Shockwaves with Molecular Dynamics

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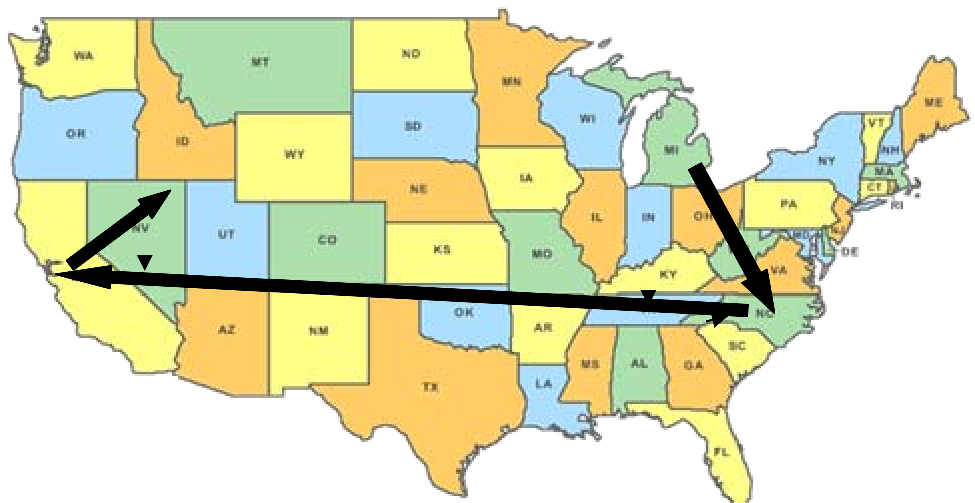
[no longer at UCDavis & LLNL!]



Ruby Valley Research Institute

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Local Ruby Valley Industry

MICRO-BREWED IN NEVADA'S HIGH COUNTRY

RUBY MOUNTAIN

BREWING COMPANY

VIENNA STYLE

LAGER

Shockwaves with Molecular Dynamics

Wm G Hoover & Carol G Hoover
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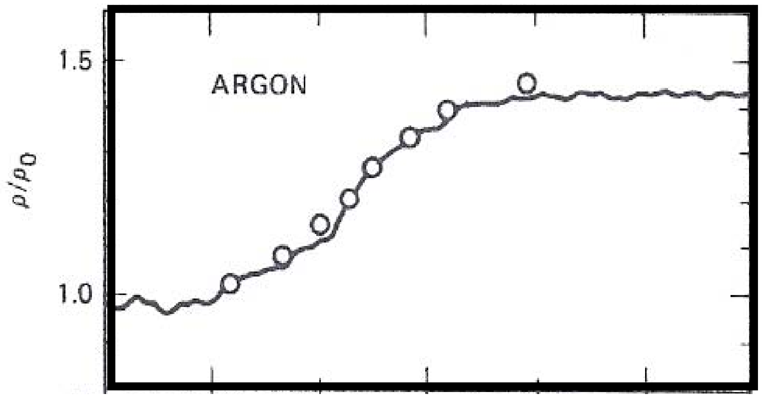
1. What are Shockwaves?
2. How are Shockwaves Generated?
3. What can Shockwaves Teach Us?
4. Shockwaves from Molecular Dynamics
5. Some Lessons + Remaining Questions

1. What are Shockwaves?

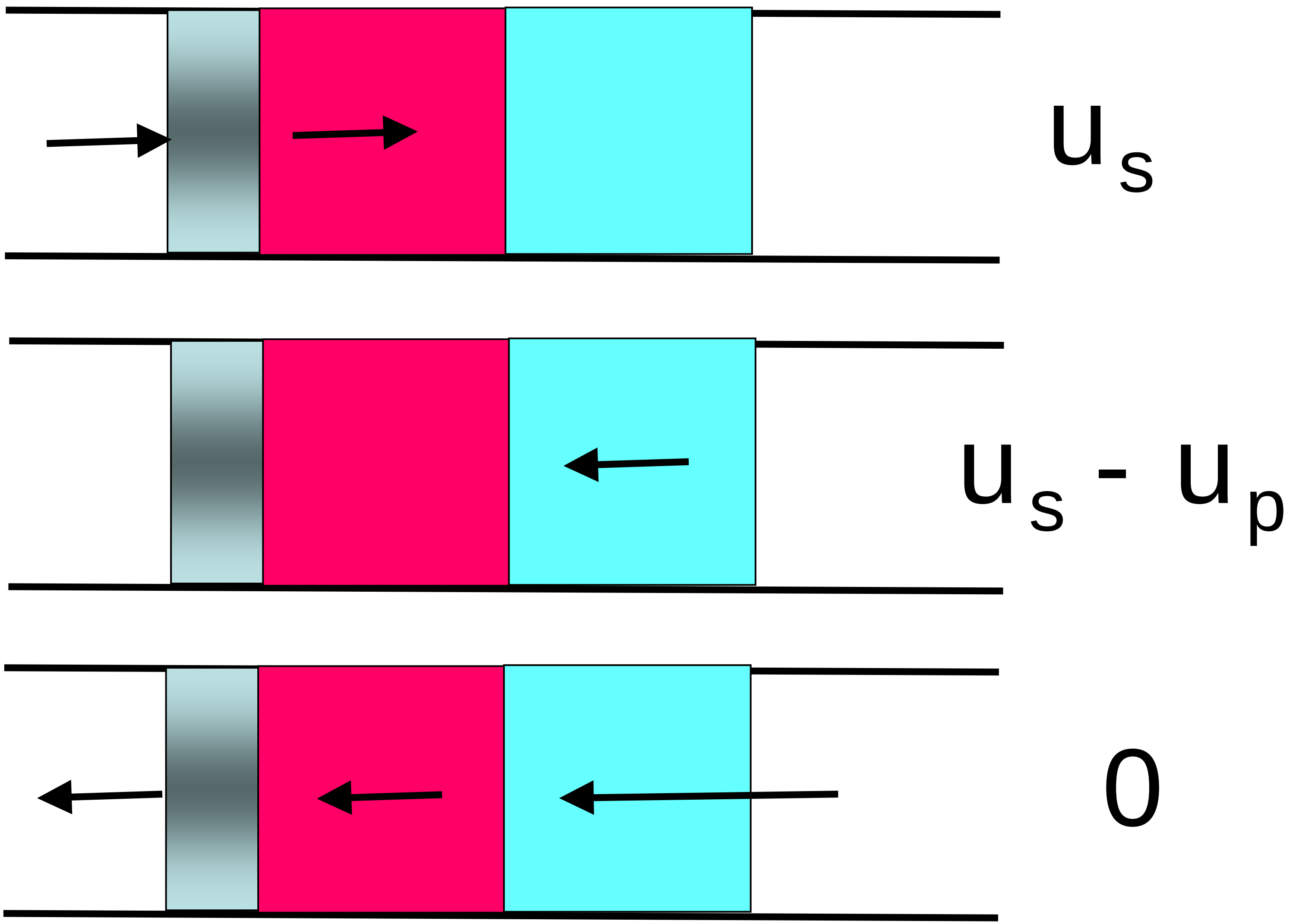
Near-Discontinuities in {v, ρ, e, σ, T}: Velocity, Density, Energy, Stress, and Temperature Jump in a few Free Paths



Phys Rev Letts 1979

Shockwaves are a Simple Laboratory for studying nonlinear Transport as the boundary conditions are equilibrium.

2. How are Shockwaves Generated?



Constants of the Motion

ρu,

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

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

with velocity changing from u_s to $(u_s - u_p)$ in Shockwave.

Newtonian Viscosity + Fourier Heat Conductivity can convert these to differential equations, to make it possible to compute P_{xx} and Q_x.

Holian says Q_x can change sign!

Fourier, Newton, and Fick

$$\mathbf{Q} = -\kappa \nabla \mathbf{T}$$

$$\mathbf{P} = [\mathbf{P}_{\mathbf{eq}} - \lambda \nabla \bullet \mathbf{v}]\mathbf{I} - \eta[\nabla \mathbf{v} + \nabla \mathbf{v}^{\mathbf{t}}]$$

$$\mathbf{J} = -\mathbf{D} \nabla \rho$$

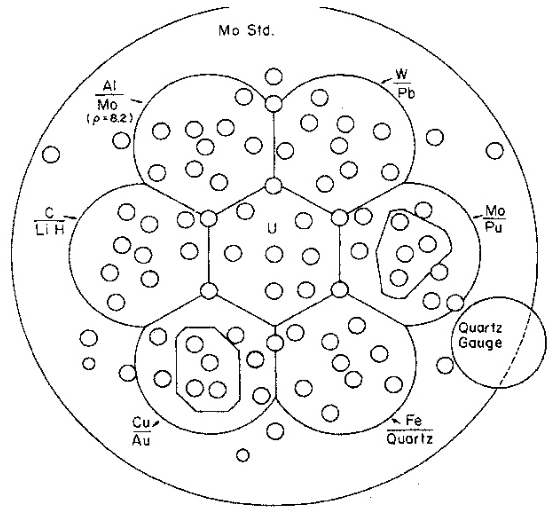
3. What can Shockwaves Teach Us?

- **High-Pressure Equation of State**
  - **Hugoniot Energy Conservation Relation**
  - **Pressure varies Linearly with Volume!**
- **Viscosity determines the distance scale**
- **Highly Nonlinear Transport Information,**
  - **such as the Temperature Tensor, with**

$$T_{xx} \neq T_{yy}$$

Threefold Compression → 6TPa

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



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Shock-wave experiments at threefold compression

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(Received 3 June 1983)

Simple Repulsive Pair Potential

Choose a weak repulsive force
Resembling a SPAM weight function
or a van der Waals type repulsion:

$$\phi(r) = (10/\pi h^2)[1 - (r/h)]^3 .$$

Then we expect to find:

$$e = (\rho/2) + T \quad \text{and} \quad P = \rho e .$$

$$Z^{1/N} \sim VTe^{-\rho/2T}$$

Although the Compression is Irreversible we Conserve Mass, Momentum → Rayleigh Line

$$\rho_0 u_s = \rho(u_s - u_p) = M$$

$$P + \rho(u_s - u_p)^2 = P_0 + \rho_0 u_s^2$$

$$P - P_0 = (M^2/\rho_0) - (M^2/\rho)$$

Cubic Spline Example: P = (9/2) - 4V

Viscosity determines ShockWidth

Momentum Conservation:

$$P - P_0 = \rho_0 u_s u_p \sim \eta u_p / \lambda_{WIDTH}$$

$$\lambda_{WIDTH} \sim \eta / \rho u_s$$

Kinetic Theory:

$$\lambda_{MFP} \sim \eta / \rho c \sim \eta / \rho u_s$$

Conclusion → Shockwaves are Thin:

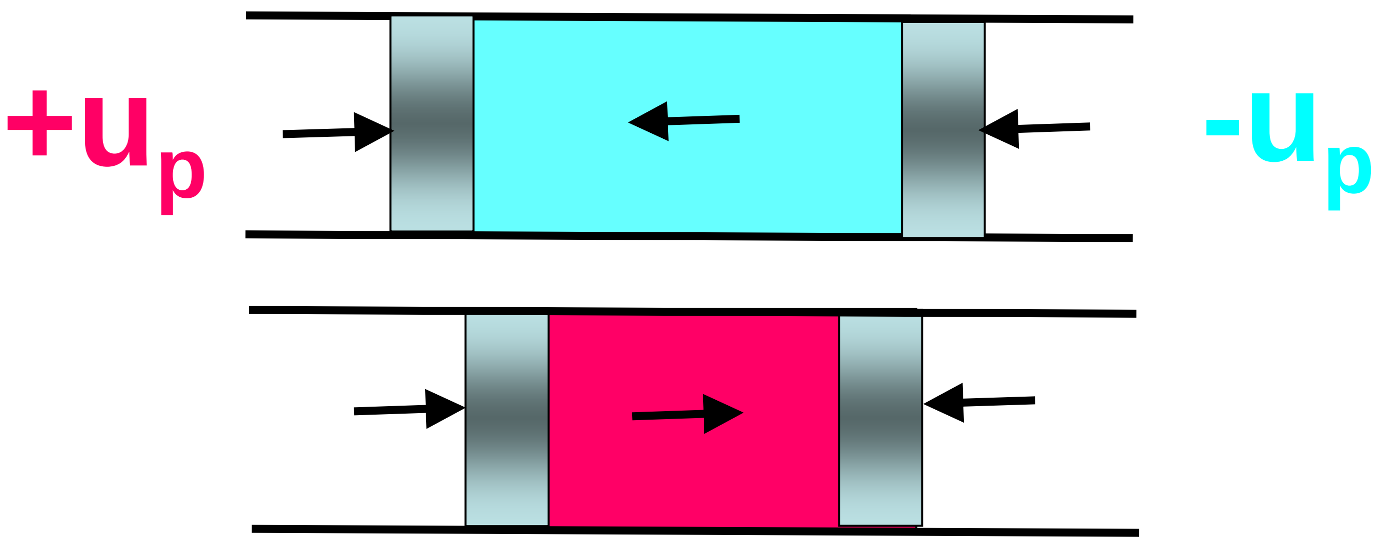
$$\lambda_{WIDTH} \sim \lambda_{MFP}$$

Energy Conservation → Hugoniot

Work done = $P_{HOT}(\Delta V/2) + P_{COLD}(\Delta V/2)$

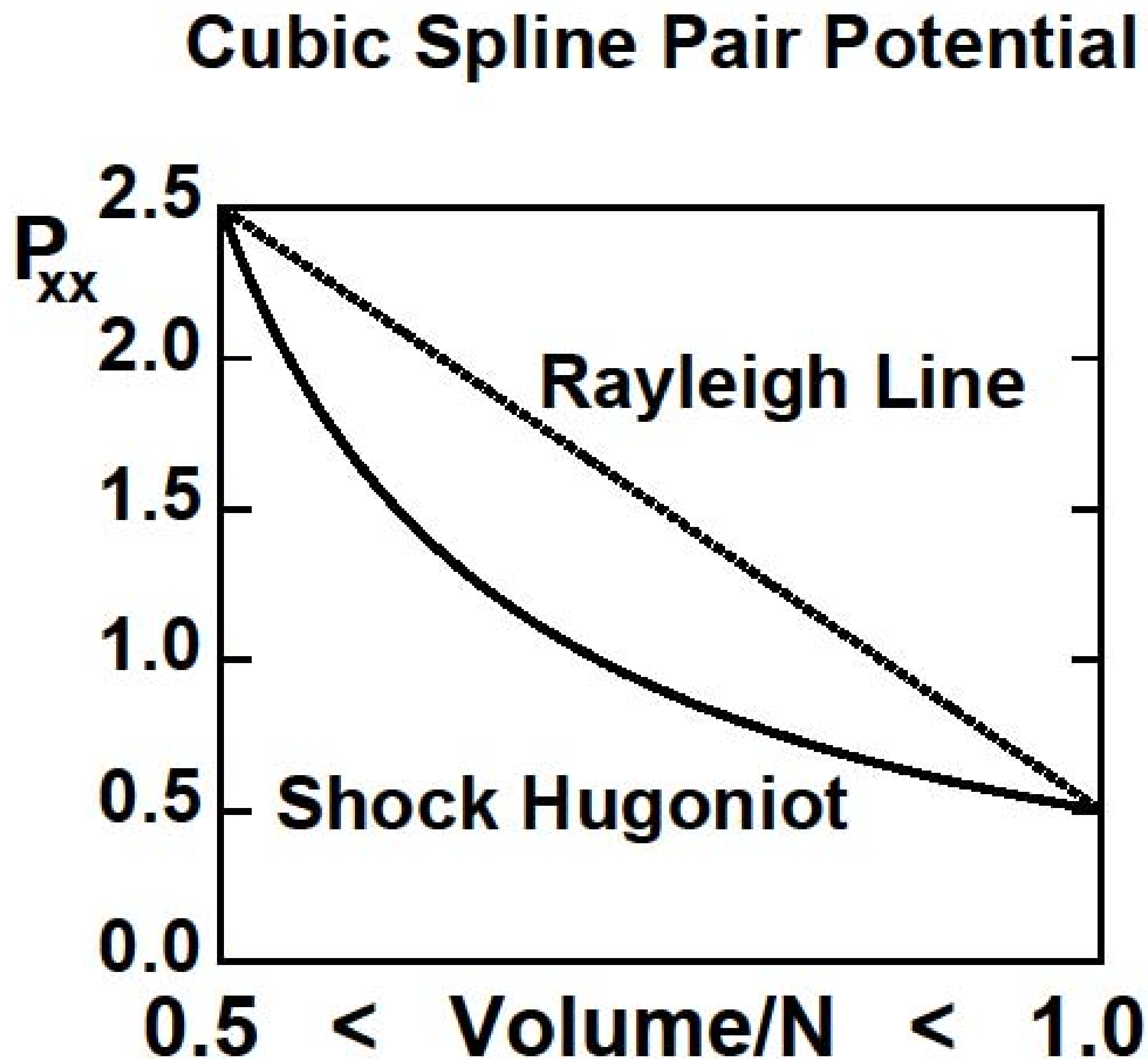
No Change in Kinetic Energy

$\Delta E = (P_{HOT} + P_{COLD})(\Delta V/2)$



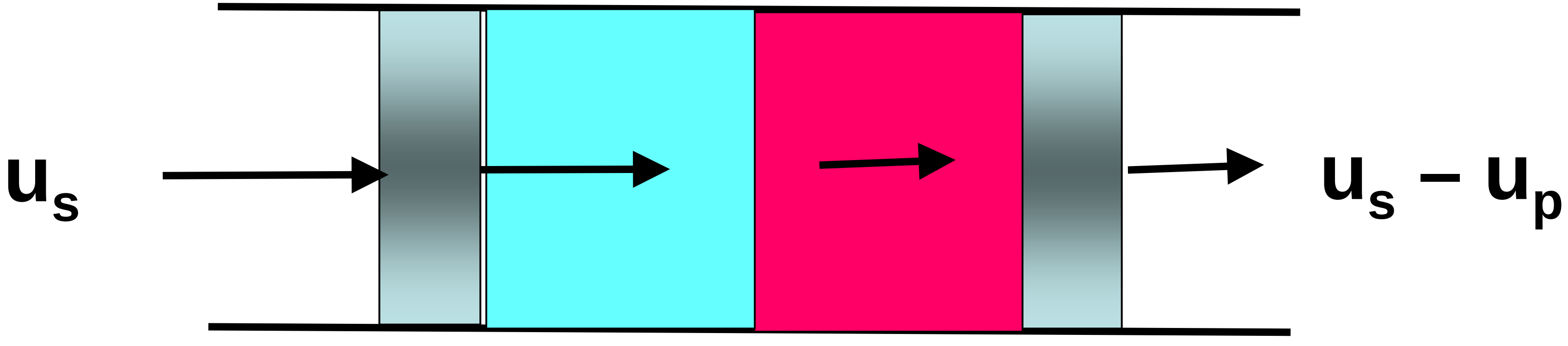
Cubic Spline Example: $P = [3 - V]/[6V - 2]$

With V = 1 and T = 0 initially.

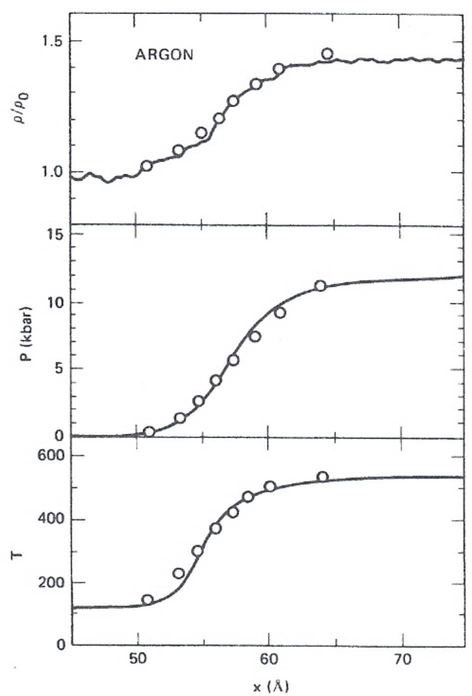

Cubic Spline Pair Potential
P_xx
2.5
2.0
1.5
1.0
0.5
0.0
Rayleigh Line
Shock Hugoniot
0.5 < Volume/N < 1.0

4. Simulation Techniques

- **1. Shrinking Boundary Conditions**
- **2. Stagnation Against a Wall**
- **3. Two Treadmills @ u_s and [$u_s - u_p$].**
  - **This last method is the best one!**

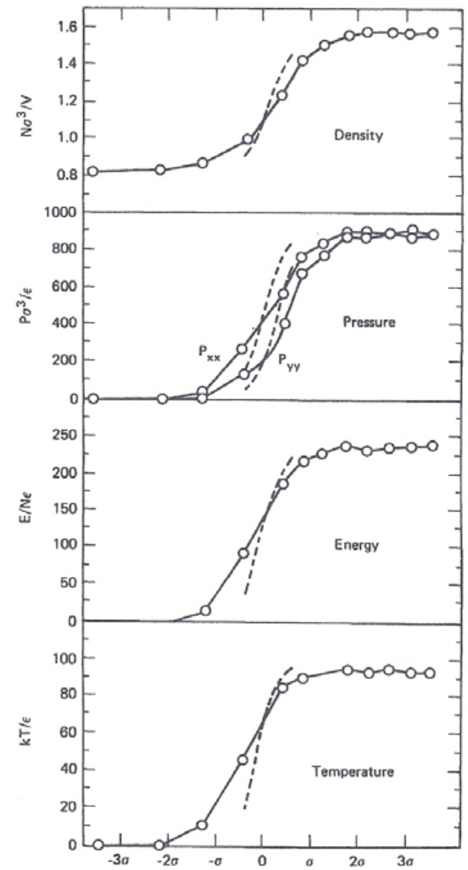


Navier-Stokes *vs* Molecular Dynamics



Navier-Stokes Shockwidths are *too Narrow* for Strong Shocks

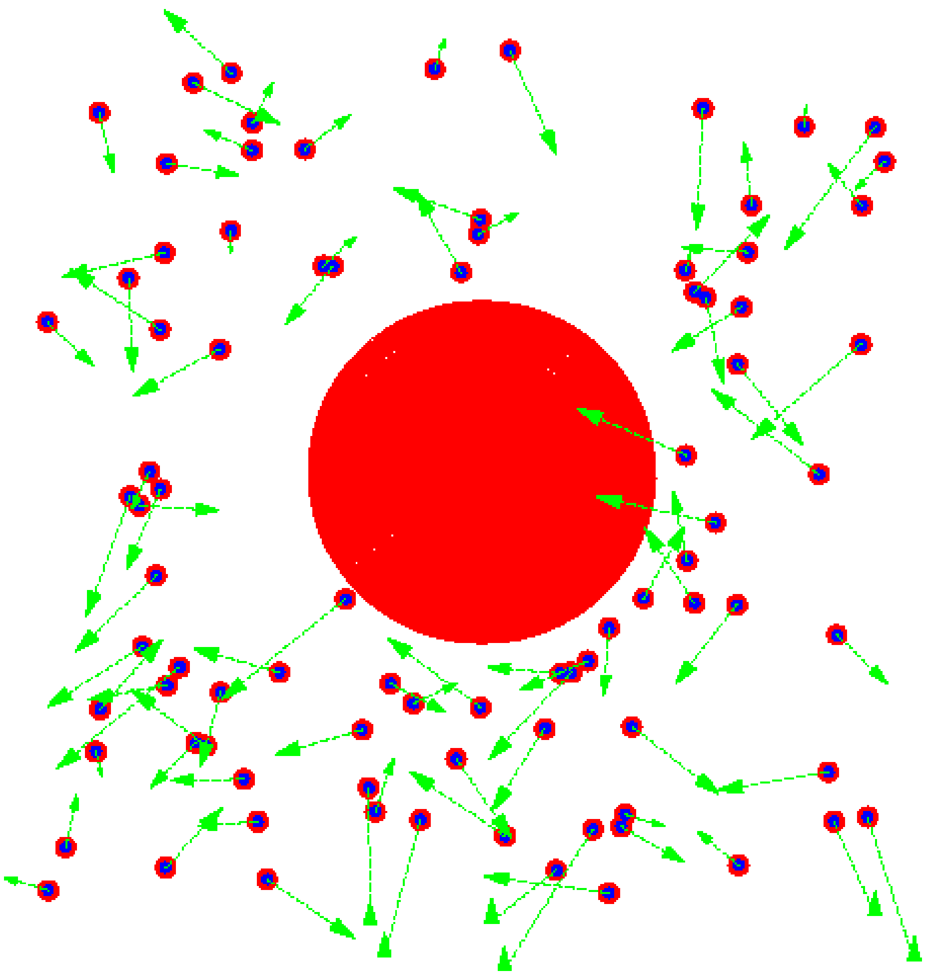
(Linear) transport Coefficients are *too Small* ! →



Weak Shocks are the same .

Analysis from Kinetic Theory

Ideal Gas Thermometer



Temperature is just the *comoving* Kinetic Energy .

Analysis from Gibbs' Ensemble

$$kT = \langle (\nabla \mathcal{H})^2 \rangle / \langle \nabla^2 \mathcal{H} \rangle$$

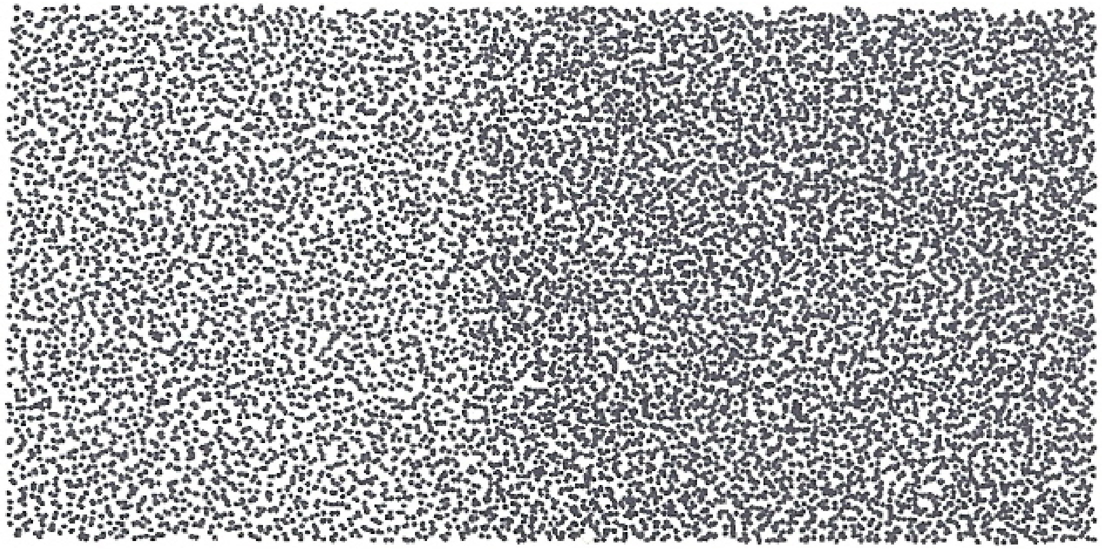
Configurational Temperature

Involves forces and their Gradients. This expression was noted by Landau and Lifshitz around 1950.

50% Compression with a Strong Shockwave

$\Rightarrow$

Cold
Fast



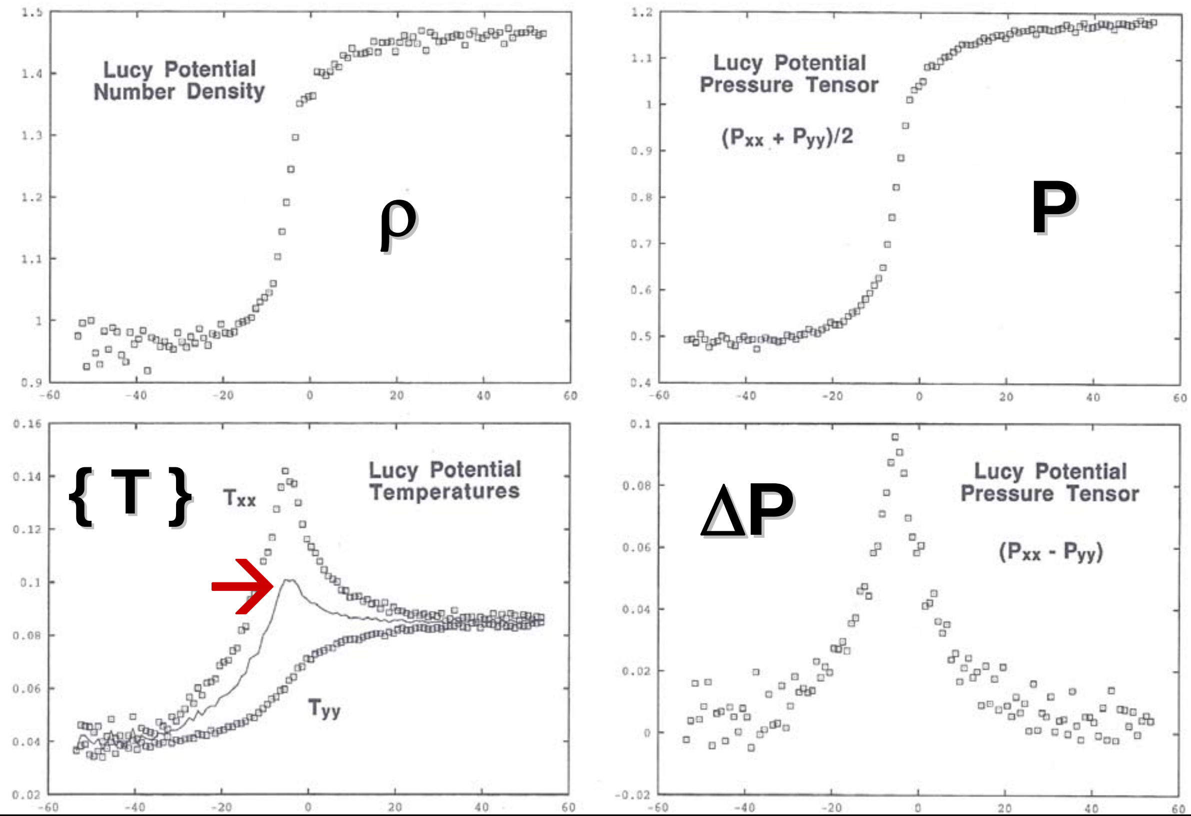
$\Rightarrow$

Hot
Slow

FIG. 1. Snapshot of the 12 960-particle shock wave simulation

This shockwave has quite an interesting temperature profile !

12,960-Particle Shock Profiles



Flagrant Violation of Fourier's Law !

Some Interesting Points

- Shockwidth gives a Viscosity estimate
- Heat Conductivity can be Negative!*
- Shockwave Stability is Interesting
- Boundaries are Equilibrium ones
- The transition is Irreversible

- *See Mott-Smith in 1951 Physical Review.

Simple Equation of State
(apologies to van der Waals)

Choose a weak repulsive force Resembling the weight function:

$$\phi(r) = (10/\pi h^2)[1 - (r/h)]^3,$$

Expecting to find:

$$e = (\rho/2) + T \quad \text{and} \quad P = \rho e$$

Stationary Shockwave Solution Satisfying Conservation Laws

$$u_{COLD} = 2 \ ; \ u_{HOT} = 1$$

$$\rho_{COLD} = 1 \ ; \ \rho_{HOT} = 2$$

$$P_{COLD} = 1/2 \ ; \ P_{HOT} = 5/2$$

$$e_{COLD} = 1/2 \ ; \ e_{HOT} = 5/4$$

$$T_{COLD} = 0/4 \ ; \ T_{HOT} = 1/4$$

$$\Delta e = (3/4) = < -P > \Delta v = (3/2)(1/2)$$

Solution for Twofold Compression

$$\rho u = 2$$

$$P + \rho u^2 = 9/2$$

$$\rho u[\ e + (P/\rho) + (u^2/2)\ ] = 10$$

Almost correct, with the shockwave moving slowly to the right.

$$u,\rho,P,e = (2, 1, 1/2, 1/2) \rightarrow (1, 2, 5/2, 5/4)$$

Development of Smooth Profiles in either One or Two Dimensions

$$\rho(x) = \Sigma_j w(x - x_j)$$

where, with $r = |x|$

$$w_{1D} = (5/4h)[1 - (r/h)]^3[1 + 3(r/h)]$$

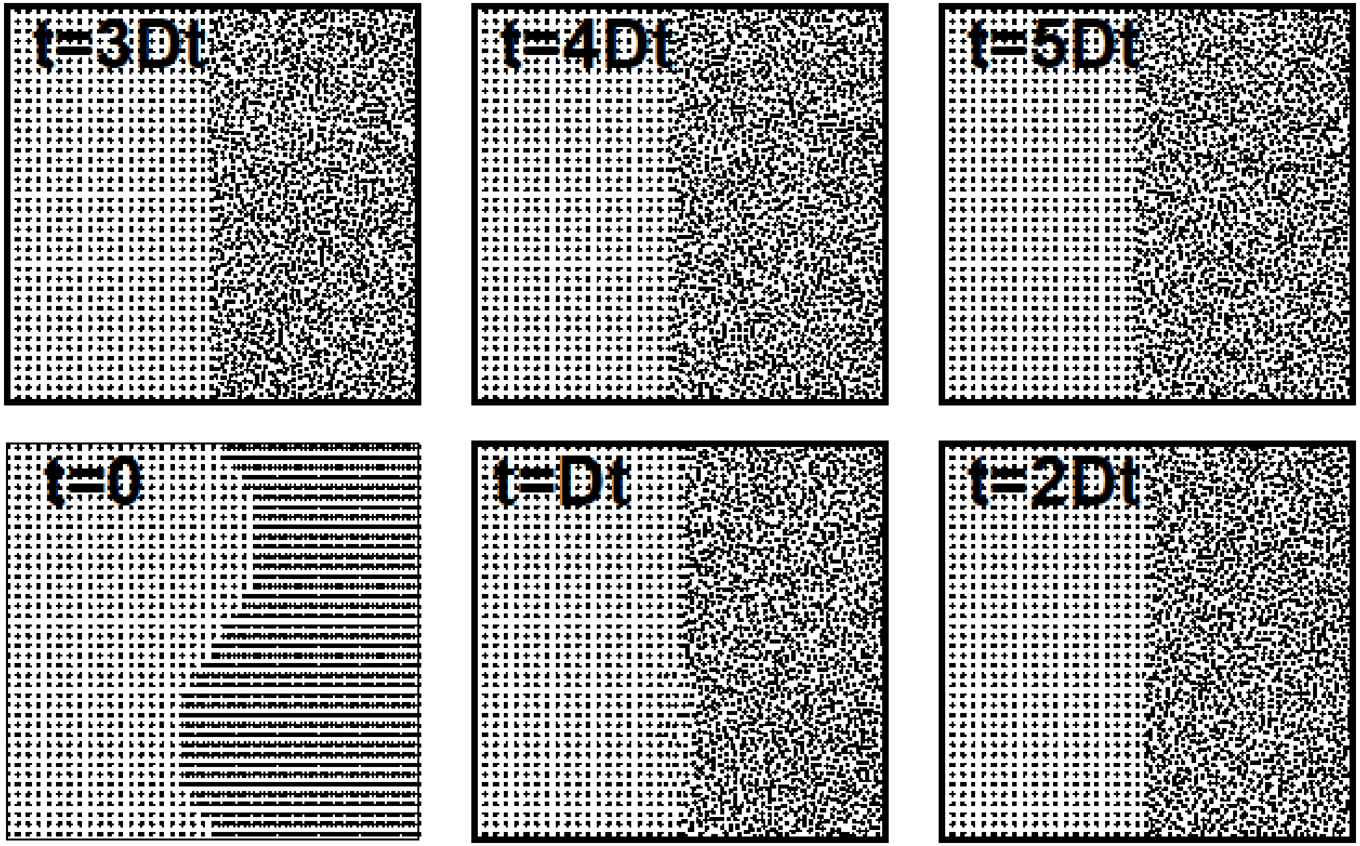
or

$$\rho(x,y) = \Sigma_j w(x - x_j, y - y_j)$$

where, with $r = [x^2 + y^2]^{1/2}$

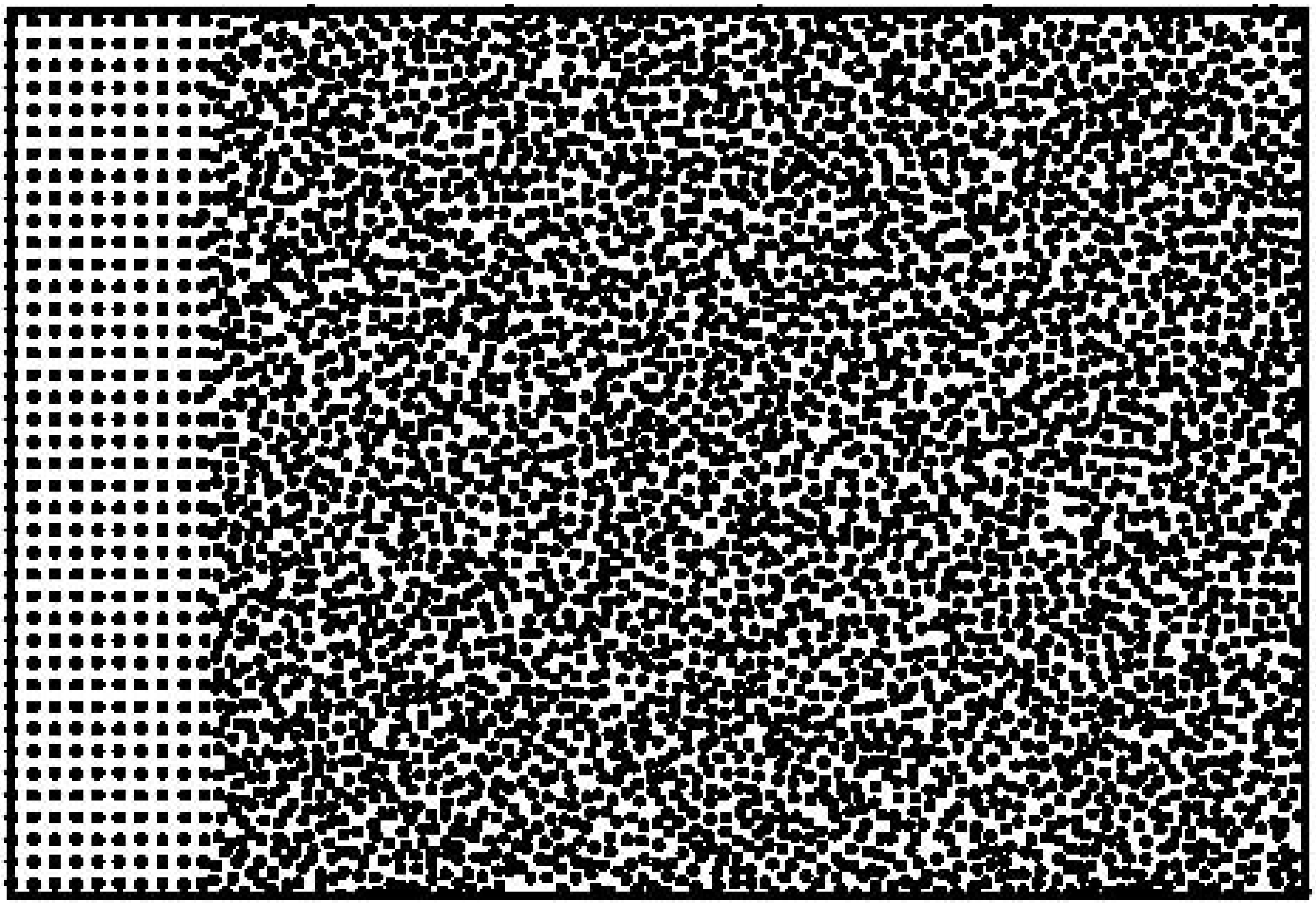
$$w_{2D} = (5/\pi h^2)[1 - (r/h)]^3[1 + 3(r/h)]$$

What about Shock Stability?

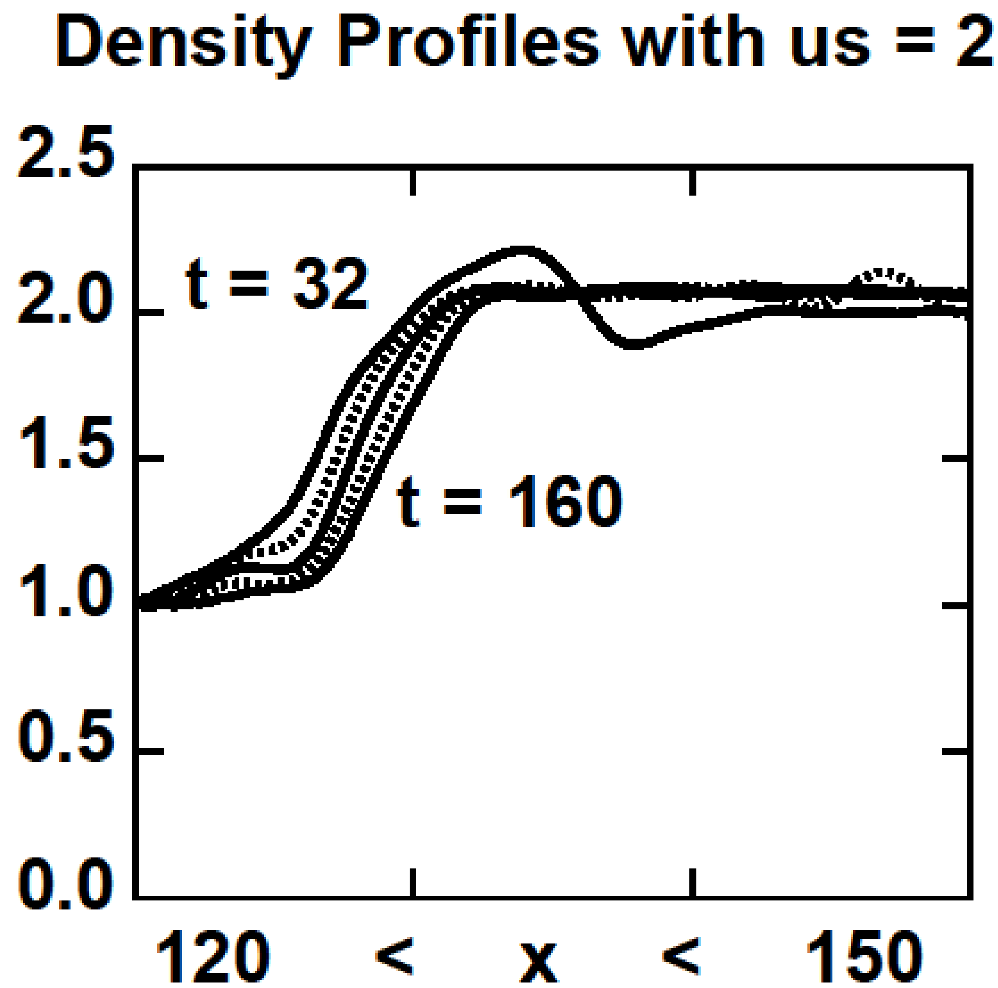


Sinusoidal Initial Condition

Twofold Compression Shockwave
Enlarged Shockfront View



The Shockwave profile narrows with time, indicating that it is **STABLE** !



What about Temperature?

Kinetic Temperature ← Momenta

Configurational Temperature ← Forces

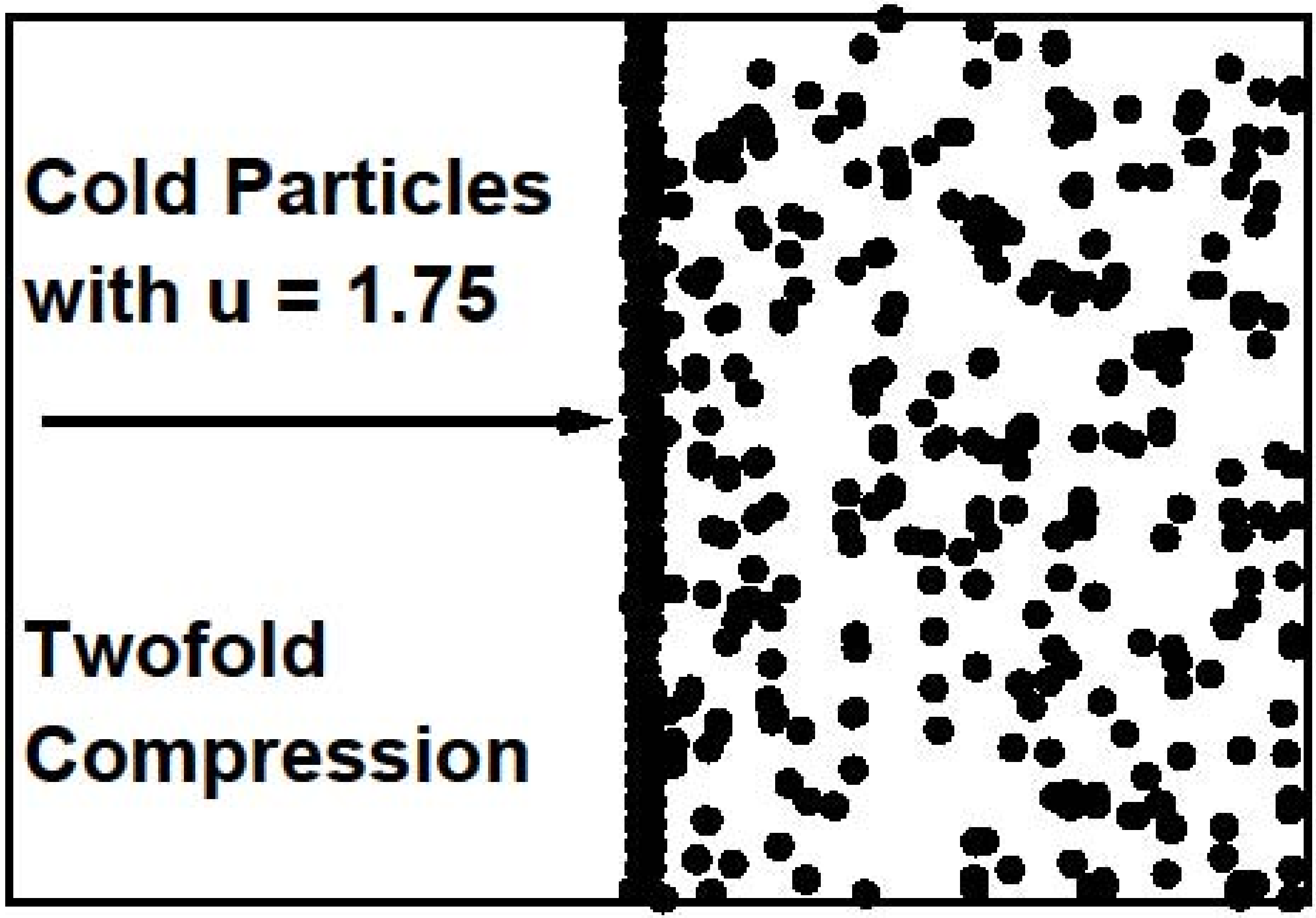
$kT_{Kinetic} = \langle p^2/m \rangle$ **relative to mean flow**

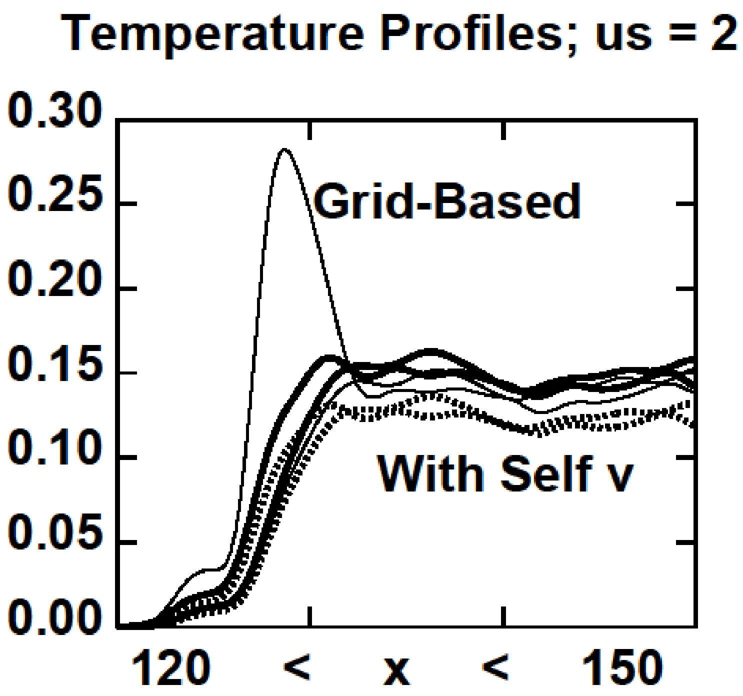
$kT_{Config} = \langle \nabla \mathcal{H}^2 \rangle / \langle \nabla^2 \mathcal{H} \rangle$

Determine the mean flow by using w(r):

$\langle v \rangle_j = \Sigma w_{ij} v_i / \Sigma w_{ij}$ **; w(r) a weight function.**

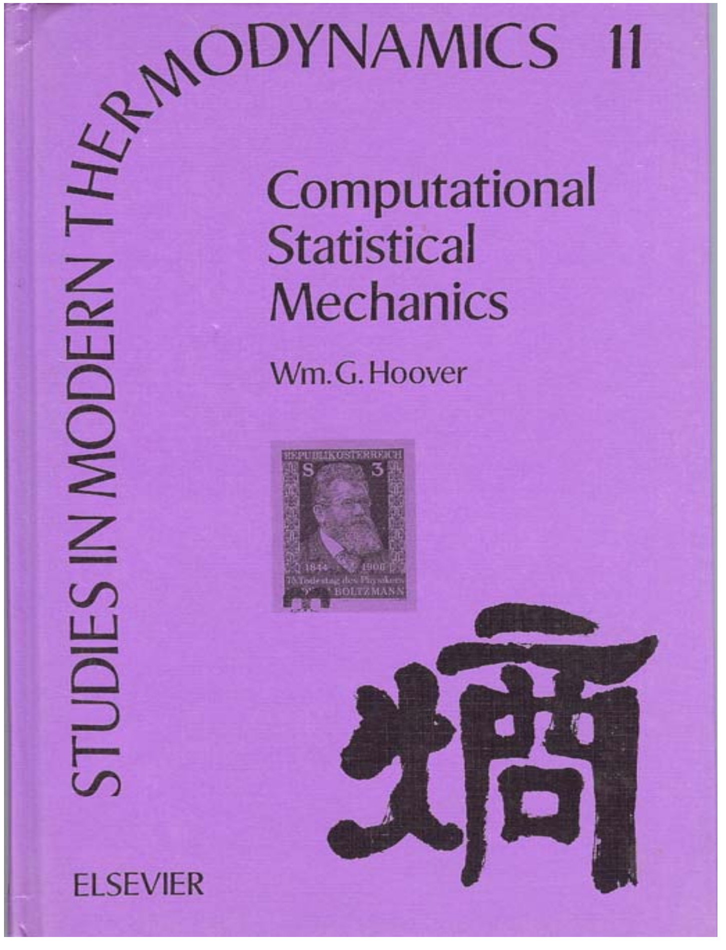
Negative Temperature Particles

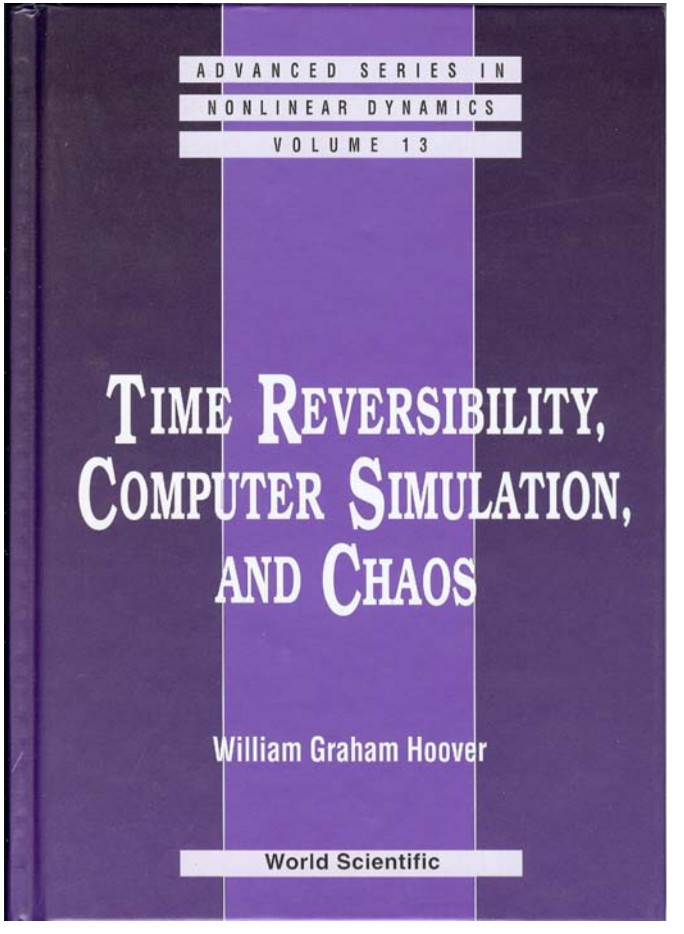




Configurational Temperature Blows up! Among the various Kinetic Temperatures only the Grid-Based temperature has a Strong maximum. Evidently local temperatures will be more useful in analyzing nonlinear flows.

Some Useful Reference Books





For a pdf file, go to
www.williamhoover.info

For a comp copy, write
hooverwilliam@yahoo.com

Remaining Puzzles

- **Description of Temperature/Heat Flow**
- **Direct Measurement of Shock Heat Flux**
- **Cell Model of the Shockwave Process**
- **Prediction of the Nonlinear Viscosity**
- **Best Definitions of P_{xx}, ρ, u, et *cetera***

- **For more details: arXiv:0905.1913**