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Temperature maxima in stable two-dimensional shock waves

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We use molecular dynamics to study the structure of moderately strong shock waves in dense two-dimensional fluids, using Lucy's pair potential. The stationary profiles show relatively broad temperature maxima, for both the longitudinal and the average kinetic temperatures, just as does Mott-Smith's model for strong shock waves in dilute three-dimensional gases. [S1063-651X(97)01507-9]

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I. INTRODUCTION

Smooth-particle applied mechanics is a particle method for solving the partial differential equations of continuum mechanics [1–3]. The moving particles have localized spheres of influence, characterized by weighting functions $\{w(r)\}$, centered on the particles. The particle motion is governed by ordinary differential equations and so resembles molecular dynamics [4]. In the special case of a two-dimensional ideal gas, the smooth-particle equations are actually isomorphic to those of molecular dynamics [4], with the smooth-particle weighting function w playing the role of a pair potential.

Recent studies of this isomorphism emphasized the transport coefficients of an ideal smooth-particle fluid [5–7]. Particles of finite size have finite transport coefficients, causing a number dependence in particulate continuum simulations. This dependence on particle number is analogous to the interpolation errors that occur when a continuum is described by a coarse grid of points. The viscosity and heat conductivity of smooth particles can be understood fairly well by applying Enskog's kinetic theory of transport [8,9].

Here we simulate a strongly nonlinear inhomogeneous flow: a stationary planar fluid shock wave in two space dimensions. We investigate three main points: (i) stability of the planar shock wave structure in two dimensions; (ii) consistency of the shock wave profiles with the known transport coefficients; and (iii) anisotropicity of the temperature tensor T_{ij}. Previous fluid studies have been devoted to these issues in three space dimensions [10,11]. Recent work has suggested that the longitudinal temperature T_{xx} is more relevant to shock wave transport than the mean temperature T is [11]. The results we find in two dimensions suggest that Mott-Smith's picture [12] of a shock wave as an intimate mixture of hot and cold particles is an apt description for dense fluids with weak repulsive potentials. In the following sections, we describe our simulation technique, give some sample results, and record our conclusions.

II. SHOCK WAVE SIMULATIONS USING LUCY'S POTENTIAL

Lucy's weight function [2], used here as a pair potential, has two continuous derivatives and a finite range h:

$$w_{Lucy}(r)=(5/\pi h^2)[1+3(r/h)][1-(r/h)]^3; \quad r<h.$$

The constitutive properties for this potential are known fairly well. Hoover and Hess provided an accurate Grüneisen description for its equation of state [7]. They pointed out that the shear viscosity η and heat conductivity κ can be usefully approximated by their low-density forms:

$$\eta=0.24\sqrt{mkT}[1+4(h^2kT)^2]/h=\kappa m/(4k).$$

For the relatively low kinetic "temperatures," $\langle mv^2\rangle/2k$, and relatively high densities, $N/V \gg h^{-2}$, considered in the present work, the combination (h^2kT) is of order unity, so that the transport properties are dominated by collective effects of order $T^{5/2}h^3$.

We first studied shock wave propagation in the two-dimensional Lucy fluid by implementing a two-dimensional analog of the algorithm discussed in Ref. [10]. There, two similar samples of cold fluid collide symmetrically, with velocities equal to the "piston velocity" $\pm u_p$, launching twin shock waves at the collision plane, which propagate into the cold fluid with the "shock velocity" $\pm u_s$. For twofold compression of a relatively cold gas, the shocked material was so slow in reaching thermal equilibrium that system lengths of several hundred particle diameters were inadequate for convergence to a stationary profile.

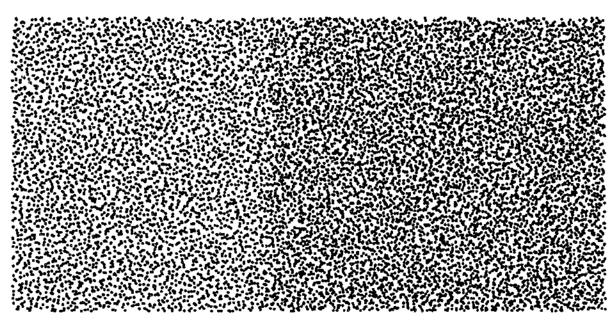

FIG. 1. Snapshot of the 12 960-particle shock wave simulation described in the text. Particles enter at the left and leave at the right. Fourth-order Runge-Kutta integration of the motion equations with a timestep of 0.025 is used.

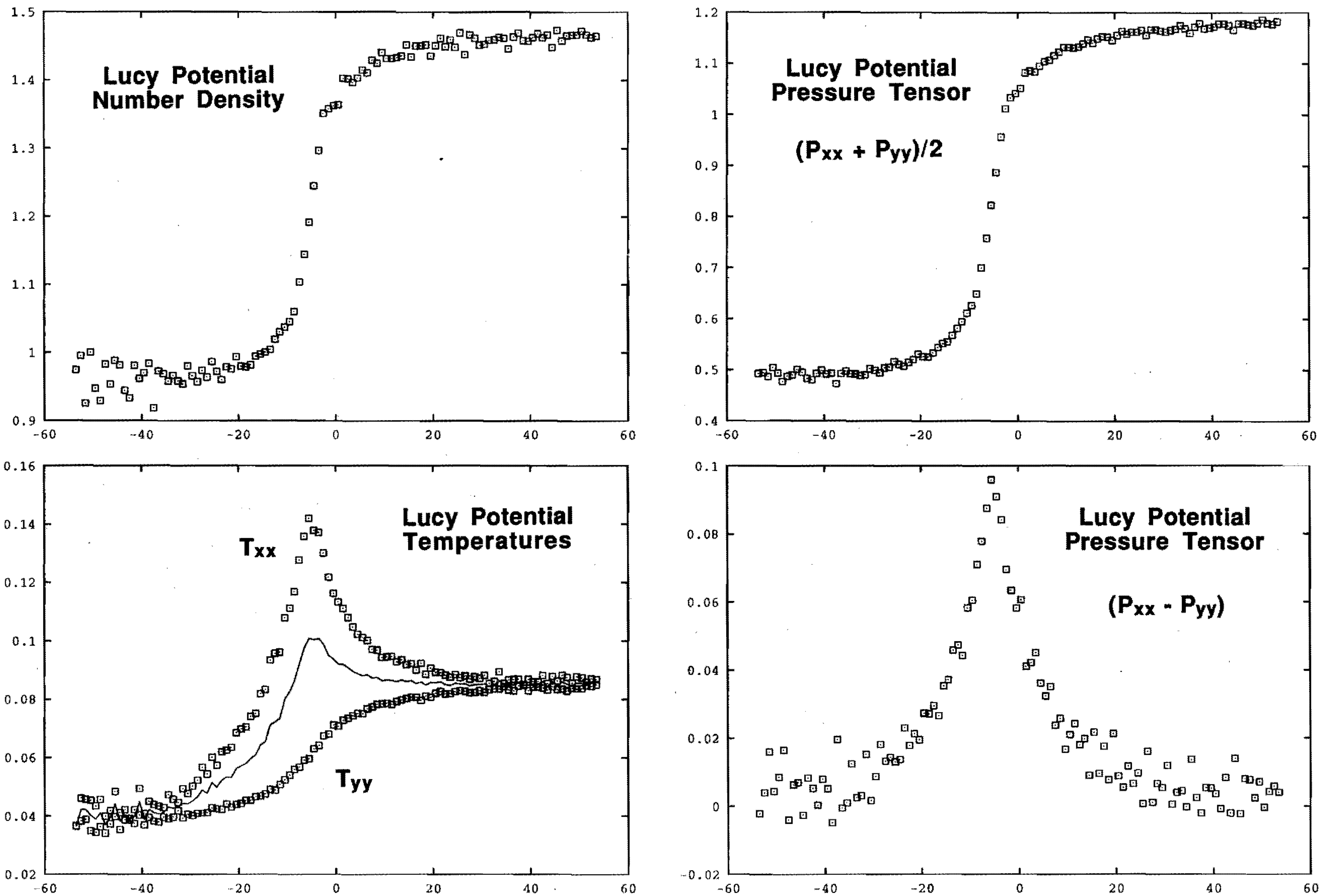

FIG. 2. Number density, temperature (the longitudinal and transverse components are labeled), and pressure-tensor components are shown for the strong shock wave described in the text. The profiles are averages over the time required to replace all particles in the system 3.6 times. The abscissa is measured in units of the square root of the area per particle in the unshocked fluid. This same distance, $(V_o/N)^{1/2}$, corresponds to the bin width used in calculating averages, following Hardy's approach. Compare the profiles shown here to the three-dimensional profiles shown in Ref. [10].

We therefore adopted a much older stationary-state approach [13], in which planes of cold particles, moving to the right at the shock velocity and selected from a square lattice with appropriate random particle displacements, periodically replace an equal number of particles, removed at the right boundary, which have velocity $u_s - u_p$. The boundary velocities and the number density of the incoming material are chosen to match a solution of the fluid conservation equations. Right and left mirror boundaries and top and bottom periodic boundaries complete the model description. See Fig. 1 for a typical snapshot.

This approach was successful. A system with 3240 particles produced a nominally stationary profile. In the vicinity of the shock front, the hydrodynamic variables are statistically indistinguishable from those for 12 960 or 51 840 particles. The profiles shown in Fig. 2 correspond to a compression ratio of 3:2, with entrance and exit velocities of 1.35 and 0.90. The range of the potential, $h = 3$, together with an initial number density of unity, corresponds to nearly 30 pair interactions for a typical dense-fluid particle. The system size was cycled smoothly from 144×72 down to 143×72, at which point three columns of 72 particles were introduced at the left boundary and the 216 hot particles nearest the right boundary were removed, readjusting the position of both mirror boundaries to the left.

Average profiles were generated using Hardy's scheme [14] over a time period corresponding to 20 complete replacements of all the particles in the system. It is noteworthy that both the longitudinal temperature T_{xx} and the mean temperature $T = [T_{xx} + T_{yy}]/2$ have pronounced maxima. The heat flux, in the comoving frame of the fluid, proceeds always from right to left, corresponding to a negative heat conductivity in the hot fluid, in contradiction to Fourier's Law, but in agreement with Mott-Smith's strong shock wave model [14]. He approximated the velocity distribution within the shock as a linear combination of the hot and cold distributions. Half the average kinetic energy of a pair of particles, one hot and one cold, exceeds the average of their temperatures by $(1/8)mu_p^2$:

$$E_{pair} = kT_{hot} + kT_{cold} + (1/4)mu_p^2.$$

The excess thermal energy provides the physical interpretation for the temperature maximum found in the stationary profiles. In the steeply rising portion of the wave, where the heat conductivity is positive, both the shear viscosity and the conductivity, as measured in the shock wave

$$\eta = -(P_{xx} - P_{yy})/(2du/dx); \quad \kappa = -Q_x/(dT/dx),$$

are in semiquantitative agreement with values from independent shear-flow and heat-flow simulations [3,5–7].

III. CONCLUSIONS

Our results characterize the (i) stability, (ii) consistency, and (iii) anisotropicity of two-dimensional strong shock waves. Because the rms displacment of two-dimensional particles diverges in *large* systems [15], and because the analysis of surface vibrations as superpositions of Rayleigh waves suggests divergence in three dimensions and an even stronger instability in two, one might suspect that planar shock waves would be unstable in the present case. On the other hand, it is usual to imagine that shock waves are stabilized by compressibility: lagging troughs in a sinusoidally perturbed wave front generate a higher pressure and catch up; any crests leading the main wave generate lower pressures and slow down. Our two-dimensional simulations support the existence of stable planar shock waves in a two-dimensional dense fluid.

Because the temperature gradients dT_{xx}/dx and dT/dx from Fig. 2 both change sign while the heat flux component dQ_x/dx does not, no positive Fourier conductivity is capable of describing our profiles. This inconsistency with linear hydrodynamics is, likewise, a feature of Mott-Smith's model for strong three-dimensional shock waves. Thus, the suggestion [11] that the transport coefficients be chosen on the basis of the longitudinal temperature T_{xx} rather than the average one $(T_{xx} + T_{yy})/2$ [11] is less useful in two dimensions than in three. The source of the substantial temperature anisotropicity is not hard to find or explain. Mott-Smith's idea that the velocity distribution is best viewed as a combination of hot and cold parts has been borne out by our simulations and establishes that a kinetic theory, as opposed to an extension of Navier-Stokes reasoning, must be used to understand these interesting far-from-equilibrium systems.

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