Shockwaves with Molecular Dynamics and Continuum Mechanics

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Nonequilibrium Simulation School
3 September 2015 Sheffield U K

For more shocking details consult :
arXiv: 0905.1913 and 1005.1525 ;
Website: http://williamhoover.info

Ruby Valley Neighbors

Local Ruby Valley Industry

MICRO-BREWED IN NEVADA'S HIGH COUNTRY

RUBY MOUNTAIN

BREWING COMPANY

VIENNA STYLE

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Shockwaves with Molecular Dynamics and Continuum Mechanics

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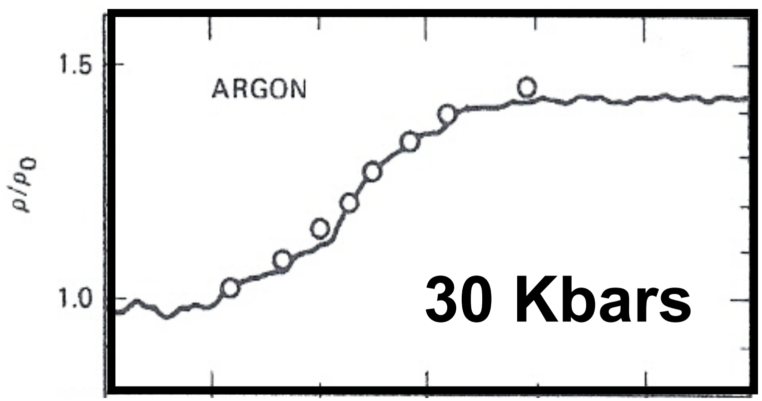
1. What are Shockwaves ?
2. How are Shockwaves Generated ?
3. What can Shockwaves Teach Us ?
4. Shockwaves from Molecular Dynamics
5. Shockwaves from Continuum Dynamics
6. “Smooth-Particle” Averaging
7. Some Lessons + Remaining Questions

#1. What are Shockwaves?

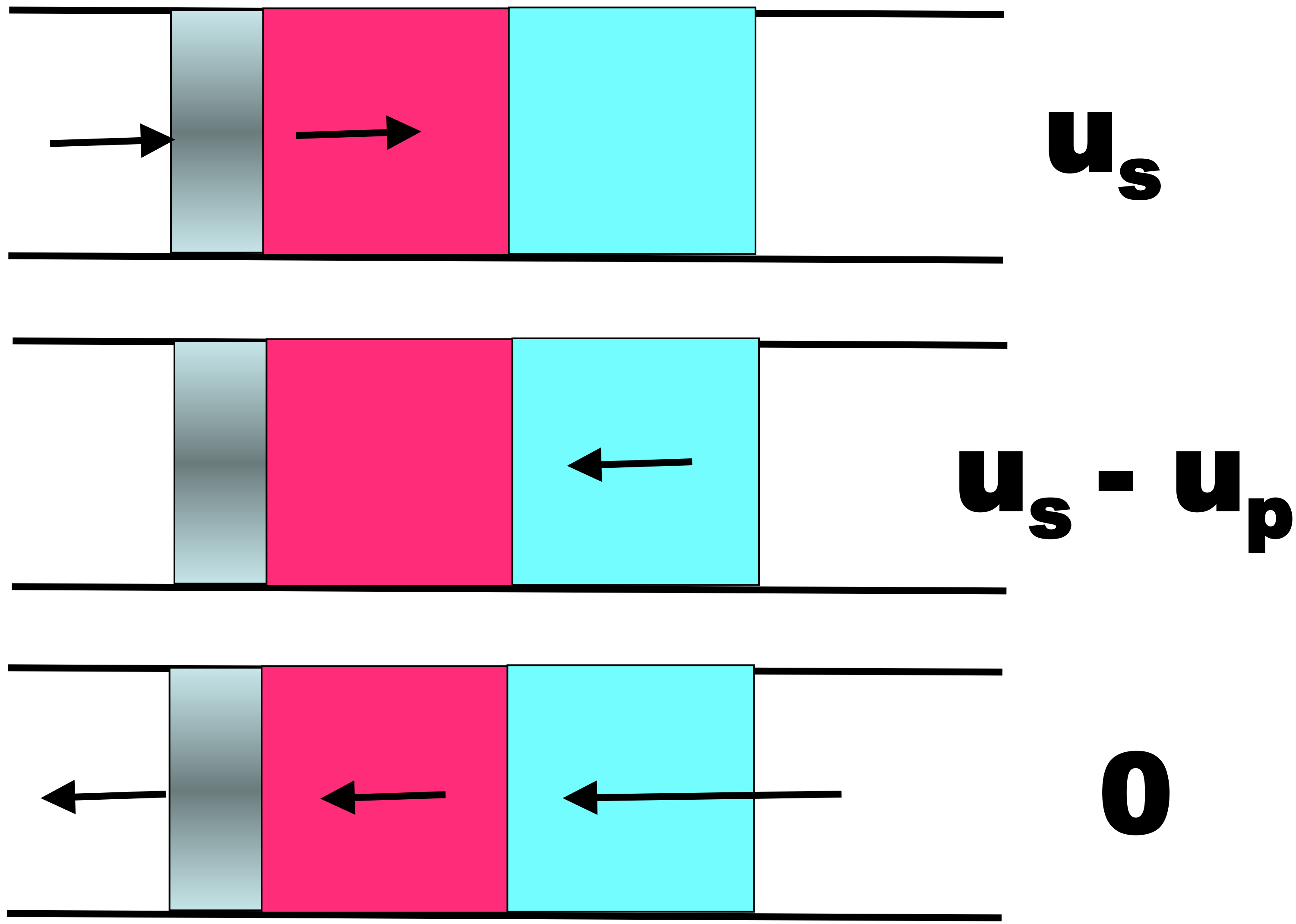
Near-Discontinuities in Macro Properties : Velocity, Density, Energy, Stress, and Temperature Jump in a few Free Paths



Phys Rev Letters
W G Hoover, 1979
Klimenko/Dremin

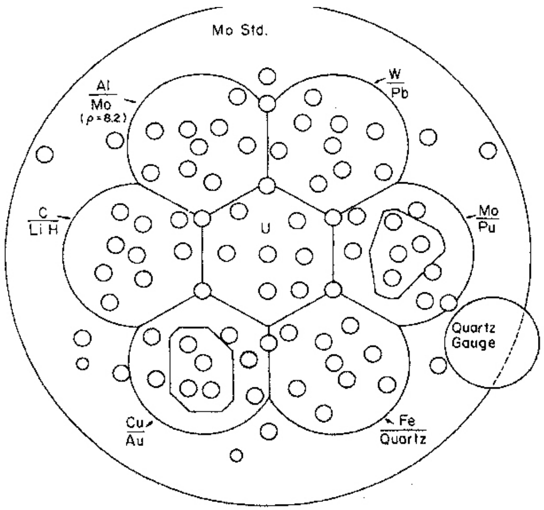
Shockwaves are a Simple Laboratory for studying Nonlinear Transport because the boundary conditions are equilibrium.

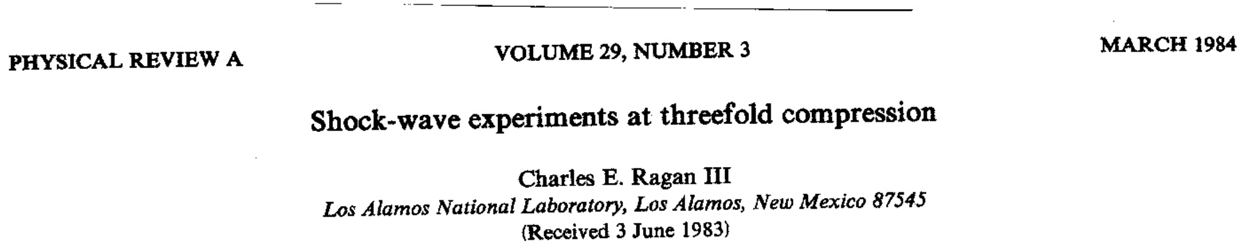
#2. Three Ways to Generate Shockwaves Give Three Different Interface Speeds



#2. Threefold Compression → 6TPa Shock Velocity ← Pin Closures

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)

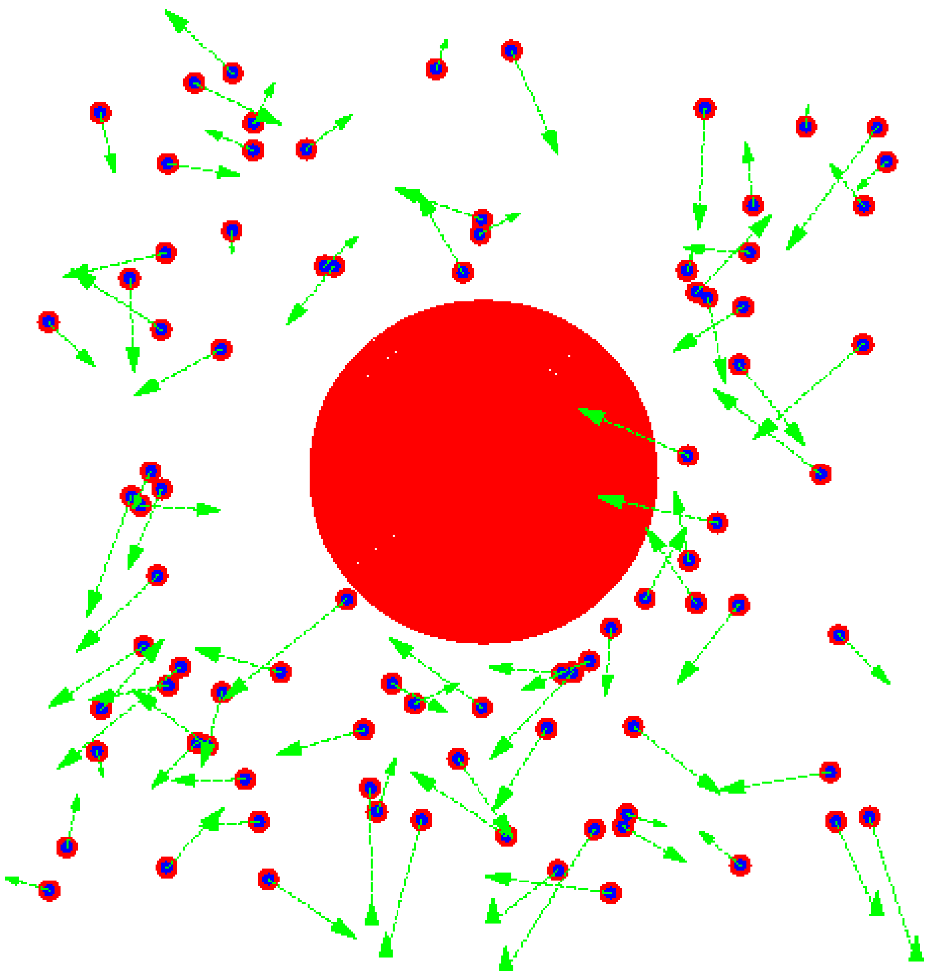
#3: What can Shockwaves Teach Us?

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

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

Analysis from Kinetic Theory

Ideal Gas Thermometer



Temperature is just the *comoving* Kinetic Energy .

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: Viscosity determines ShockWidth

Newtonian Viscosity:

$$P - P_0 = \sim \text{viscosity} \times u_p/\text{width}$$

Kinetic Theory:

$$\text{Viscosity} \sim \text{Mean free path} \times c$$

Conclusion → Shockwaves are Thin:

$$\text{Shock Width} \sim \text{Mean Free Path}$$

#3: Constants of the Motion

$$u/V\ ,$$

$$P_{xx} + (u^2/V)\ ,$$

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

Velocity changes : $u_s \rightarrow (u_s - u_p)$.

#5: Newtonian Viscosity + Fourier Heat Conductivity can convert these to first-order differential equations for u(x) and T(x), which makes it possible to compute P_{xx} and Q_x from the velocity and temperature gradients.

#3: 50% Compression using MD with a Strong Shockwave

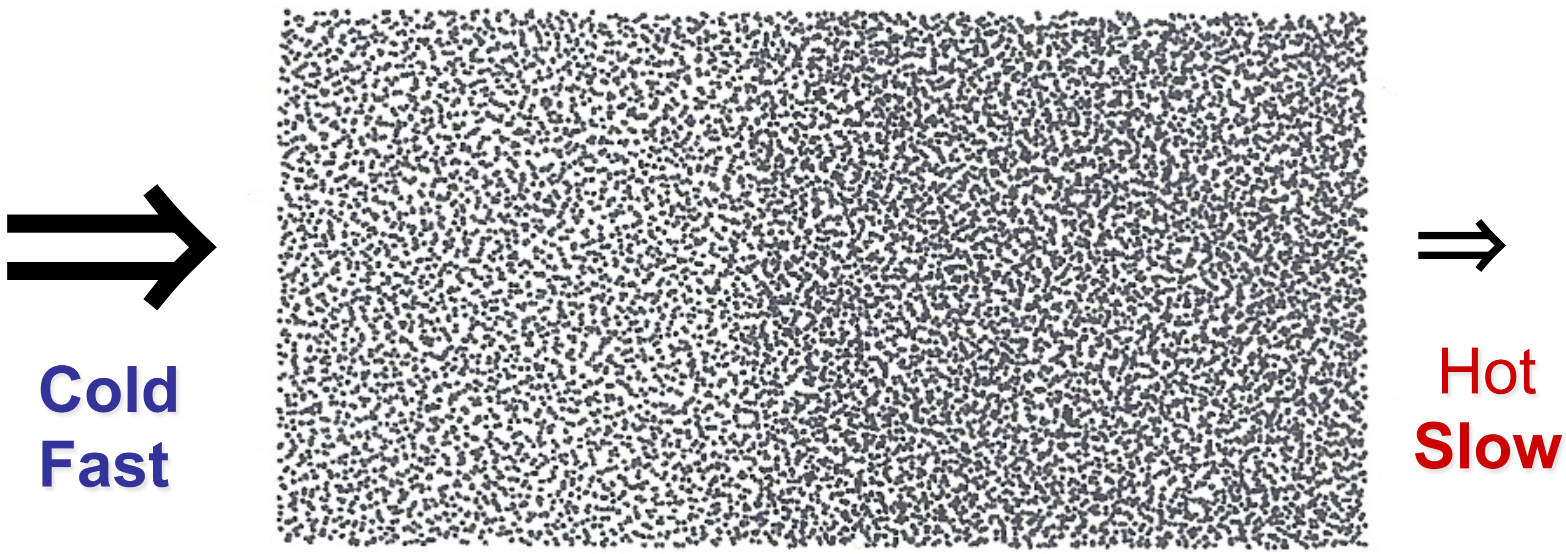
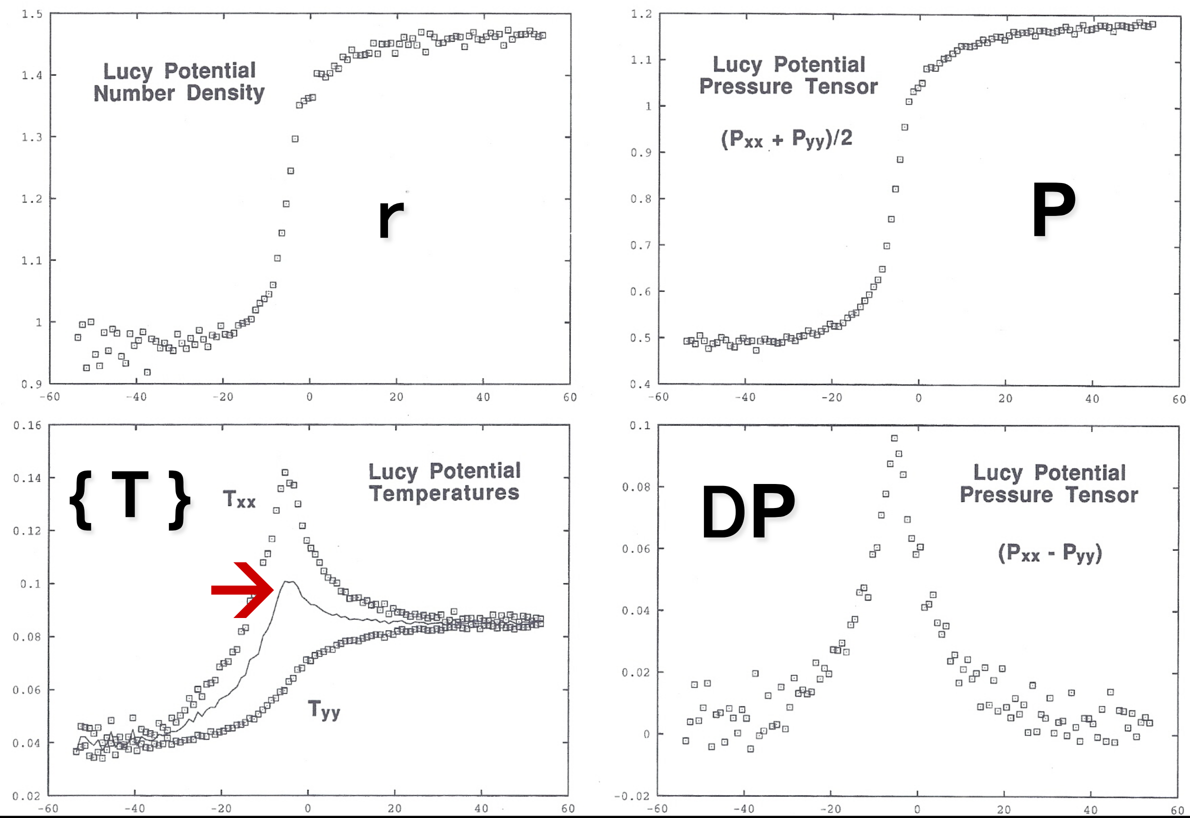


FIG. 1. Snapshot of the 12 960-particle shock wave simulation

This shockwave has quite an interesting temperature profile !

#3: 12,960-Particle Shock Profiles



Flagrant Violation of Fourier's Law !

#4 & #5: Microscopic *versus* MACROSCOPIC viewpoints

#4: microscopic particle mechanics :

Hamiltonian → F = ma

P and Q come from the Virial & Heat Theorems

P is time-reversible while Q is irreversible .

#5: MACROSCOPIC *CONTINUUM* MECHANICS :

Fluxes depend on *gradients* of P and Q ,

[comoving fluxes of momentum and energy]

Typically P and Q depend on gradients of u and e

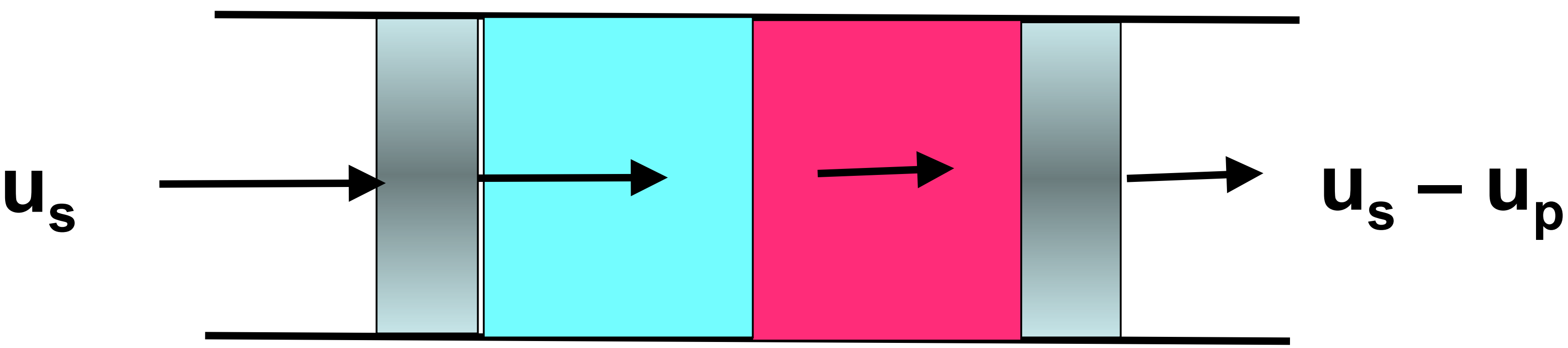
Typically these relations aren't time-reversible

P is irreversible while Q is time-reversible .

How can or do these two prescriptions *ever* agree ?

#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!



#4: Simple Equation of State (with apologies to van der Waals)

Choose a weak repulsive force Resembling the weight function:

Force varies as $[\ 1 - (r/h)\ ]^n$ and is normalized to unity

Expecting to find:

$$e = (1/2V) + T \quad \text{and} \quad P = (e/V)$$

#4: Stationary Shockwave Solution Satisfying Conservation Laws

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

$V_{COLD} = 1$; $V_{HOT} = 1/2$

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

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

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

constant fluxes : 2, (9/2), 2x3

$$\Delta e = (3/4) = \langle -P \rangle \Delta v = (3/2)(1/2)$$

#4 and #5: $P = (1/2V^2) + (T/V) = (e/V)$
→ Solutions for Twofold Compression

$$(u/V) = 2 \; ;$$

$$P_{xx} + (u^2/V) = 9/2 \; ;$$

$$(u/V)\,[\; e + (P_{xx}V) + (u^2/2)\;] + Q_x = 2\text{x}3 = 6$$

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

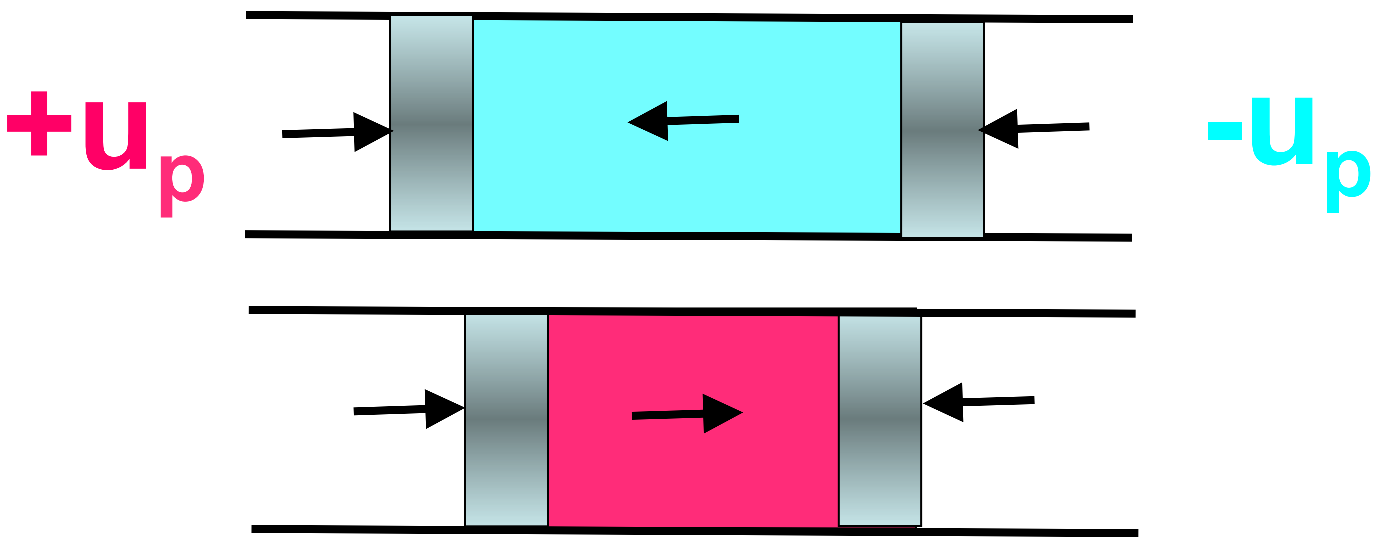
$(u, V, P, e) = (2, 1, 1/2, 1/2) \rightarrow (1, 1/2, 5/2, 5/4)$

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.

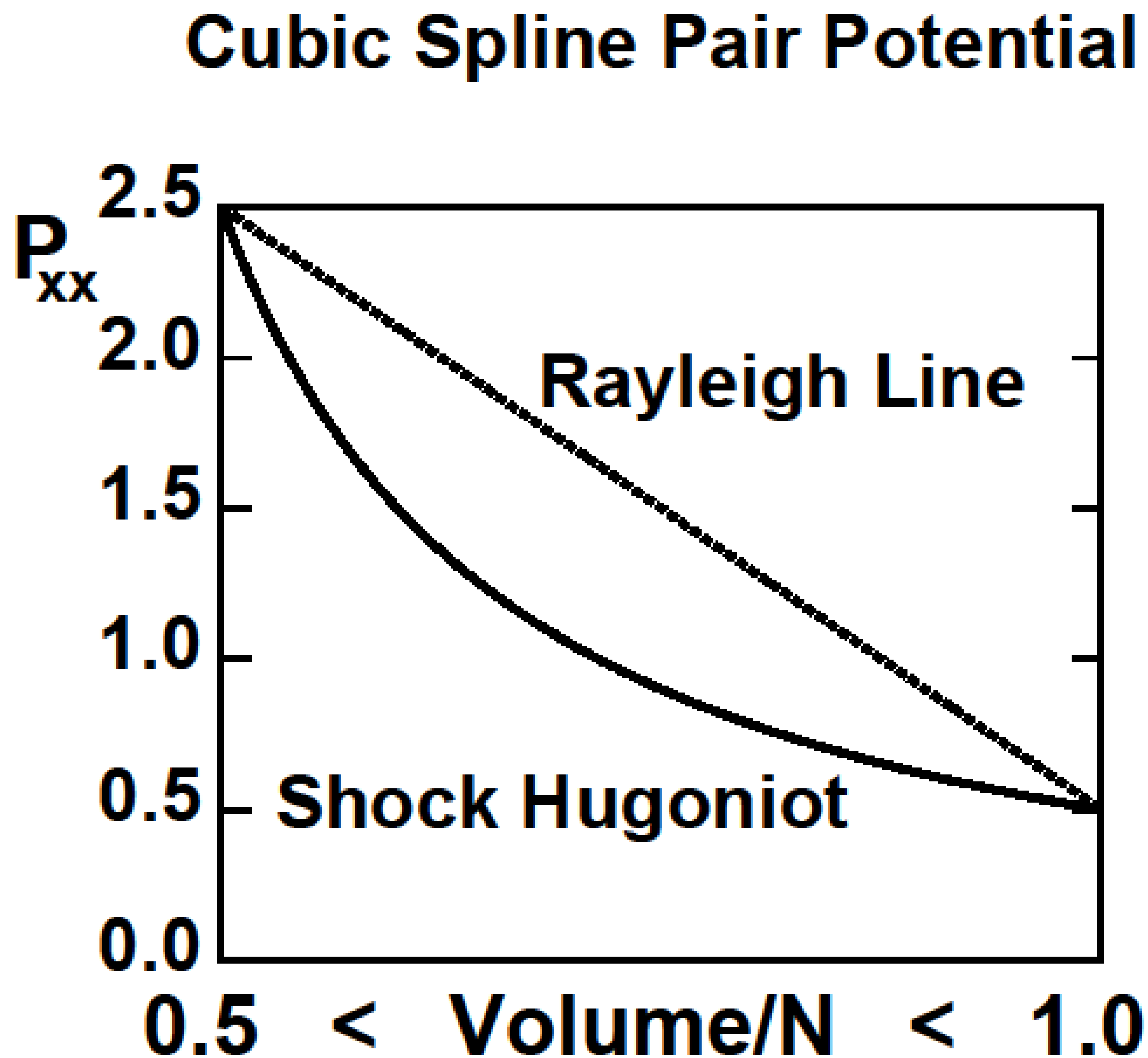
Although the Compression is Irreversible we Conserve Mass, Momentum → Rayleigh Line

$$(u_s / V_0) = (u_s - u_p)/V = M$$

$$P + (u_s - u_p)^2/V = P_0 + u_s^2/V_0$$

$$P - P_0 = (M^2 V_0) - (M^2 V)$$

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


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

#5: MACROSCOPIC CONTINUUM Definitions of Smooth Profiles for "Field Variables" at R

Consider averaging { m, mv, me, . . . }

or pressure, heat flux, gradients, . . .

Each particle's influence is w(r < h) :

$(1/V) = \sum m_i w(r_i - R)$; $u(R)/V(R) = \sum m_i v_i w(r_i - R)$

Gradients of (1/V), (u/V), (e/V), . . .

Give sums with gradients of $w(r_i)$

w is a smooth-particle weight function

CONTINUUM MODELS depend on h !

#4 microscopic *versus* #5 MACROSCOPIC viewpoints

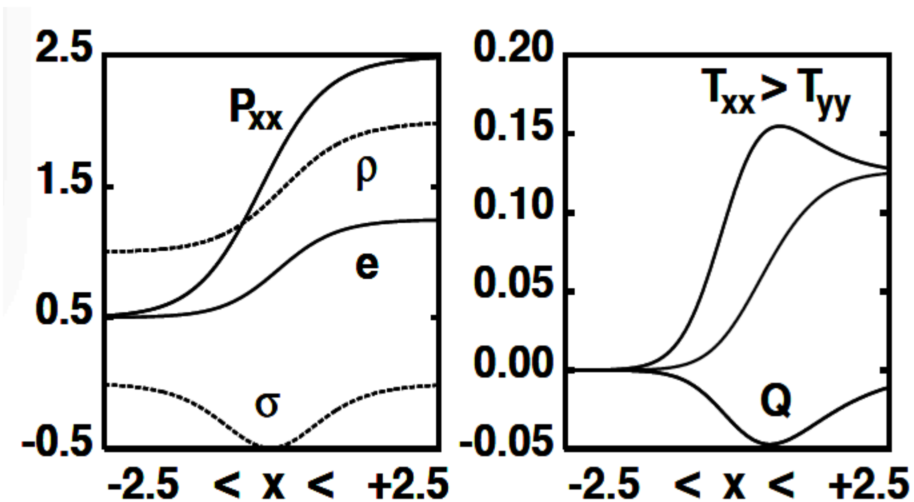
How can these two prescriptions ever agree ?

1: The smoothing length h can be chosen arbitrarily

2: A delay time tau can also be chosen for the heat flux Q and the shear stress $(P_{xx} – P_{yy})/2$:

$$Q + \text{tau}(dQ/dt) = - K(dT/dx)$$

But, remember that T_{xx} and T_{yy} are quite different :



#6: Smooth-Particle Profiles in either One or Two Dimensions

$$\mathrm{rho}(x) = \sum_j w(x - x_j)$$

where, with $r = | x |$

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

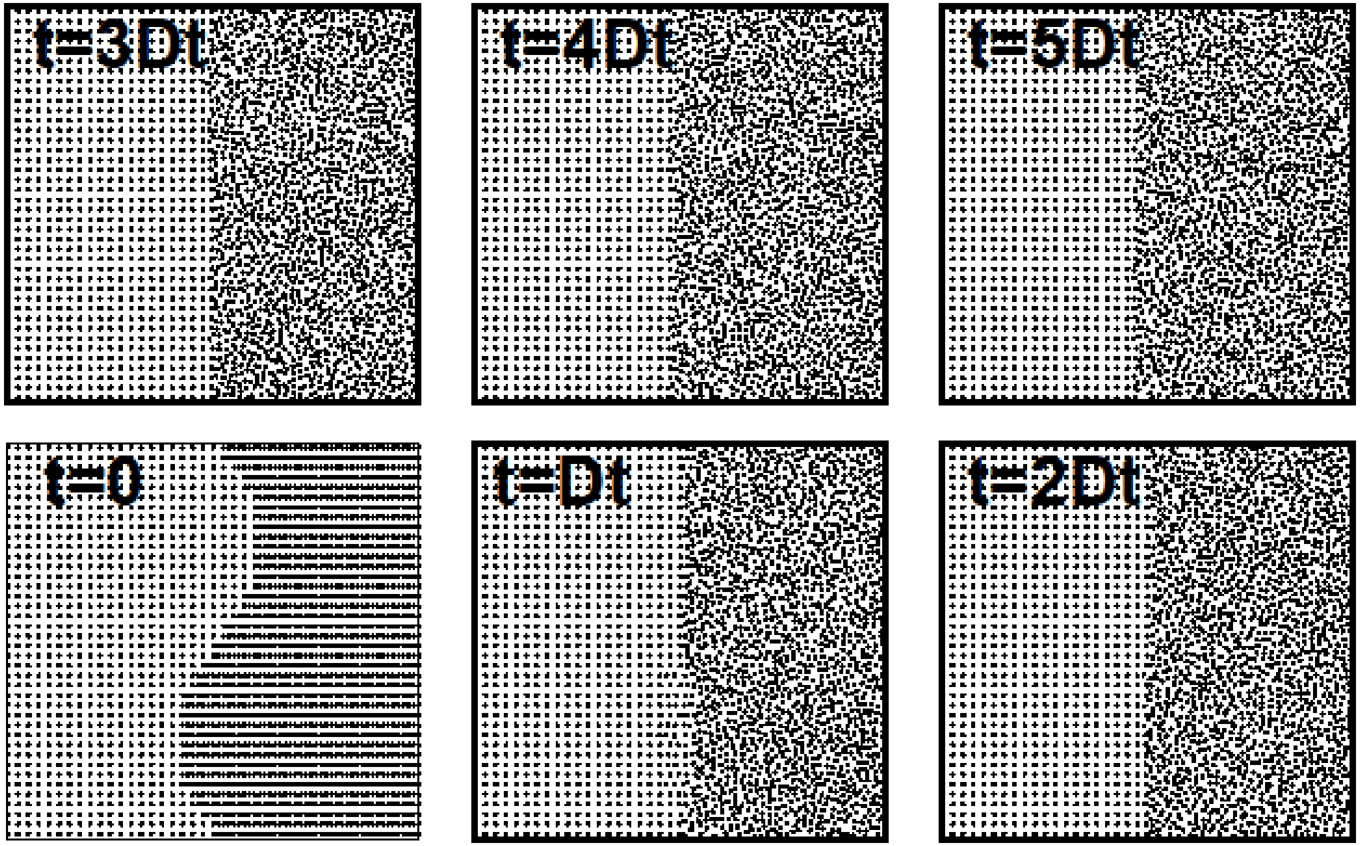
or

$$\mathrm{rho}(x,y) = \sum_j w(x - x_j, y - y_j)$$

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

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

#6: What about Shock Stability?



Sinusoidal Initial Condition

#6: What about Temperature?

Kinetic Temperature $\leftarrow$ Momenta

Configurational Temperature $\leftarrow$ Forces

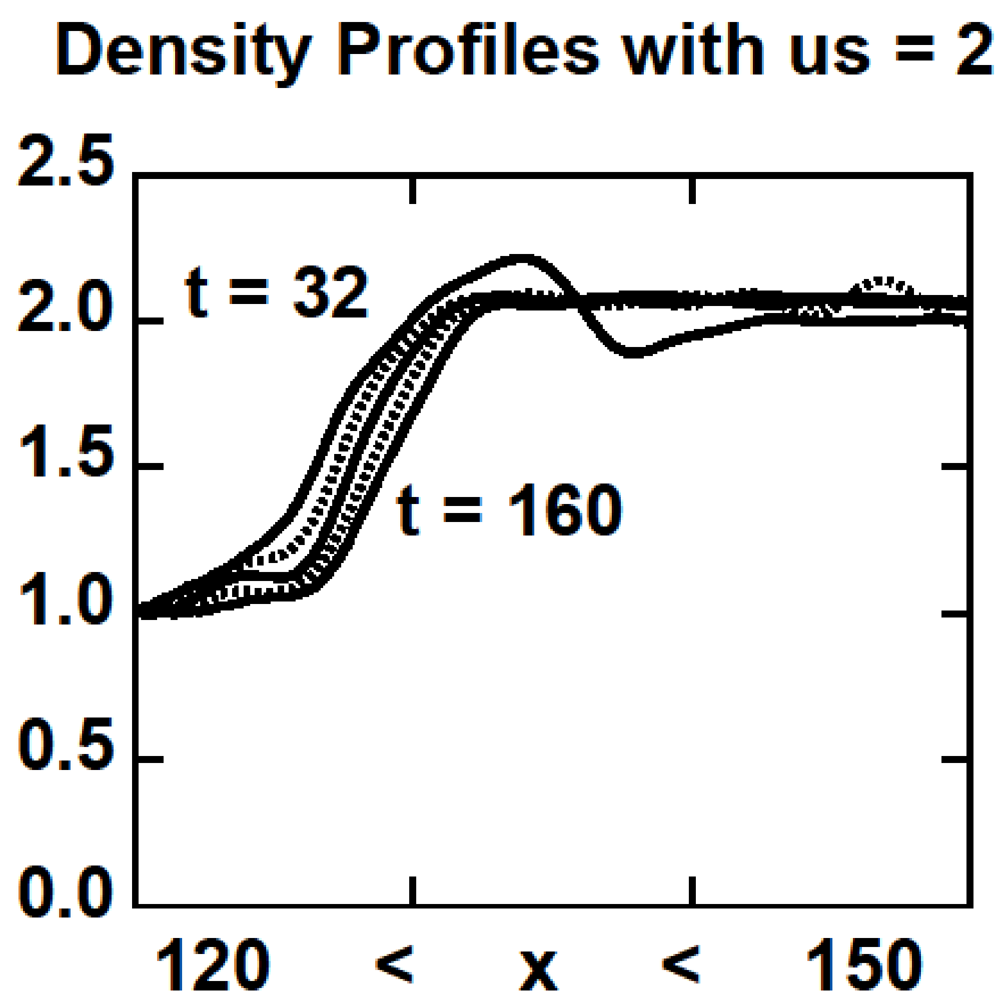
$kT_{Kinetic} = \langle p^2/m \rangle$ **relative to mean flow**

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

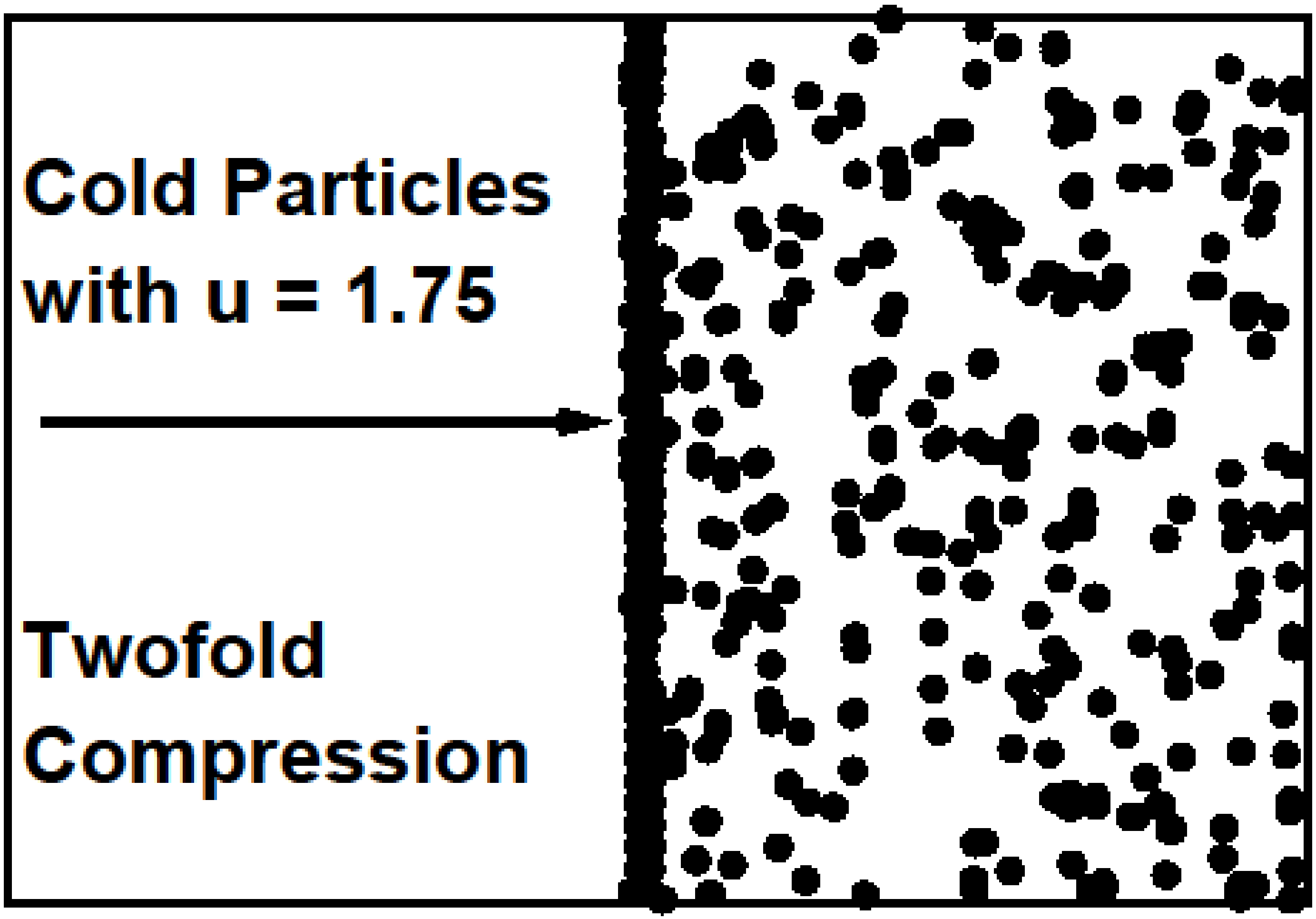
Determine the mean flow by using w(r):

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

#6: The Shockwave profile narrows with time, indicating that it is STABLE !



Negative Temperature Particles



#6: Development of Smooth Profiles for "Field Variables" at R

Consider averaging { m, mv, me, . . . } within a radius h of R :

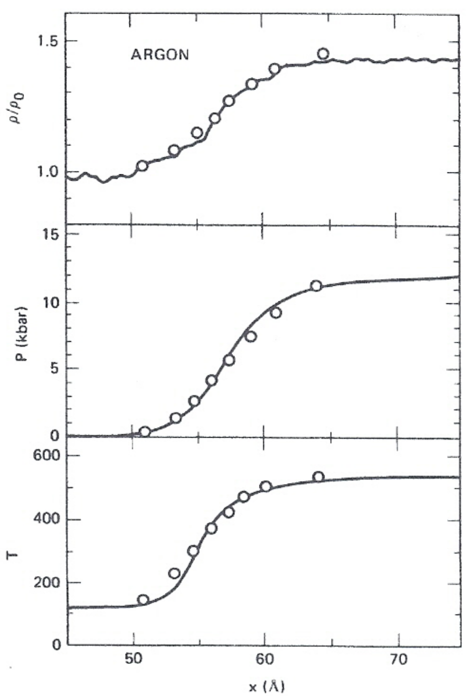
$$\mathrm{rho}(R) \approx \sum_i m_i(r_i)w(r_i-R) \text{ where}$$

$$w_{2D} = (10/\pi h^2)[\ 1 - (r/h)\ ]^3 \text{ or}$$

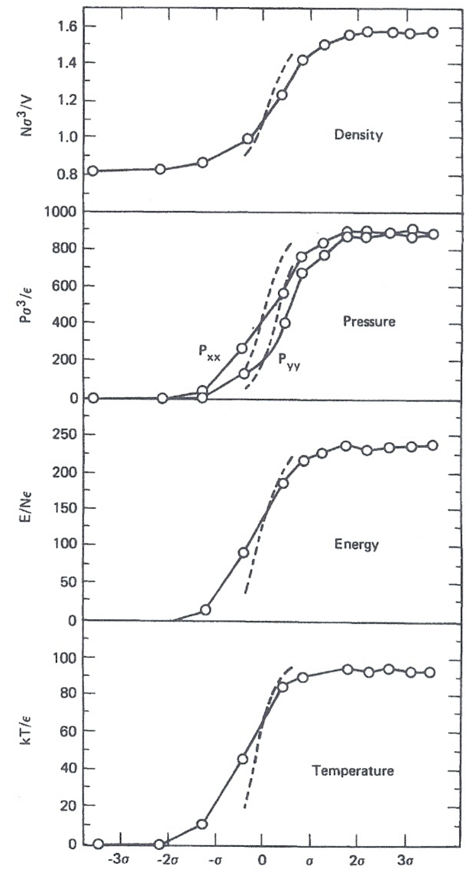
$$w_{2D} = (10/\pi h^2)[\ 1 - (r/h)\ ]^3[\ 1 + 3(r/h)\ ]$$

w is *normalized* with integral = 1

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 .

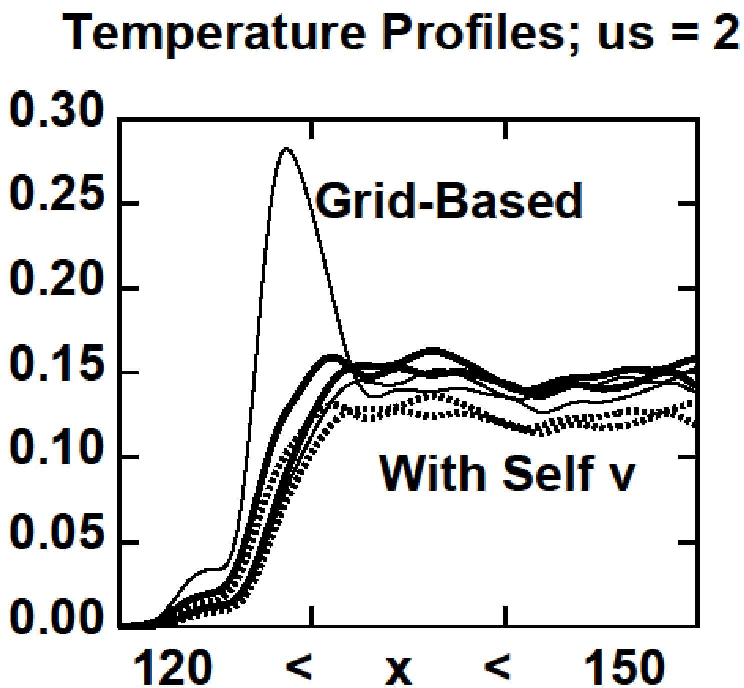
N-S ←→ MD

#7: 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 in fact

* See Mott-Smith in 1951 Physical Review.

#7 : Lessons So Far



Normalized potential ~ $(1 - r)^3$

The spatial integral is set equal to unity. The choice of the local Temperature depends on whether or not the "Self" contribution is included in the sums.

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.

#7: Lessons So Far*

- Thickness is of order the Mean Free Path
- One-dimensional shocks are Stable
- Kinetic Temperature is a Tensor
- Configurational Temperature is Poor
- Nonlinear Viscosity is Complex
- Time Delay is Typical

* arXiv:0905.1913 : T and Stability

* arXiv:1005.1525 : work, heat, relaxation

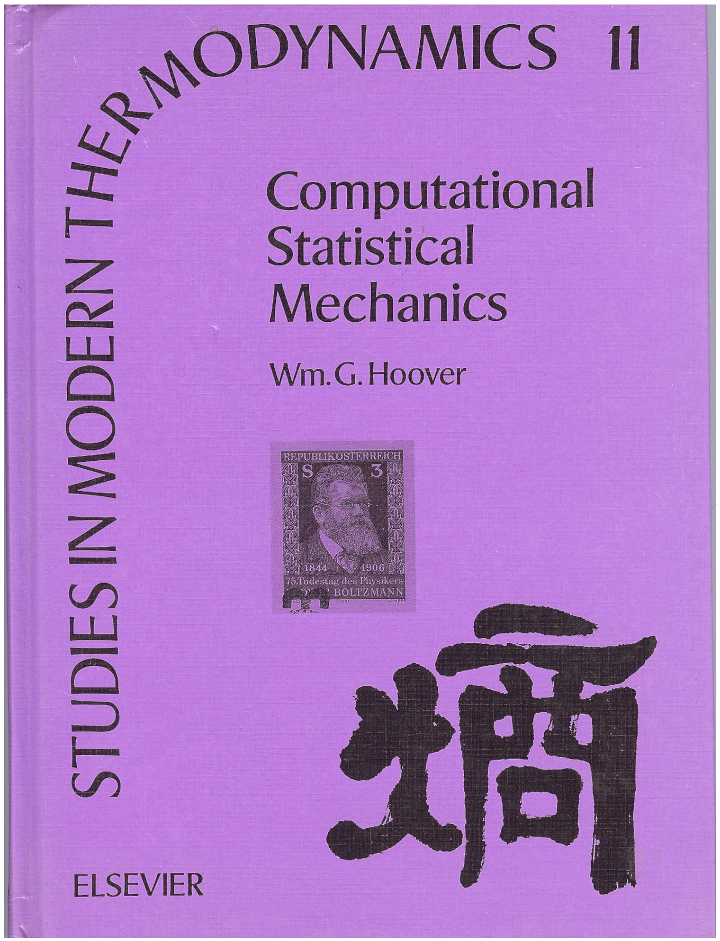
#7: Remaining Puzzles*

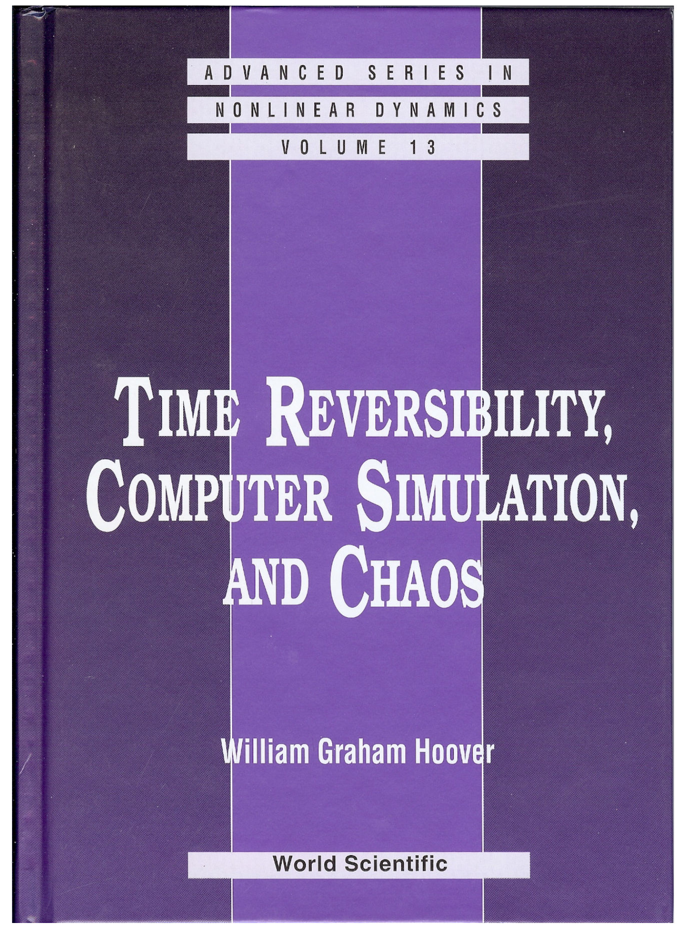
- Description of Temperature/Heat Flow
- Direct Measurement of Shock Heat Flux
- Cell Model of the Shockwave Process
- Prediction of the Nonlinear Viscosity
- Best Definitions of P_{xx}, rho, u, h, *et cetera*

* arXiv:0905.1913 : T and Stability

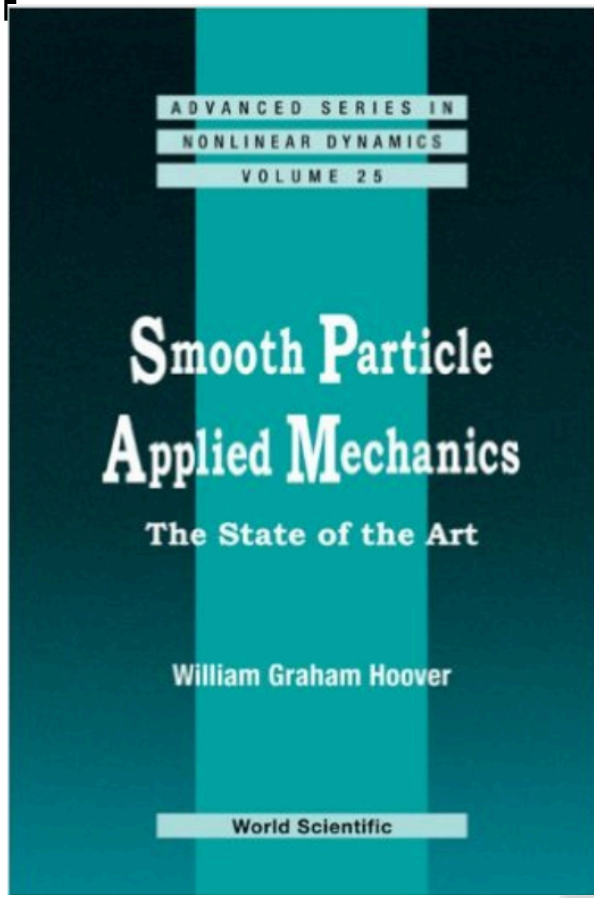
* arXiv:1005.1525 : work, heat, relaxation

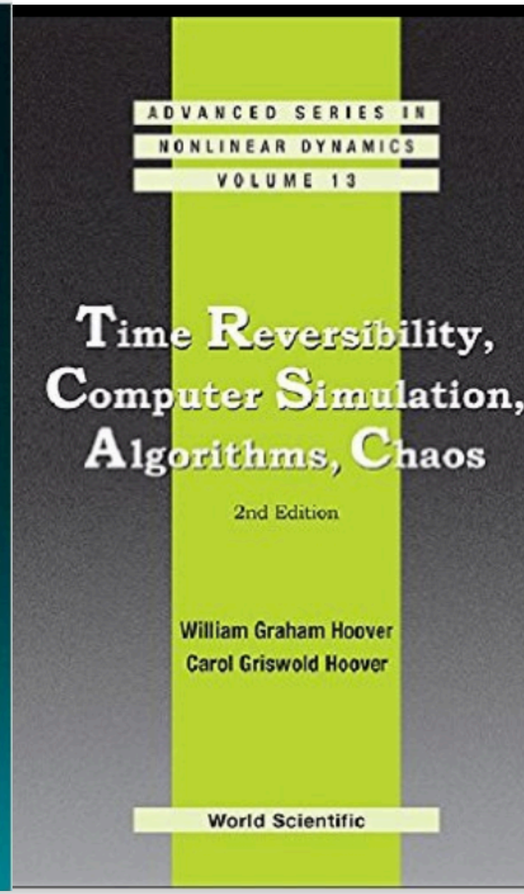
Some Useful Reference Books

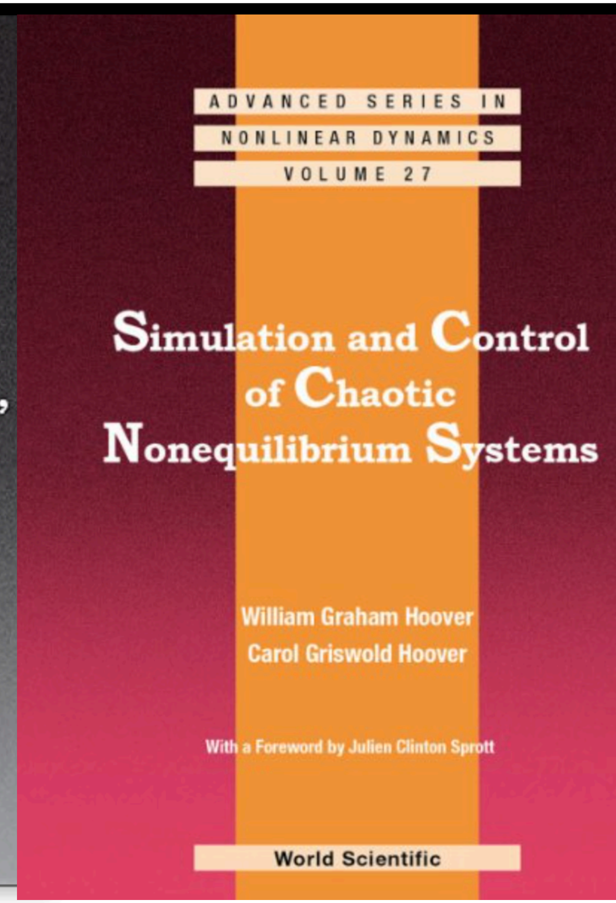


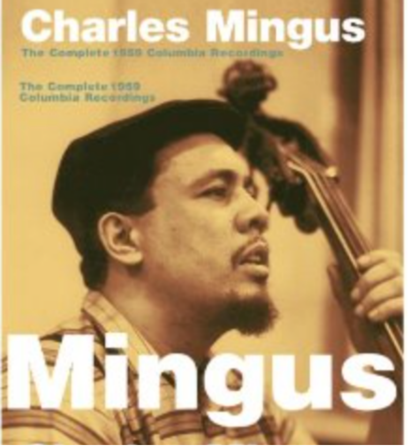


Some Useful Reference Books



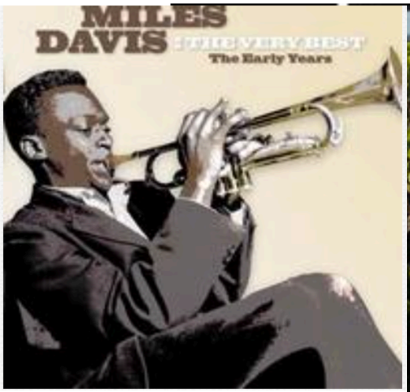






2015 Ian Snook Prize :
$1000 US for the most interesting
Ergodic Time-Reversible Map
Of Unit Square Into Itself

← 1996 Computational Methods in
Science and Technology
21(3) [2015]



2007 with
Ian & Marie →