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Note

An Artificial Energy Method for Calculating Flows with Shocks*

INTRODUCTION

Many important processes in fluid dynamics may be treated as adiabatic except in certain exeptional regions where dissipative effects play an essential role, e.g., shocks, boundary layers, etc. The artificial-viscosity method, first introduced by von Neumann and Richtmyer, provides a physically intuitive and computationally effective technique for treating flows with embedded shocks. Simply stated, this method introduces an artificial viscous pressure term in regions of compression in such a manner that an increase in entropy occurs shock transition zones.

This approach allows one to separately view the entropy production within a physical model from that inherent in any one of a number of numerical techniques for calculating solutions of the model. Certain difficulties arise, however, in attempting to adapt this technique directly to transonic flow problems. Although the resolution of these difficulties is not itself the subject of this paper, the questions they raise have motivated this study and have led to a viewpoint which may be of more general interest.

Briefly, this paper describes how dissipative flows can be induced by reducing the total energy available for adiabatic processes in shock zones. Section 1 describes a class of inviscid fluid flows, here called semiflows, which differ from one another through the law expressing the conservation of a modified "total energy" expresion. Section 2 discusses the thermodynamic differences among semiflows and establishes a condition which produces dissipative flows. This has the effect of modifying the pressure in regions of compression in a manner analogous to the artificial-viscosity method. For a perfect gas the effect is equivalent to suitably modifying the gas constant in the equation of state.

In order to test the validity of the concepts discussed in the paper a comparison of numerical solutions of a Riemann problem employing MacCormack's method was made using the usual non-adiabatic equations and the artificial energy method of this paper. The result indicates that the dissipation effect predicted by the analytical formulation is reflected in the numerical method as well.

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1. Conservatiion Laws for Inviscid Fluids

The basic variables describing inviscid fluids are $\rho =$ density, $e =$ specific internal energy, $p =$ pressure, and $\mathbf{u} =$ velocity. An important auxiliary variable is the total specific energy $E(\mathbf{u})$ given by $E(\mathbf{u}) = \frac{1}{2}\mathbf{u}^2 + e$.

Certain differentiation operators with respect to a velocity $\mathbf{u}$ will be useful:

$$\dot{D}_{\mathbf{u}}\phi \equiv \partial_t \phi + \operatorname{div}(\mathbf{u}\phi), \qquad D_{\mathbf{u}}\phi \equiv \partial_t \phi + \mathbf{u} \cdot \operatorname{grad} \phi \tag{1.1}$$

in which ϕ is a scalar function.

The following discussion assumes that p is given by an equation of state: $p = p(\rho, e)$. An adiabatic inviscid flow is then described by the conservation laws

$$\begin{aligned} &\text{(mass)} && \dot{D}_{\mathbf{u}}\rho = 0, \\ &\text{(momentum)} && \dot{D}_{\mathbf{u}}(\rho(\mathbf{u} \cdot \zeta_i)) + \operatorname{div}(p \cdot \zeta_i) = 0, \quad i = 1, 2, 3, \\ &\text{(energy)} && \dot{D}_{\mathbf{u}}(\rho E(\mathbf{u})) + \operatorname{div}(p\mathbf{u}) = 0, \end{aligned} \tag{1.2}$$

where ζ_i, $i = 1, 2, 3$, denote fixed vectors in the direction of the coordinate axes.

The following provides a concise description of these laws:

THEOREM. *A necessary and sufficient condition that* $(\rho, \mathbf{u}, e)$ *satisfy* (1.2) *is that*

$$\dot{D}_{\mathbf{u}}(\rho E(\mathbf{v})) + \operatorname{div}(p\mathbf{v}) = 0 \tag{1.3}$$

for every $\mathbf{v}$ *such that* $\mathbf{v} - \mathbf{u} =$ const.

The proof follows by noting that for every $\zeta =$ const, if $\mathbf{v} = \mathbf{u} + \zeta$, then $E(\mathbf{v}) = E(\mathbf{u}) + (\mathbf{u} \cdot \zeta) + (\zeta \cdot \zeta)/2$ and the result follows by equating like powers of ζ in (1.3).

Consider the artificial total energy expression $\hat{E}(\mathbf{v})$ given by

$$\hat{E}(\mathbf{v}) = E(\mathbf{v}) - f(\mathbf{u}^2/2, e) \tag{1.4}$$

in which f is a suitable convex function of its arguments as explained in the following section. Flows determined by the condition that

$$\dot{D}_{\mathbf{u}}(\rho \hat{E}(\mathbf{v})) + \operatorname{div}(p\mathbf{v}) = 0 \tag{1.5}$$

for every $\mathbf{v}$ such that $\mathbf{v} - \mathbf{u} =$ const will be called *semiflows*; thus semiflows differ from (1.2) in that conservation of "energy" is expressed by

$$\dot{D}_{\mathbf{u}}(\rho \hat{E}(\mathbf{u})) + \operatorname{div}(p\mathbf{u}) = 0. \tag{1.6}$$

As discussed in the next section, differences among semiflows arise from differences in thermodynamic assumptions arising from the choice of $\hat{E}(\mathbf{v})$.

2. Dissipative Semiflows

An important thermodynamic relationship is

$$de + p\,d\rho^{-1} = T\,ds \tag{2.1}$$

in which s is the entropy and T is the temperature. Since semiflows conserve mass, it follows that

$$\dot{D}_{\mathbf{u}}(\rho e) = \rho T D_{\mathbf{u}} s - p \operatorname{div} \mathbf{u}. \tag{2.2}$$

Since semiflows also conserve momentum, there results, after some manipulation,

$$\dot{D}_{\mathbf{u}}(\rho \mathbf{u}^2/2) = -\mathbf{u} \cdot \operatorname{grad} p. \tag{2.3}$$

Thus, referring to (1.2), there follows

$$\dot{D}_{\mathbf{u}}(\rho E(\mathbf{u})) + \operatorname{div}(p\mathbf{u}) = \rho T D_{\mathbf{u}} s$$

so that the semiflow ($f = 0$ in (1.4)) describing (1.2) implies, and is implied by, $D_{\mathbf{u}} s = 0$ which is the condition for adiabatic flow.

When $f \not\equiv 0$ in (1.4) the semiflows described by (1.5) will, generally, be non-adiabatic. The physically important class of such flows are those which are *dissipative*, i.e., $D_{\mathbf{u}} s \geqslant 0$. For simplicity suppose $f = \alpha \mathbf{u}^2/2 + \beta e$, where $0 \leqslant \alpha, \beta < 1$. The conservation of "energy" as expressed by (1.6) yields, using (2.2) and (2.3),

$$\begin{aligned} 0 &= \dot{D}_{\mathbf{u}}(\rho \hat{E}(\mathbf{u})) + \operatorname{div}(p\mathbf{u}) \\ &= \alpha \mathbf{u} \cdot \operatorname{grad} p + \beta p \cdot \operatorname{div} \mathbf{u} + (1-\beta)\,\rho T D_{\mathbf{u}} s; \end{aligned} \tag{2.4}$$

this class of semiflows will therefore be dissipative if

$$\alpha \mathbf{u} \cdot \operatorname{grad} p + \beta p \cdot \operatorname{div} \mathbf{u} \leqslant 0. \tag{2.5}$$

The essential features of this argument can be expected to remain valid when the parameters α and β are allowed to vary in certain regions. In particular, by taking α and β as non-negative parameters in regions of compression ($\mathbf{u} \cdot \operatorname{grad} p < 0$, $p \cdot \operatorname{div} \mathbf{u} < 0$) and zero elsewhere f will measure the energy lost by entropy production in regions of compression. The resulting dissipative semiflows should furnish solution of (2.4) which, as $\alpha \to 0$, $\beta \to 0$, converge in a weak sense to the physically relevant solution of (1.2) when shocks are present.

Clearly, (2.5) will be satisfied by setting

$$\begin{aligned} \alpha &= \lambda_\alpha \,|\mathbf{u} \cdot \operatorname{grad} p|, & \mathbf{u} \cdot \operatorname{grad} p < 0 \\ &= 0, & \mathbf{u} \cdot \operatorname{grad} p \geqslant 0 \end{aligned}$$

and

$$\beta = \lambda_\beta |\text{div}\,\mathbf{u}|, \qquad \text{div}\,\mathbf{u} < 0$$
$$= 0, \qquad \text{div}\,\mathbf{u} \geqslant 0,$$

where λ_α and λ_β are non-negative. Other, more computationally effective, choices can also be employed. For a perfect gas the ratio p/ρ will then be given by

$$p/\rho = (\gamma - 1)(\hat{E} - (1 - \alpha)\mathbf{u}^2/2)/(1 - \beta) \tag{2.6}$$

since $E = (1 - \alpha)\mathbf{u}^2 + (1 - \beta)e$ and $e = (\gamma - 1)^{-1}p/\rho$; the effect is thus a modification of the pressure.

In order to test the application of this idea to shock capturing techniques a numerical study of a Riemann problem was made. For a gas with $\gamma = 1.4$ initial conditions were chosen as

$x < 0$	$x > 0$
$\rho = 0.445$	$\rho = 0.5$
$u = 0.698$	$u = 0.$
$p = 3.528$	$p = 0.571$

The exact solution of Eqs. (1.2) with these initial conditions is shown by the solid lines in Figs. 1 and 2. Figure 1 shows the result of integrating the adiabatic invisicdflow (1.2) by a second-order MacCormack finite-difference scheme. Figure 2 shows the result of applying the same numerical scheme to calculate the semiflow described by (2.4) in which $\alpha = 0$ and

$$\beta = 0 \qquad \text{if} \quad \Delta_i u_i^n \equiv u_{i+1}^n - u_{i-1}^n \geqslant 0$$
$$= \frac{(0.3)\Delta_i u^n}{\min_k(\Delta_k u^n)} \qquad \text{if} \quad \Delta_i u_i^n < 0,$$

where $u_i^n = u(i\,\Delta x, n\,\Delta t)$ in which Δx and Δt denote space and time mesh parameters, respectively. From (2.6),

$$\frac{p}{\rho} = \frac{(\gamma - 1)}{(1 - \beta)}(\hat{E} - \tfrac{1}{2}u^2).$$

This is equivalent to treating the adiabatic Eqs. (1.2) using the modified equation of state $p = (\gamma' - 1)\rho e$ with $\gamma' - 1 = (\gamma - 1)(1 - \beta)^{-1}$.

As Fig. 2 indicates, the artificial energy method produced a slightly broader shock transition zone than the solution obtained in Fig. 1; however, the solution obtained by this method effectively eliminated the oscillations behind the shock and ahead of the rarefaction which are evident in Fig. 1. No difference in these solutions occurred at

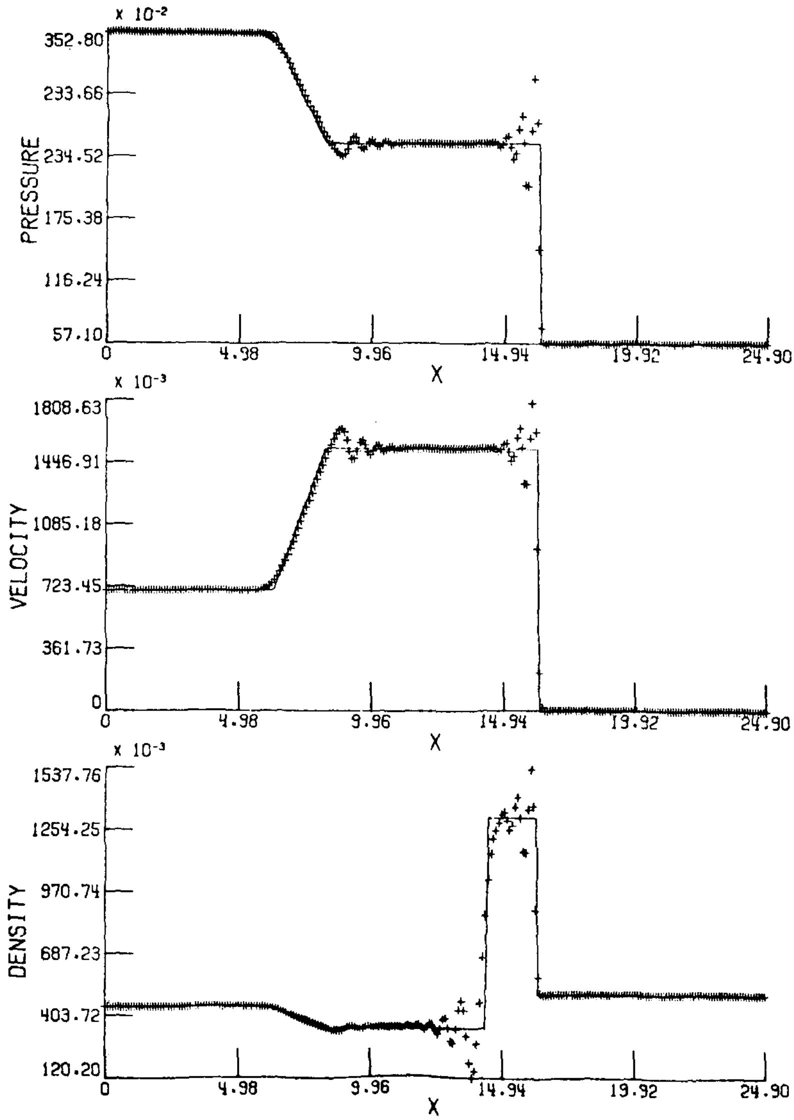

FIG. 1. Numerical solution (MacCormack) of the adiabatic conservation laws (Eq. (1.2)).

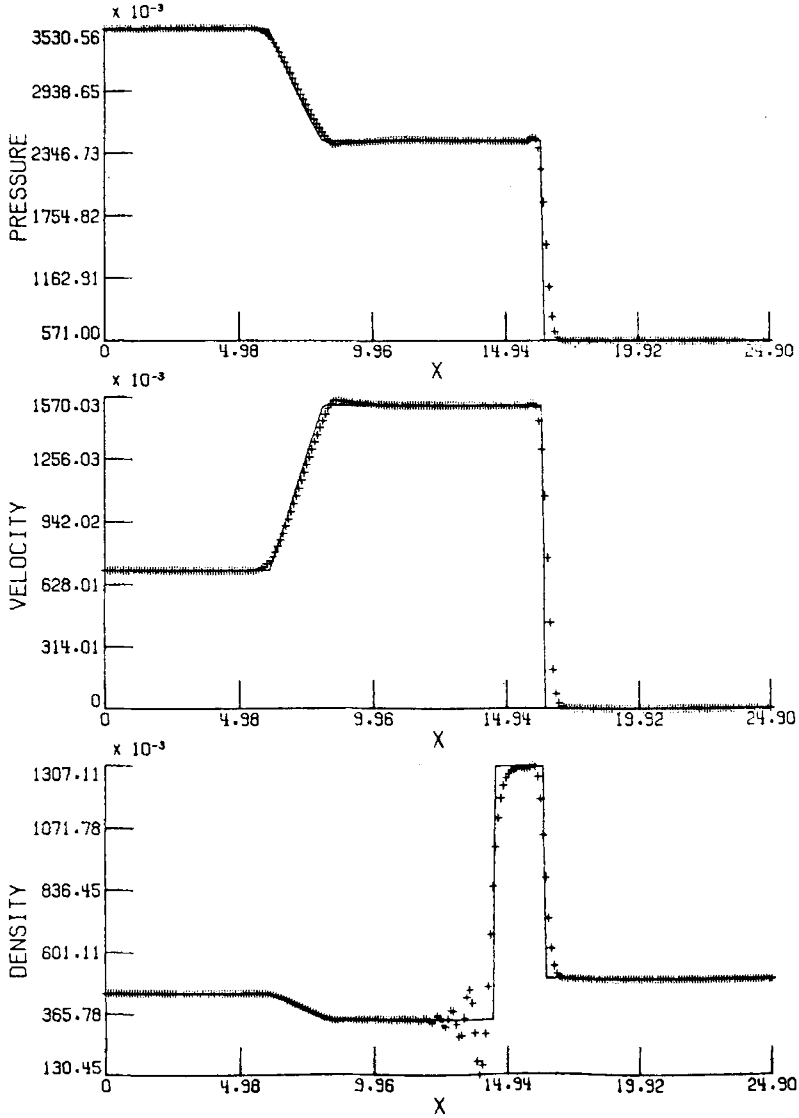

FIG. 2. Numerical solution (MacCormack) by the artificial energy method (Eq. (2.4)).

the contact discontinuity where both the pressure and velocity are continuous because no dissipation is added at the contact as a result of condition (2.5).

For steady isentropic flows the conservation of energy may be expressed by the Bernoulli law. The above discussion suggests that steady dissipative semiflows can be induced by a suitable modification of the Bernoulli expression in regions of compression. This may prove useful in numerical methods for treating transonic flows past bodies.

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