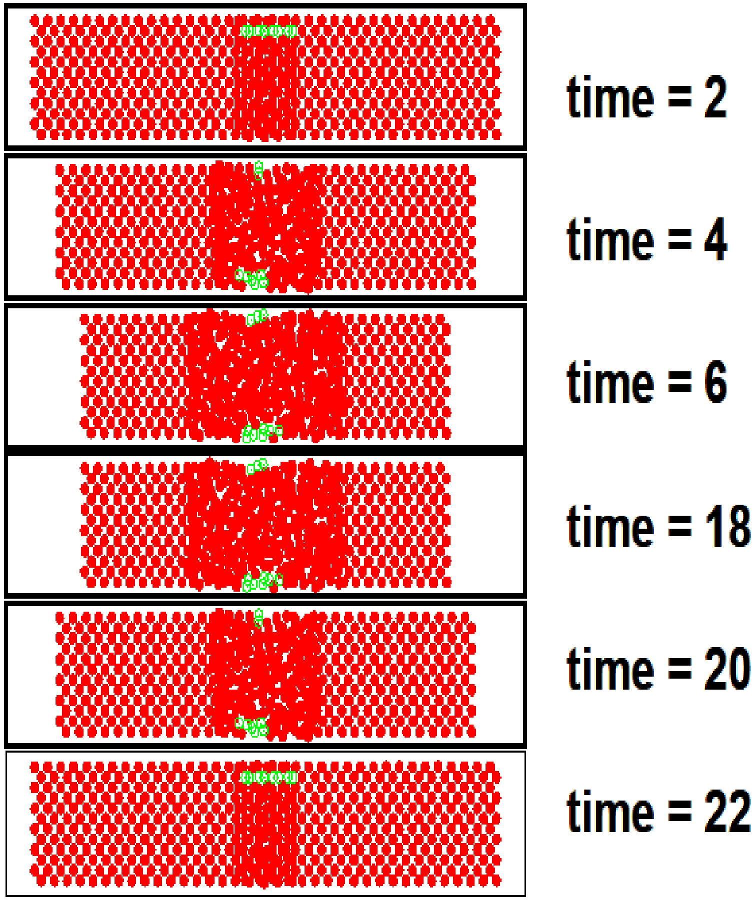
From Physical Review E 81 (2010)

7.1 Instantaneous Growth Rates { Λ }

Particles with above-average linear growth rates can be located by diagonalizing the propagator I + Ddt ,

where

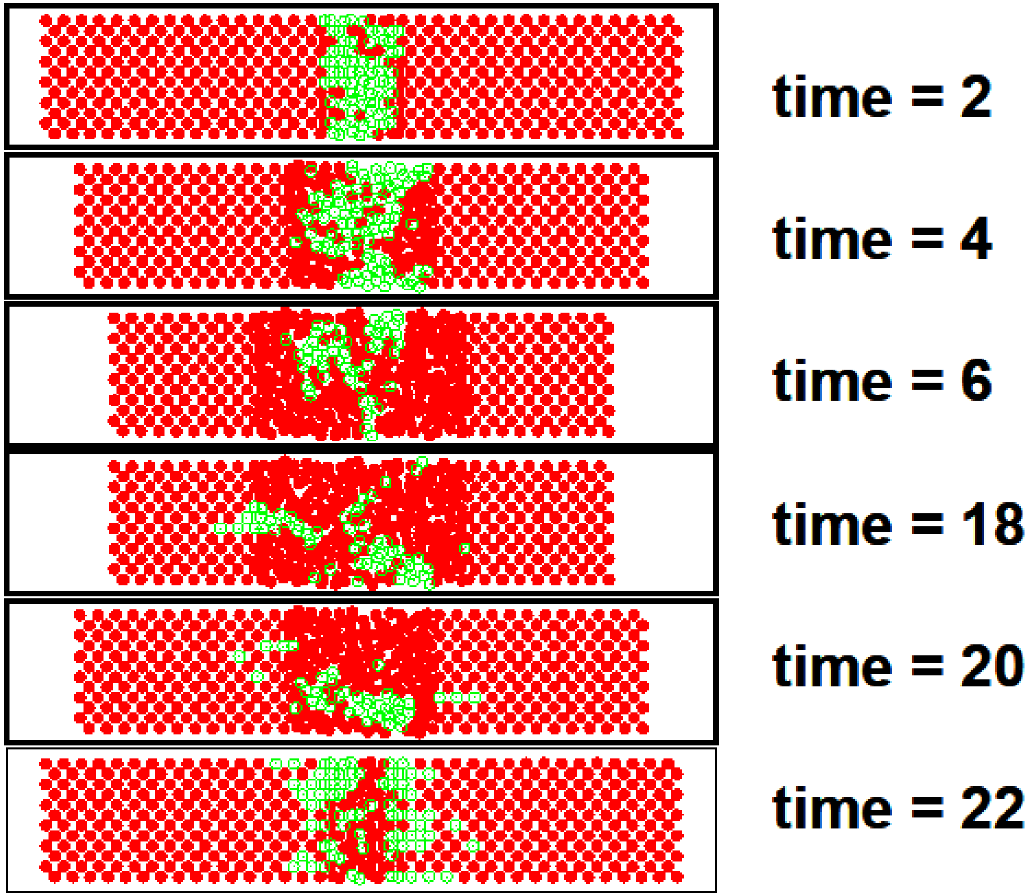
$$D = \partial(\dot{q},\dot{p})/\partial(q,p)$$



Runge-Kutta Reversibility is quite good !

7.2 Irreversible Lyapunov Vectors { λ }

Instantaneous
Growth Vectors { λ }
following the motion
kept Orthonormal
by using a set of
Lagrange Multipliers



***Bit*-Reversibility is the right way !**

8.1 Summary and Prospects (for more see arXiv 1001.1015)

IRREVERSIBLE Shockwaves can be generated by REVERSIBLE dynamics .

Temperature is a TENSOR !

Gradients of (u, T) precede (σ, Q) .

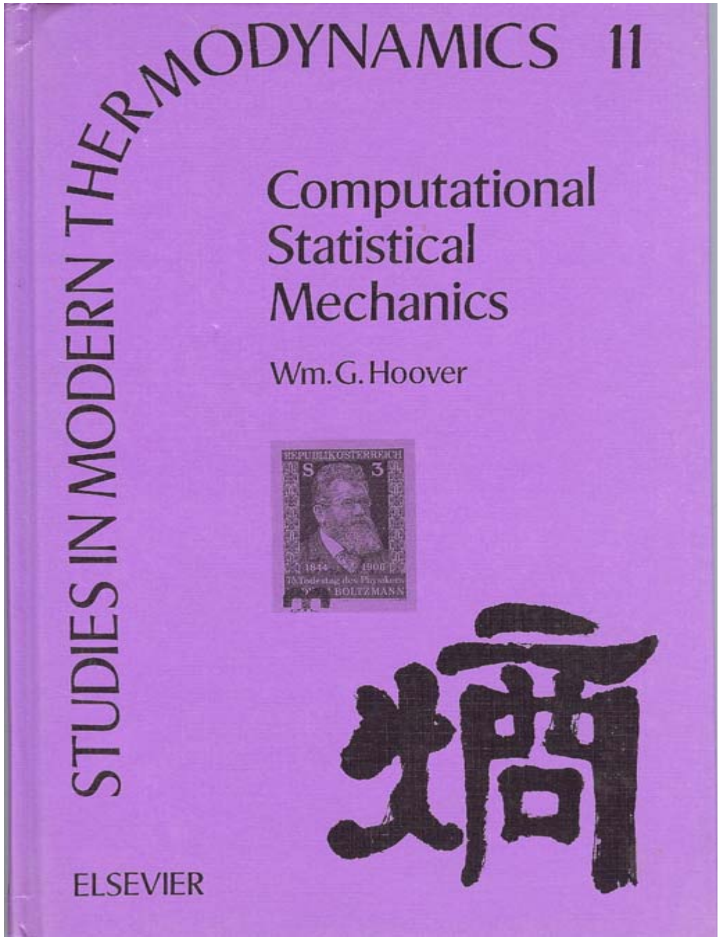
Partitioning thermal contributions of (P, e, σ, Q) to (Work, Heat) provides successful shockwave simulations .

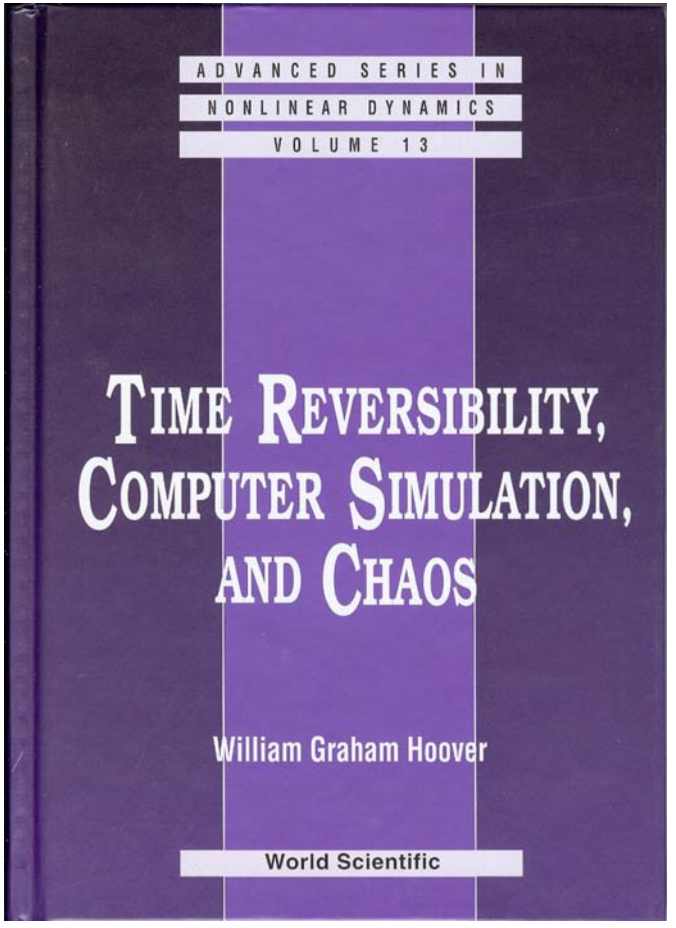
8.2 Some Things to Work on

- **Stability Analyses: Understanding how irreversibility and entropy production can be described in this time-reversible problem by analyzing the Lyapunov spectra , Covariant Lyapunov spectra , and Phase-Space Growth Rates .**

- **Constitutive Relations: Optimizing the weight function for two and three dimensional flows (Rayleigh-Bénard) .**

7.3 Some Useful Reference Books





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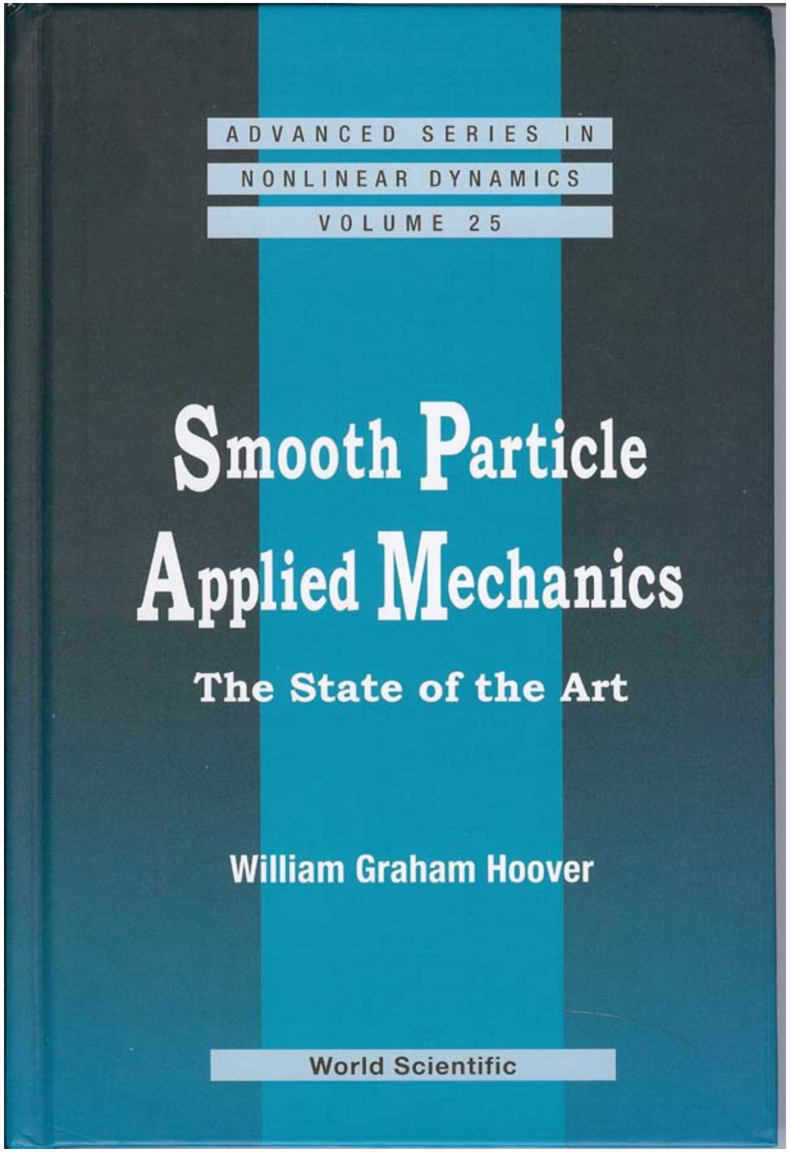

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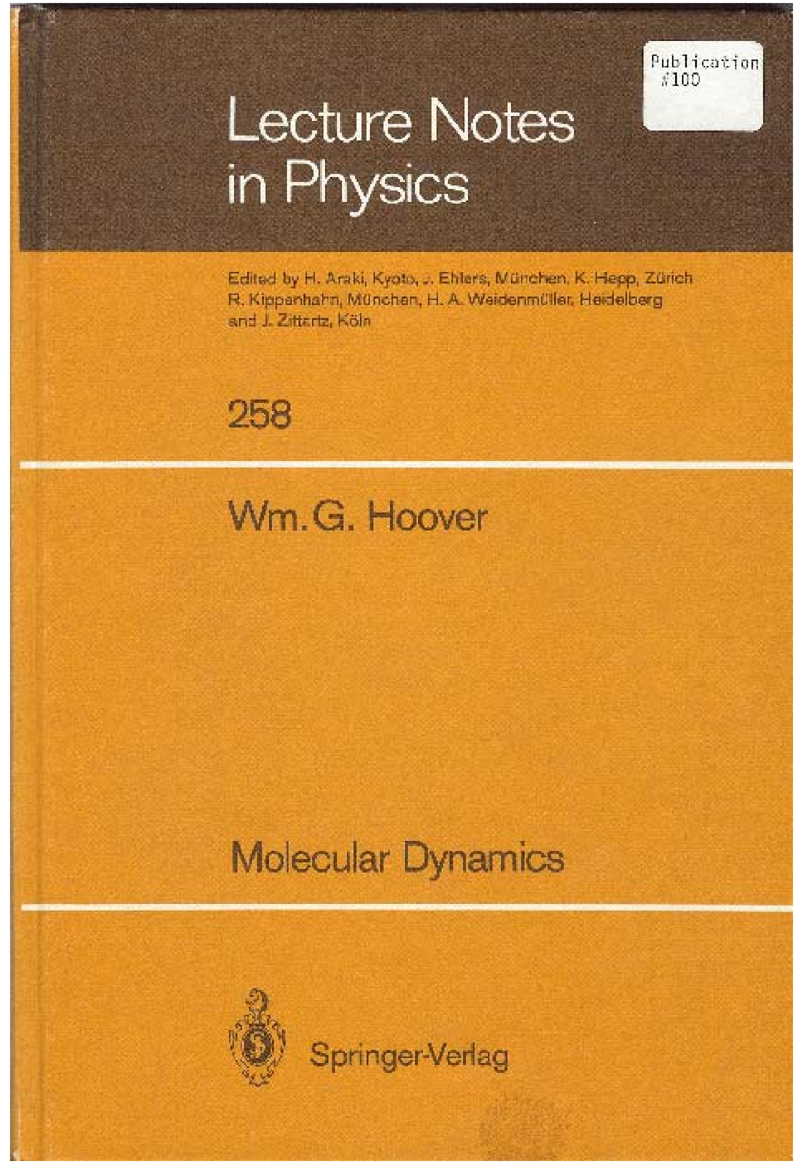

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