LAX-FRIEDRICHS AND THE VISCOSITY-CAPILLARITY CRITERION

BY

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IMA Preprint Series #49

December 1983

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS
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Lax-Friedrichs and the Viscosity-Capillarity Criterion

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* This research was supported in part by the Air Force Office of Scientific Research, Air Force Systems Command, USAF, under contract/grant no. AFOSR-81-0172. The United States Government is authorized to reproduce and distribute reprints for government purposes notwithstanding any copyright hereon.

Research supported in part with grants from AFOSR and NSF while a visitor at the Institute for Mathematics and Its Applications, University of Minnesota.

0. Introduction.

It has been shown by Lax [1] some time ago that for hyperbolic conservation laws solutions obtained as limits of the Lax-Friedrichs finite difference scheme will actually satisfy an "entropy" admissibility criterion. The goal of this paper is to attempt to extend Lax's idea to a form which is amenable to mixed problems as well, e.g. the dynamics of a van der Waals fluid. Specifically, we compare shocks obtained by the Lax-Friedrichs scheme with those permitted by the viscosity-capillarity criterion of [2], [3]. We show that for isothermal motion it is expected that shocks produced by Lax-Friedrichs will satisfy the viscosity-capillarity criterion.

1. Shock structure for an isothermal van der Waals fluid.

The equations of isothermal compressible fluid flow written in Lagrangian coordinates are:

$$\left\{ \begin{array}{l} u_t = -p(w)_x, \\ w_t = u_x, \quad -\infty < x < \infty, \end{array} \right. \quad (1.1)$$

where u is the velocity, w is the specific volume. Of course, as is well known, for the case $p' < 0$, $p'' \neq 0$, (1.1) is a genuinely nonlinear (in the sense of Lax) hyperbolic system of conservation laws and will develop shocks for arbitrarily smooth choices of initial data. Furthermore, in the case $p' > 0$ in some region (α, β) , (1.1) will be an elliptic initial value problem (at least initially) for initial data $w = w_0 \in (\alpha, \beta)$. In this case (1.1) loses well posedness due to classical Hadamard instability.

We shall be concerned here with the van der Waals fluid for fixed temperature θ the constitutive relation for p is:

$$\left\{ p(w) = \frac{R\theta}{w-b} - \frac{a}{w^2}, \quad 0 < b < w < \infty, \quad R, a > 0. \right. \quad (1.2)$$

For $\theta < \theta_{\text{crit.}} = \frac{8a}{27br}$ a typical isotherm is shown in Figure 1. We assume $\theta < \theta_{\text{crit.}}$ from here on. From Figure 1 we see that for a certain range of pressures p , $p_\alpha < p < p_\beta$ the van der Waals fluid can simultaneously exist in liquid and vapor phases. Furthermore, we see $p(\gamma) = p(\beta)$, $p(\alpha) = p(\delta)$, and

$$p' < 0 \quad \text{for } w \in (b, \alpha) \cup (\beta, \infty), \quad (1.1 \text{ is hyperbolic}),$$

$$p' > 0 \quad \text{for } w \in (\alpha, \beta), \quad (1.1 \text{ is elliptic}),$$

and from our earlier remarks in either region we can expect loss of smooth solutions. One way to deal with this difficulty is to expand our horizons and seek weak solutions to (1.1). Unfortunately, as is also well known, weak solutions for quasi-linear hyperbolic equations are notoriously nonunique. Hence we are motivated to seek admissibility criteria which hopefully will pick out physically meaningful weak solutions.

In this work we only consider the weak solutions which are piecewise constant solutions to the Riemann initial value problem. Specifically consider the initial value problem for (1.1) with initial data

$$\begin{aligned} u &= u_- , \quad x < 0 , \quad u = u_+ , \quad x > 0 , \\ w &= w_- , \quad x < 0 , \quad w = w_+ , \quad x > 0 , \end{aligned} \quad (1.3)$$

where u_- , w_- , u_+ , w_+ are constants satisfying the Rankine-Hugoniot jump conditions

$$\begin{aligned} -U[u] &= -[p] , \\ -U[w] &= [u] \end{aligned} \quad (1.4)$$

for some constant U . Here $[u] = u_+ - u_-$, etc. Then

$$\begin{aligned} u &= u_- , & x < Ut , & & u &= u_+ , & x > Ut , \\ w &= w_- , & & & w &= w_+ , & \end{aligned} \quad (1.5)$$

is a weak solution of (1.1), (1.3).

The propagating singular surface $x = Ut$ is a shock wave. Furthermore, for the van der Waals fluid if $w_- \in (b, \alpha)$, $w_+ \in (\beta, \infty)$ or vice-versa the shock-wave is a propagating phase boundary. Since (b, α) denotes the liquid phase, (β, ∞) the vapor phase, the propagating phase boundary will represent a propagating liquid-vapor interface.

One possible way to determine when a solution of the form (1.5) is "admissible" is to see if it is the limit of solutions of a physically meaningful higher order system. In [2], [3] it has been suggested that a reasonable higher order system to consider is

$$\boxed{\begin{aligned} u_t &= -p(w)_x + \mu u_{xx} - A\mu^2 w_{xxx}, \\ w_t &= u_x . \end{aligned}} \quad (1.6)$$

Here μ denotes the viscosity and $A\mu^2$ denotes the coefficient of interfacial capillarity. For simplicity we take A, μ positive constants, μ is thought of as being a small parameter. (For equilibrium problems this approach was originally formulated by van der Waals himself [4] in terms of interfacial energy; Korteweg [5] extended the idea of a capillarity contribution to the stress tensor itself.)

We shall attempt to approximate (1.5) by a solution of (1.6) of the form

$$u = \hat{u}(\xi), \quad w = \hat{w}(\xi), \quad \xi = \frac{x-Ut}{\mu}.$$

We find $\hat{w}$ satisfies

$$A \hat{w}'' + U \hat{w}' + p(\hat{w}) - p(w_-) + U^2(\hat{w} - w_-) = 0 \quad (1.7)$$

$$\hat{w}(-\infty) = w_-, \quad \hat{w}(+\infty) = w_+ \quad (1.8)$$

Definition. If (1.7), (1.8) possesses a solution we say (1.5) satisfies the viscosity-capillarity shock criterion.

If we set $y(\hat{w}(\xi)) = \hat{w}'(\xi)$ (1.7) becomes

$$\frac{A}{2} \frac{d}{dw} y^2(w) + U y(w) + p(w) - p_- + U^2(w - w_-) = 0 \quad (1.9)$$

where we have dropped the $\hat{\cdot}$'s and set $p(w_-) = p_-$. From (1.8) we see y must satisfy the boundary conditions

$$y(w_-) = 0, \quad y(w_+) = 0. \quad (1.10)$$

If we keep w_- fixed (say in the interval (b, α)) (1.9) is an initial value problem for $y(w)$ with $y(w_-) = 0$ for which we are trying to find U so that $w_+(U)$ (as determined by (1.4)) satisfies $y(w_+(U)) = 0$. If $w_+(U)$ is in the interval (β, ∞) then this traveling wave is a structured phase transition. This idea has been successfully used in [2], [3] to obtain interfacial shocks which satisfy the viscosity-capillarity criterion. For example we can state

Lemma 4.12 of [3]. Assume either

$$(I) \quad \alpha > w_- > \gamma \quad \text{and} \quad \int_{w_-}^{w^*(0)} f(\zeta, 0) d\zeta < 0, \quad \text{or}$$

$$(I') \quad b < w_- < \gamma, \quad \text{and}$$

$$(II) \quad \text{there is } U_M \text{ such that}$$

$$\int_{w_-}^{w^*(U_M)} f(\zeta, U_M) d\zeta = 0;$$

where $f(\zeta, U) = U^2(\zeta - w_-) + p(\zeta) - p(w_-)$ and $w^*(U)$ denotes the smallest solution of (1.4) lying in the interval (β, ∞) . Then for some $\bar{U}$, $0 < \bar{U} < U_M$, (1.7), (1.8) possesses a solution with $w_+ = w^*(\bar{U})$.

2. Finite differences.

In the previous section we saw that the introduction of viscosity and capillarity terms to (1.1) provides a way of picking out admissible weak solutions. Motivated by the work of Lax [1] we shall examine here the role of discretization of (1.1).

Consider the Lax-Friedrichs scheme for (1.1) given by

$$\begin{aligned} \frac{1}{\Delta t} \left\{ u(x, t + \Delta t) - \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \right\} + \\ \frac{1}{2\Delta x} \left\{ p(w(x + \Delta x, t)) - p(w(x - \Delta x, t)) \right\} &= 0, \\ \frac{1}{\Delta t} \left\{ w(x, t + \Delta t) - \frac{w(x + \Delta x, t) + w(x - \Delta x, t)}{2} \right\} - \\ \frac{1}{2\Delta x} \left\{ u(x + \Delta x, t) - u(x - \Delta x, t) \right\} &= 0. \end{aligned} \quad (2.1)$$

Set $\lambda = \frac{\Delta t}{\Delta x}$. If (2.1) has a smooth solution u, w we may expand them in a Taylor series about x, t . From (2.1) we then find

$$\begin{aligned} u_t + p(w)_x &= \frac{\Delta t}{2} (\phi(w, \lambda) u_x)_x + O(|\Delta t|^2), \\ w_t - u_x &= \frac{\Delta t}{2} (\phi(w, \lambda) w_x)_x + O(|\Delta t|^2), \end{aligned} \quad (2.2)$$

where $\phi(w, \lambda) = p'(w) + \lambda^{-2}$.

From (2.2) we see (2.1) is first order accurate with respect to (1.1) but second order accurate with respect to

$$\boxed{\begin{aligned} u_t + p(w)_x &= \frac{\Delta t}{2} (\phi(w, \lambda) u_x)_x, \\ w_t - u_x &= \frac{\Delta t}{2} (\phi(w, \lambda) w_x)_x. \end{aligned}} \quad (2.3)$$

In order to force well posedness on (2.3) a natural assumption is $\phi(w, \lambda) > 0$ which makes (2.3) parabolic. In regions where $p' > 0$ (e.g. in the region (α, β) for the van der Waals fluid) $\phi(w, \lambda) > 0$ automatically. In hyperbolic regions where $p' < 0$ we need

$$\lambda^2 \max_w \{-p'; w \text{ s.t. } p' < 0\} < 1. \quad (\text{CFL})$$

which is just Courant-Friedrichs-Lewy condition. CFL will hold if λ is sufficiently small. Hence if CFL is satisfied, (2.3) is a well posed parabolic system and should (2.1) converge for some fixed λ , (2.1) will provide a second order accurate approximation of (2.3).

We now examine how (2.3) approximates (1.1) in the vicinity of a shock wave. To do this we again look for structured solutions (now of (2.3)) of the form

$$u(x, t) = \hat{u}(\xi), \quad w(x, t) = \hat{w}(\xi), \quad \xi = \frac{x - Ut}{\Delta t}.$$

We easily find $\hat{w}$ satisfies

$$\phi(\phi \hat{w}') + U \phi \hat{w}' + U^2(\hat{w} - w_-) - p(\hat{w}) + p_- = 0 \quad (2.4)$$

where $p_- = p(w_-)$ and where we have imposed the boundary conditions

$$\hat{w}(-\infty) = w_-, \quad \hat{w}(+\infty) = w_+ \quad (2.5)$$

If we let $y(\hat{w}(\xi)) = \phi \hat{w}'$ and drop the $\hat{\cdot}$'s we see $y(w)$ satisfies

$$\frac{1}{4} \frac{d}{dw} (y^2(w)) + U y(w) + U^2(w - w_-) - p(w) + p_- = 0, \quad (2.6)$$

$$y(w_-) = 0, \quad y(w_+) = 0. \quad (2.7)$$

But this is precisely the same shooting problem as presented earlier (see (1.9), (1.10)) with $A = \frac{1}{2}$. Hence the $A = \frac{1}{2}$ case of viscosity-capillarity criterion and the shock structure problem associated with (2.3) will produce identical admissible end states u_-, w_-, u_+, w_+ and admissible shock speed U .

The above analysis suggests that if (i) Δt , λ are sufficiently small, and (ii) the difference scheme (2.1) converges, then (2.1) will produce shocks satisfying the viscosity-capillarity criterion. Since the shock structure problem for (2.3) is only an approximation to the interfaces produced by (2.1) getting beyond such suggestive analysis will require further study.

3. Eulerian coordinates.

In the first two sections we considered shock structure problems for an isothermal compressible fluid in Lagrangian coordinates. In this section we derive analogous results for Eulerian coordinates.

The isothermal compressible fluid flow equations in Eulerian coordinates are

$$\boxed{\begin{aligned} \rho_t + m_x &= 0 \\ m_t + \left(\frac{m^2}{\rho} + p\right)_x &= 0 \end{aligned}}, \quad -\infty < x < \infty. \quad (3.1)$$

Here ρ is density, u is velocity, $m = \rho u$ is momentum, p is pressure, $\bar{p}(\rho) = p(w) = p\left(\frac{1}{\rho}\right)$.

Consider the shock front

$$\begin{aligned} m &= m_- & x < 0 & & m &= m_+ & x > 0 \\ \rho &= \rho_- & & & \rho &= \rho_+ & \end{aligned} \quad (3.2)$$

for which the fluid is moving through the stationary front. The Rankine-Hugoniot conditions in this case are

$$\begin{aligned} [m] &= 0, \\ \left[\frac{m^2}{\rho} + \bar{p}\right] &= 0, \end{aligned} \quad (3.3)$$

from which we see

$$m_- = m_+$$

and

$$m_-^2 = - \frac{[p]}{[w]}.$$

Following Korteweg's theory of capillarity [5], [6], [7], [8], [9] we imbed (3.1) in the higher order system

$$\boxed{\begin{aligned} \rho_t + m_x &= 0, \\ m_t + \left(\frac{m^2}{\rho} + p\right)_x &= \left(\mu \rho u_x + A \mu^2 \rho_{xx} - \frac{A \mu^2}{\rho} \rho_x^2\right)_x. \end{aligned}} \quad (3.4)$$

Here $\mu\rho$ is the viscosity, $A\mu^2$ and $\frac{A\mu^2}{\rho}$ are capillarity coefficients. This choice of the capillarity coefficients forces the equilibrium configuration of the fluid to satisfy the Maxwell equal area rule (see [7], [9]). For simplicity we assume μ, A are positive constants so that $\mu\rho$ is the von Neumann-Richmyer [10] form of the viscosity. Furthermore μ is assumed to be a small parameter.

As is the usual technique, we look for steady state solutions of (3.4) i.e. $m_t = 0, \rho_t = 0$. Also we set $\xi = \frac{x}{\mu}$ so that (3.3) becomes

$$\begin{aligned} m' &= 0 \\ \left(\frac{m^2}{\rho} + \bar{p}\right)' &= (\rho u' + A\rho'' - \frac{A}{\rho}\rho'^2)' \end{aligned} \quad (3.5)$$

In order to force solutions of (3.5) to approximate (3.2) as $\mu \rightarrow 0+$ we require

$$\begin{aligned} m(-\infty) &= m_- , & m(+\infty) &= m_+ , \\ \rho(-\infty) &= \rho_- , & \rho(+\infty) &= \rho_+ , \end{aligned} \quad (3.6)$$

A straightforward integration of (3.5) shows $m = m_- = m_+$ and that ρ must satisfy

$$-A\rho'' + \frac{A}{\rho}\rho'^2 + \frac{m}{\rho}\rho' + m^2\left(\frac{1}{\rho} - \frac{1}{\rho_-}\right) + \bar{p}(\rho) - \bar{p}(\rho_-) = 0$$

If we rewrite this equation in terms of $w = \frac{1}{\rho}$ we see

$$\frac{1}{w}A(\ln w)'' - m(\ln w)' + m^2(w - w_-) + p(w) - p(w_-) = 0 \quad (3.8)$$

Finally set $y(w) = (\ln w(\xi))'$. We then see $y(w)$ satisfies

$$\frac{A}{2} \frac{d}{dw} y^2(w) - my(w) + m^2(w - w_-) + p(w) - p(w_-) = 0 \quad (3.9)$$

$$y(w_-) = 0 , \quad y(w_+) = 0 \quad (3.10)$$

This is precisely the "shooting" problem encountered in Section 1 where now U is replaced by $-m$. As in Section 1 a solution of (3.9), (3.10) will determine w_-, w_+, m which yield a weak solution (3.6) of (3.1) which is admissible according to the viscosity-capillarity criterion.

Now let us consider the Lax-Friedrichs difference scheme for (3.1) i.e.

$$\begin{aligned}
 & \frac{1}{\Delta t} \left\{ \rho(x, t + \Delta t) - \frac{\rho(x + \Delta x, t) + \rho(x - \Delta x, t)}{2} \right\} \\
 & + \frac{1}{2\Delta x} \left\{ m(x + \Delta x, t) - m(x - \Delta x, t) \right\} = 0, \\
 & \frac{1}{\Delta t} \left\{ m(x, t + \Delta t) - \frac{m(x + \Delta x, t) + m(x - \Delta x, t)}{2} \right\} \\
 & + \frac{1}{2\Delta x} \left\{ \left(\frac{m^2}{\rho} + \bar{p} \right) (x + \Delta x, t) - \left(\frac{m^2}{\rho} + \bar{p} \right) (x - \Delta x, t) \right\} = 0.
 \end{aligned} \tag{3.11}$$

As in Section 2 assume (3.11) has smooth solutions ρ, m and expand about (x, t) . We find

$$\begin{aligned}
 \rho_t + m_x &= \left(\frac{\Delta t}{2} \right) \left[-\rho_{tt} + \lambda^{-2} \rho_{xx} \right] + O(|\Delta t|^2) \\
 m_t + \left(\frac{m^2}{\rho} + \bar{p} \right)_x &= \left(\frac{\Delta t}{2} \right) \left[-m_{tt} + \lambda^{-2} m_{xx} \right] + O(|\Delta t|^2),
 \end{aligned}$$

where $\lambda = \frac{\Delta t}{\Delta x}$. Hence (3.11) is first order accurate to (3.11) but second order accurate to

$$\boxed{
 \begin{aligned}
 \rho_t + m_x &= \frac{\Delta t}{2} \left[-\rho_{tt} + \lambda^{-2} \rho_{xx} \right], \\
 m_t + \left(\frac{m^2}{\rho} + \bar{p} \right)_x &= \frac{\Delta t}{2} \left[-m_{tt} + \lambda^{-2} m_{xx} \right].
 \end{aligned}
 } \tag{3.13}$$

We now examine the shock structure problem for (3.13) by looking for steady state solutions of (3.13) $\rho_t = 0, m_t = 0$ of the form $m = m(\xi), \rho = \rho(\xi), \xi = \frac{x}{\Delta t}$. As before we require m, ρ to satisfy (3.6). We see m, ρ are solutions of

$$\begin{aligned}
 m' &= \frac{\lambda^{-2}}{2} \rho'', \\
 \left(\frac{m^2}{\rho} + \bar{p} \right)' &= \frac{\lambda^{-2}}{2} m''.
 \end{aligned} \tag{3.14}$$

Integrating (3.14) shows ρ satisfies

$$-\frac{\lambda^{-4}}{4} \rho'' + \frac{\lambda^{-4}}{4\rho} \rho'^2 + m_- \lambda^{-2} \frac{\rho'}{\rho} m_- \left(\frac{1}{\rho} - \frac{1}{\rho_-} \right) + \bar{p}(\rho) - \bar{p}(\rho_-) = 0 . \quad (3.15)$$

But (3.15) is just (3.7) with $A = \frac{\lambda^{-4}}{4}$. Thus the shock admissibility problem for (3.13) is identical to the one for the viscosity-capillarity problem (3.4) with $A = \frac{\lambda^{-4}}{4}$. This result again suggests that if (3.11) converges and Δt is sufficiently small, (3.11) will produce shocks satisfying the viscosity-capillarity criterion.

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