

Chapter 1

Shockwaves and Local Hydrodynamics; Failure of the Navier-Stokes Equations

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Shockwaves provide a useful and rewarding route to the nonequilibrium properties of simple fluids far from equilibrium. For simplicity, we study a strong shockwave in a dense two-dimensional fluid. Here, our study of nonlinear transport properties makes plain the connection between the observed local hydrodynamic variables (like the various gradients and fluxes) and the chosen recipes for defining (or “measuring”) those variables. The *range* over which nonlocal hydrodynamic averages are computed turns out to be much more significant than are the other details of the averaging algorithms. The results show clearly the incompatibility of microscopic time-reversible cause-and-effect dynamics with macroscopic instantaneously-irreversible models like the Navier-Stokes equations.

1.1. Introduction

Leopoldo García-Colín has studied nonequilibrium fluids throughout his research career. In celebrating his Eightieth Birthday we conform here to his chosen field of study. Though Leo’s approach is typically quite general, looking for improvements on linear transport theory, he has studied particular problems too. A specially interesting and thought-provoking study, with Mel Green, of the nonuniqueness of bulk viscosity [1], emphasised the general problem of finding appropriate definitions for state variables far from equilibrium. The magnitude of the bulk viscosity gives the additional viscous pressure due to the compression *rate*. The pressure difference evidently depends upon the underlying definition of the equilibrium reference pressure. The reference pressure itself in turn depends upon the choice between temperature and energy in *defining* the reference state. In the end,

the same physics results, as it always must; the valuable lesson is that many different languages can be used to describe the underlying physics. There is the tantalizing possibility that some one approach is better than others.

In fact, temperature itself can have *many* definitions away from equilibrium [2]. Away from equilibrium the *thermodynamic* temperature would depend upon defining a nonequilibrium entropy – and there is good evidence that there is no such entropy. This is because nonequilibrium distribution functions are typically fractal, rather than smooth [3]. The *kinetic* temperature, a measure of the velocity fluctuation, becomes a *tensor* away from equilibrium [2,4]. At low density this temperature is the same as the pressure tensor, $P = \rho T$. For dense fluids the potential energy introduces *nonlocality*, complicating the definition of constitutive averages. The simplest of the many *configurational* temperatures [5–7] depends on force fluctuations, and so likewise has tensor properties. Because configurational temperature can be negative [8] and because thermodynamic temperature is undefined away from equilibrium, we focus our attention on kinetic temperature here.

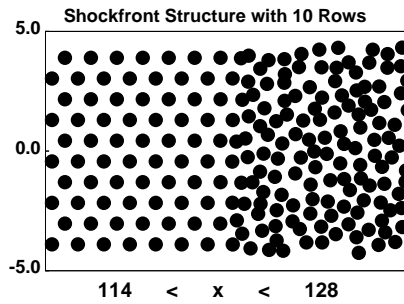


Fig. 1.1. Closeup of a strong shockwave. The cold stress-free solid on the left moves to the right at twice the speed of the hot fluid, which exits to the right. The boundaries in the vertical y direction are periodic. The pair potential is $\phi(r < 1) = (10/\pi)(1 - r)^3$. The overall density change is $\sqrt{4/3} \rightarrow 2\sqrt{4/3}$ and $u_s = 2u_p = 1.93$. The system height is $10\sqrt{3/4} \simeq 8.66$.

Shockwaves are irreversible transition regions linking a “cold” and a “hot” state [8–11]. Such a shock region contains nonequilibrium gradients in density, velocity, and energy. The irreversible change from cold to hot takes place in just a few free paths in a time of just a few collision times [11]. The localized nature of shockwaves makes them ideal for computer simulation. Their gross one-dimensional nature, illustrated in Figure 1, makes it possible to compute *local* averages in a region of width h . Because

h is necessarily small it is evident that the average values depend on it. Thus the average temperature depends upon both the underlying definition of temperature and additionally on the details of the local averaging.

In this work we begin by describing molecular dynamics simulations, for a strong, nominally stationary and one-dimensional shockwave, in a two-dimensional fluid. Next, we discuss the Navier-Stokes description of such a wave and then set out to compare the two approaches, focusing on the definition of local hydrodynamic variables. A close look at the momentum and heat fluxes shows clear evidence for the incompatibility of the microscopic and macroscopic constitutive relations.

1.2. The Microscopic Model System and a Continuum Analog

We consider structureless particles of unit mass in two space dimensions interacting with the short-ranged purely-repulsive pair potential,

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

As shown in Figure 1, particles enter into the system from the left, moving at the shock velocity u_s . Likewise, particles exit at the right with a lower mean speed, $u_s - u_p = u_s/2$, where u_p is the “Particle” or “piston” velocity. The velocity ratio of two which we choose throughout is consistent with twofold compression. We carried out series of simulations, all with a length of 250 and the shock near the system center, with system widths of from 10 to 160 rows. Figure 1 shows a closeup of the center of such a 10-row flow for the narrowest system width, $10\sqrt{3}/4 \simeq 8.66$.

To analyze the results from molecular dynamics one and two-dimensional average values of the density, energy, pressure, heat flux and the like were computed using the one- and two-dimensional forms of Lucy’s weight function [12,13]:

$$w^{1D}(r < 1) = (5/4h)(1 - r)^3(1 + 3r) ; r \equiv |x|/h .$$

$$w^{2D}(r < 1) = (5/\pi h^2)(1 - r)^3(1 + 3r) ; r \equiv \sqrt{x^2 + y^2}/h .$$

The averages are not significantly different to those computed with Hardy’s more cumbersome approach [14].

A preview of the one-dimensional averages results from molecular dynamics’ simplest continuum analog, a solution of the stationary Navier-Stokes equations. For simplicity, in the Navier-Stokes analog we use the

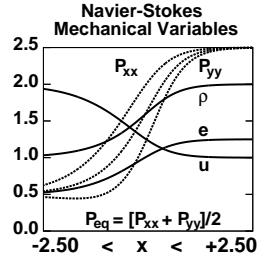


Fig. 1.2. The nonzero pressure-tensor components from the Navier-Stokes equations solution, P_{xx} and P_{yy} , as well as their average, $P = (\rho^2/2) + \rho T$, are shown as dashed lines along with the velocity, energy, and density profiles. In this simple example it is assumed that the bulk viscosity vanishes so that the average of the longitudinal and transverse components is equal to the equilibrium pressure.

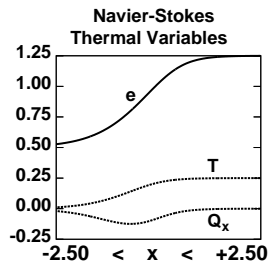


Fig. 1.3. The energy, (scalar) temperature, and heat flux vector from the Navier-Stokes equations are shown here. The heat conductivity and shear viscosity coefficients were assumed equal to unity in the underlying calculation.

constitutive relations for the van-der-Waals-like model with shear viscosity and heat conductivity of unity:

$$P = \rho e = (\rho^2/2) + \rho T ; e = (\rho/2) + T$$

$$(P_{xx} - P_{yy})/2 = -du/dx ; (P_{xx} + P_{yy})/2 = P ;$$

$$Q_x = -dT/dx .$$

This model is similar to our microscopic simulation model, but has a nonzero initial pressure and energy. A set of self-consistent cold and hot boundary conditions for the Navier-Stokes velocity, pressure, energy, and scalar temperature is as follows:

$$u : [2 \rightarrow 1] ; \rho : [1 \rightarrow 2] ; P : [1/2 \rightarrow 5/2] ; e : [1/2 \rightarrow 5/4] ; T : [0 \rightarrow 1/4] .$$

These boundary conditions satisfy conservation of mass, momentum, and energy. The (constant) mass, momentum, and energy fluxes *throughout* the shockwave (not just at the boundaries) are:

$$\rho u = 2 ; P_{xx} + \rho u^2 = 5/2 ; \rho u [e + (P_{xx}/\rho) + (u^2/2)] + Q_x = 6 .$$

The most noteworthy feature of the numerical solution is the slight decrease of P_{yy} below the equilibrium value on the cold side of the shock. Figure 2 shows the mechanical variables and Figure 3 the thermal variables near the center of the shock as computed from the Navier-Stokes equations [11]. A serious shortcoming of the Navier-Stokes equations is their failure to distinguish the longitudinal and transverse temperatures.

1.3. Averaged Results from Molecular Dynamics

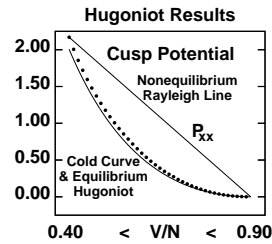


Fig. 1.4. The longitudinal pressure tensor component P_{xx} varies linearly with volume, and follows the Rayleigh line. The cold curve corresponds to the pressure of a perfect static triangular lattice. The equilibrium Hugoniot, indicated by dots, corresponds to thermodynamic equilibrium states accessible from the initial cold state by shockwave compression. For P_{yy} see Figure 7.

One-dimensional averages reproduce the linear dependence of P_{xx} on the volume very well. That linear dependence is the “Rayleigh Line”, shown in Figure 4. The “cold curve” in that Figure is the calculated pressure for a cold triangular lattice:

$$P_{\text{cold}}V = 3NrF(r); r = \sqrt{(V/V_0)}; V_0 = \sqrt{3/4}N; F(r) = (30/\pi)(1-r)^2 .$$

That pressure lies a bit below the Hugoniot curve (the locus of all equilibrium states which can be reached by shocking the initial state). The Hugoniot pressure at each volume was generated by trial-and-error isothermal (isokinetic) molecular dynamics runs, leading to the temperatures satisfying

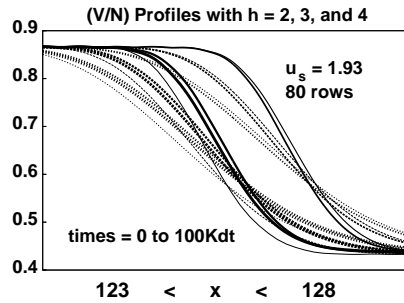


Fig. 1.5. Shockwave profiles at five equally-spaced times. The five line widths correspond to times of 0, 25,000dt, 50,000dt, 75,000dt, and 100,000dt. The steepest profiles correspond to $h = 2$. Results for $h = 3$ and $h = 4$ are also shown. The fourth-order Runge-Kutta timestep, here and throughout, is given by $dt = 0.02/u_s \simeq 0.01$.

the Hugoniot relation:

$$E_{\text{hot}} - E_{\text{cold}} = +\Delta V [P_{\text{hot}} + P_{\text{cold}}]/2; \quad \Delta V = V_{\text{cold}} - V_{\text{hot}} .$$

Figure 5 shows typical one-dimensional snapshots of the shockwave profile, $V(x)$. The averages shown in the Figure were computed at 5 equally-spaced times, separated by 25,000 timesteps. The fluctuating motion of the shockwave, of order unity in 100,000 timesteps, corresponds to fluctuations in the averaged shock velocity of order 0.001.

The apparent shockwidth is sensitive to the range of the weighting function h . $h = 2$ is evidently *too small*, as it leads to discernable wiggles in the profile. The wider profiles found for $h = 3$ and $h = 4$ indicate that the constitutive relation describing the shockwave must depend explicitly on h . That is, h must be chosen sufficiently large to avoid unreasonable wiggles, but must also be sufficiently small to capture and localize the changes occurring within the shockwave.

Two-dimensional averages are no more difficult to evaluate. The density at a two-dimensional gridpoint, for instance, can be evaluated by summing the contributions of a few dozen nearby particles:

$$\rho_r \equiv \sum_j w_{rj}^{2D} = \sum_j w^{2D}(|r - r_j|) .$$

Such sums are automatically continuous functions of the gridpoint location r . They necessarily have continuous first and second derivatives too, provided that the weight function has two continuous derivatives, as does Lucy's weight function [12,13]. Linear interpolation in a sufficiently-fine grid can then provide *contours* of macroscopic variables. Figure 6 is an

illustration, and shows the contour of average density at 10 equally-spaced times. The boundary value of u_s for that Figure was chosen as 1.92 rather than the shock velocity of 1.93. Thus the shockfront moves slowly to the left in the Figure, with an apparent picture-frame velocity of -0.01 .

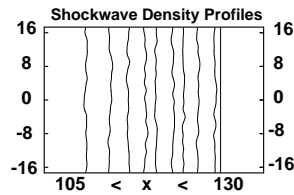


Fig. 1.6. Ten average-density contours (corresponding to the shockfront position) at equally-spaced times for a 40-row system. The amplitude of the fluctuations, of order unity, is similar to the range of the weight function h . The total timespan is 225,000 timesteps. Because the entrance velocity, at $x = 0$, is $u_s = 1.92$, rather than 1.93, the shockfront moves slowly toward the left, with a picture-frame velocity of about -0.01 .

Figure 7 shows the nonequilibrium equation of state within the shockwave, the variation of the pressure tensor components P_{xx} and P_{yy} with the specific volume, $(V/N) \equiv (1/\rho)$. P_{xx} is insensitive to the smoothing length h (as is required by the momentum conservation condition defining the Rayleigh line) while P_{yy} shows a slight dependence on h . This lack of sensitivity of the pressure tensor suggests that nonequilibrium formulations of the equation of state within the shock can be successful.

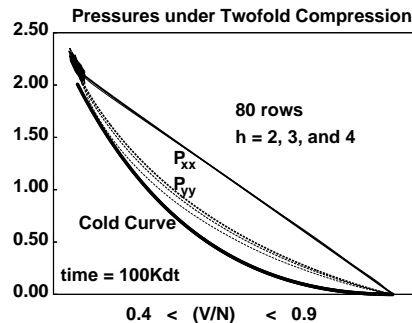


Fig. 1.7. Typical snapshot of the dependence of P_{xx} and P_{yy} on the volume (V/N) . The line width increases with the range $h = 2, 3, \text{ and } 4$. The range-dependence of P_{xx} is too small to be seen here while it is possible to see a small increase in P_{yy} with increasing h .

The conventional Newton and Fourier constitutive relations require that gradients be examined too. *Gradients* can be evaluated directly from sums including ∇w . Consider the gradient of the velocity at a gridpoint r as an example (where w_{rj} is the weight function for the distance separating the gridpoint from Particle j):

$$(\rho \nabla \cdot v + v \cdot \nabla \rho)_r \equiv \nabla \cdot (\rho v) \equiv \nabla_r \cdot \sum_j w_{rj} v_j = \sum_j v_j \cdot \nabla_r w_{rj} .$$

Using the identity,

$$\rho = \sum_j w_{rj} ,$$

gives

$$(\rho \nabla \cdot v)_r = \sum_j (v_j - v_r) \cdot \nabla_r w_{rj} .$$

The tensor temperature gradient can be evaluated in the same way:

$$(\rho \nabla \cdot T)_r = \sum_j (T_j - T_r) \cdot \nabla_r w_{rj} .$$

Figure 8 compares the velocity gradients as calculated using three values of h to the pressure tensor using the same three values. We see that the velocity gradient is much more sensitive than is the stress to h , suggesting a sensitive dependence of the Newtonian viscous constitutive relation on the range of the weight function. The data in the Figure indicate a shear viscosity of the order of unity. Gass' Enskog-theory viscosity [15] confirms this estimate.

Figure 9 shows the temperature gradients. There are two of these for each h because the longitudinal and transverse temperatures differ. Again the magnitudes of the gradients are relatively sensitive to h while the maximum in the nonequilibrium flux Q_x is less so. Again the heat conductivity from the data is of the order of Gass' Enskog-theory estimate.

1.4. Conclusion: Failure of Navier-Stokes Equations

Results from earlier shockwave simulations [9,11,16] have uniformly been described as showing "good" or "fairly good" agreement with continuum predictions. Examining the more nearly accurate profiles made possible with improved averaging techniques shows that the agreement is actually limited, and in a qualitative way. A more detailed look at the data shown

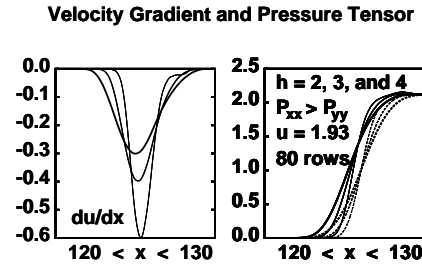


Fig. 1.8. The velocity gradient, for three values of h , is much more sensitive than is the shear stress, $(P_{yy} - P_{xx})/2$, to h . The gradient extrema, at 125.35, 125.18, and 125.01 precede the shear stress extrema at 125.67, 125.61, and 125.57 for $h = 2, 3$, and 4.

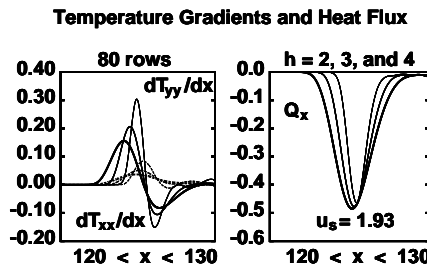


Fig. 1.9. The temperature gradients (the dashed lines correspond to the transverse temperature) for three values of h correspond to the heat fluxes found with the same h values. The pronounced maximum in T_{xx} indicates a violation of Fourier's Law, as the heat flux does not show a corresponding change of sign. The maxima in dT_{xx}/dx occur at distances 124.93, 124.49, and 124.09, significantly leading the flux maxima at 125.44, 125.29, and 125.15 for $h = 2, 3$, and 4.

in Figures 8 and 9 reveals a consistent “fly in the ointment” pattern: the largest fluxes are *not* located at the largest values of the gradients. The fluxes lag behind the gradients by a (relaxation) time of order unity. This shows that no simple instantaneous relationship links the fluxes to the gradients. *In molecular dynamics the instantaneous stress cannot be proportional to the instantaneous strain rate.*

The reason for this apparent contradiction of linear transport theory is plain enough: the underlying molecular dynamics is time-reversible, so that pressure is necessarily an *even* function of velocity and time. This same symmetry must be true also of any spatially-averaged instantaneous pressure. Because there is no possibility to find an instantaneous irreversible constitutive relation with time-reversible molecular dynamics, it is apparent

that any attempt to “explain” local molecular dynamics averages through irreversible macroscopic constitutive relations is doomed to failure.

There is of course no real difficulty in carrying out the instantaneous averages, in one or two or three space dimensions, for today’s molecular dynamics simulations. On the other hand, the gap between the microscopic and macroscopic pictures becomes an unbridgable chasm when the detailed spatiotemporal contradictions between the two approaches are considered.

1.5. Prospects

The prospect of understanding shockwaves in gases has stimulated studies of dilute gases, based on the Boltzmann equation [17–20]. Leo has been a driving force for this work. Though the analysis is highly complex [19, 20] it has become apparent that the Boltzmann equation is itself nicely consistent with corresponding solutions using molecular dynamics [17,18], up to a Mach number $M = u_s/c_{\text{cold}}$ of 134. The applicability of the Burnett equations, which include all second-order contributions of the gradients to the fluxes, is still in doubt for strong shockwaves in dilute gases [17,18].

Dense fluids will require a new approach. Local averages must be defined. Longitudinal and transverse temperatures must be treated separately. The causal timelag between the forces (velocity and temperature gradients) and the resulting momentum and heat fluxes must be included in the modelling. Although these challenges are enormous, today’s fast computers place the responsibility for successfully meeting them squarely on physicists’ imaginations. The excuse that the problem is too hard to tackle is no longer valid. We can look forward to many more contributions from Leo, his coworkers, and those inspired and stimulated by his work.

Acknowledgment

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