NASA Contractor Report 3526

A Variational Principle for Compressible Fluid Mechanics

Discussion of the One-Dimensional Theory

Robert Joel Prozan

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A Variational Principle for Compressible Fluid Mechanics

Discussion of the One-Dimensional Theory

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1.0 SUMMARY AND INTRODUCTION

Conventional numerical analyses of fluid dynamic systems variously use finite element or finite difference analogs to satisfy the governing equations of motion. To date, numerical solutions are more of an art than a science.

In this report it is proposed that the second law of thermodynamics, a neglected principle of physics, is of paramount importance to a successful solution to the governing equations of motion. The second law is not new, nor is the post priori use of the second law in ascertaining the physical correctness of the solution. What is new is the incorporation of the second law as a fundamental statement of motion which is of equal importance to the solution as are the familiar conservation equations. It is hypothesized that the second law of thermodynamics is actually a variational principle and, in point of fact, is used as such in the subsequent discussion.

Many years of experience with the frustrations of numerical modeling have convinced the author that something is missing in the conventional numerical approaches. Even if the conservation equations are satisfied the solution may fail. There must be other governing criterion that have heretofore been lacking.

The ensuing discussion will use the second law of thermodynamics as a variational statement to derive a numerical procedure which provides insight to some fundamental questions not previously resolved. The procedure, based on numerical experimentation, appears to be stable provided the CFL condition is satisfied. This stability is manifested no matter how severe the gradients (compression or expansion) are in the flow field.

For reasons of simplicity only one-dimensional inviscid compressible unsteady flow will be discussed here; however, the concepts and techniques are not restricted to one dimension nor are they restricted to inviscid non-reacting flow. The solution here is explicit in time. Further study is required to determine the impact of the variational principle on implicit algorithms.

2.0 DISCUSSION

2.1 The Variational Principle

In the subsequent discussion vector notation will be used rather than the more frequently used Einstein notation. The equations of motion for compressible, inviscid, unsteady flow of a perfect gas are;

$$\frac{\partial \bar{f}}{\partial t} + \frac{\partial \bar{g}}{\partial x} = 0 \tag{1}$$

where $\bar{f} = (\rho, \rho u, \rho E)$; $\bar{g} = (\rho u, p+\rho u^2, \rho u H)$

and where $p = \rho Z T$; $E = \frac{ZT}{(\gamma-1)} + \frac{1}{2}u^2$; $H = E + \frac{p}{\rho}$

so that $p = (\gamma-1)(\rho E - \frac{1}{2}\rho u^2)$

In text definitions will be used throughout. The symbols introduced above are: ρ(density); u(axial velocity); T(temperature); p(pressure); t(time); x(space coordinate); Z(gas constant); γ(ratio of specific heats); E(specific internal + kinetic energy); H(total enthalpy).

The Second Law of Thermodynamics is written;

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \rho u s}{\partial x} \geq 0 \tag{2}$$

The integral of the above equation over the region of interest and over an interval of time is;

$$\int_{t_1}^{t_2} \int_V \left(\frac{\partial \rho s}{\partial t} + \frac{\partial \rho u s}{\partial x}\right) dv dt \geq 0 \tag{3}$$

Equation (3) may be further integrated to yield;

$$\int_{t_1}^{t_2} \left(\int_V \frac{\partial \rho s}{\partial t} dv + \int_{CS} \rho \bar{u} s \cdot d\bar{A} \right) dt \geq 0 \tag{4}$$

Thus the Second Law states that the entropy generated internal to the region under investigation must be stationary or increase. Another view of the Second Law results when equation (3) is expanded;

$$\int_V \left(\frac{\partial \rho s}{\partial \rho}\left(\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}\right)+\frac{\partial \rho s}{\partial \rho u}\left(\frac{\partial \rho u}{\partial t}+\frac{\partial p+\rho u^2}{\partial x}\right)+\frac{\partial \rho s}{\partial \rho E}\left(\frac{\partial \rho E}{\partial t}+\frac{\partial \rho u H}{\partial x}\right)\right)dv \geq 0 \quad (5)$$

Equation (5) states that if the conservation equations are satisfied exactly everywhere then the system entropy generation is zero. In a numerical analysis, however, the equations of motion are only satisfied approximately so that in general the equality will not be satisfied. The Second Law is therefore interpreted as stating that the "numerical" entropy created by the inexact scheme must be positive. There are many choices made during the construction of a numerical analog. Whether by accident or design, these choices must not (in the long run at least) violate the Second Law.

The equations of motion which must be satisfied can be viewed as constraints to the entropy formation. Therefore, the constrained entropy function (S) can be written as;

$$S = \int_{t_1}^{t_2}\left(\int_V \left(\frac{\partial \rho s}{\partial t} + \overline{\lambda}\cdot\left(\frac{\partial \overline{f}}{\partial t}+\frac{\partial \overline{g}}{\partial x}\right)\right)dv + \int_{CS} \rho u s \cdot dA\right)dt \quad (6)$$

where the $\overline{\lambda}=(\lambda_\rho, \lambda_{\rho u}, \lambda_{\rho E})$ are the Lagrange multipliers.

Note that the constraint term looks very much like the familiar Method of Weighted Residuals (MWR). Now let the time interval be small and let $\Delta t = t_2 - t_1$. The one-dimensional domain will consist of N nodes which, for simplicity, will be subdivided into (N-1) elements of length Δx. (See figure 1 below.)

Figure 1 Schematic of region

The numbering system is such that the element (e) is bounded by nodes (n) and (n+1) or that element (n) is bounded by nodes (n) and (n+1).

We will first develop the constraint term (Φ). Let $t=\Delta t\tau$ and $x-x_n=\Delta x\xi$. The constraint term is then;

$$\Phi = \Delta t\Delta x\int_{\tau=0}^{\tau=1}\sum_{e=1}^{E}\int_{\xi=0}^{\xi=1}\bar{\lambda}\cdot\left(\frac{1}{\Delta t}\frac{\partial\bar{f}}{\partial\tau}+\frac{1}{\Delta x}\frac{\partial\bar{g}}{\partial\xi}\right)d\xi d\tau \qquad (7)$$

For the element shown in figure 2 below

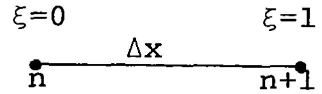

Figure 2 Schematic of element

the functions $\bar{f}$ and $\bar{g}$ are assumed to vary linearly. That is $\bar{f} = (1-\xi)\bar{f}_n+\xi\bar{f}_{n+1}$; $\bar{g} = (1-\xi)\bar{g}_n+\xi\bar{g}_{n+1}$. Then

$$\frac{\partial\bar{f}}{\partial\tau} = (1-\xi)\frac{\partial\bar{f}_n}{\partial\tau}+\xi\frac{\partial\bar{f}_{n+1}}{\partial\tau};\quad \frac{\partial\bar{g}}{\partial\xi} = \bar{g}_{n+1}-\bar{g}_n \qquad (8)$$

We will also assume a linear functional for $\bar{\lambda}$ viz;

$$\bar{\lambda} = \bar{\bar{\Lambda}}_{1n}\cdot\bar{\lambda}_n + \bar{\bar{\Lambda}}_{2n}\cdot\bar{\lambda}_{n+1} \qquad (9)$$

In the above expression the superscript ($\bar{\bar{\ }}$) is used to denote a dyad. Only diagonal dyads will occur during this development so that a vector pre or post multiplying the dyad will give the same result. There are also some occasions when it is necessary to redefine a vector as a dyad. It is felt that no undue interpretation problems to the reader should result.

Now $\bar{\bar{\Lambda}}_{1n}=\bar{\bar{\Lambda}}_{1n}(\xi)$ and $\bar{\bar{\Lambda}}_{2n}=\bar{\bar{\Lambda}}_{2n}(\xi)$. These functions are associated with the element (e) (left node (n) and right node (n+1)). The constraint term becomes;

$$\Phi=\Delta x\Delta t\sum_{n=1}^{N-1}\int_{\xi=0}^{\xi=1}(\bar{\bar{\Lambda}}_{1n}\cdot\bar{\lambda}_n+\bar{\bar{\Lambda}}_{2n}\cdot\bar{\lambda}_{n+1})\cdot((1-\xi)\dot{\bar{f}}_n+\xi\dot{\bar{f}}_{n+1}+\frac{\bar{g}_{n+1}-\bar{g}_n}{\Delta x})d\xi$$

where (the time integration has been performed),

$$\dot{\bar{f}}_n = \frac{\bar{f}_n^{m+1}-\bar{f}_n^m}{\Delta t};\quad \dot{\bar{f}}_{n+1} = \frac{\bar{f}_{n+1}^{m+1}-\bar{f}_{n+1}^m}{\Delta t}$$

and where the superscripts denote the time level.

Since the stated objective was to create an explicit scheme (this has nothing to do with the variational statement but is of great practical importance), the weight functions (to use MWR terminology) are chosen such that;

$$\int_{\xi=0}^{\xi=1}\bar{\bar{\Lambda}}_{1n}\xi d\xi = 0;\quad \int_{\xi=0}^{\xi=1}\bar{\bar{\Lambda}}_{2n}(1-\xi)d\xi = 0.$$

If $\bar{\bar{\Lambda}}_{1n}$, $\bar{\bar{\Lambda}}_{2n}$ are linear we find that;

$$\bar{\bar{\Lambda}}_{1n} = \bar{\bar{b}}'_{1n}(\xi-\tfrac{2}{3});\quad \bar{\bar{\Lambda}}_{2n} = \bar{\bar{b}}'_{2n}(\xi-\tfrac{1}{3}) \qquad (10)$$

where $\bar{\bar{b}}'_{1n}$, $\bar{\bar{b}}'_{2n}$ are arbitrary constants. Now;

$$\int_{\xi=0}^{\xi=1}(\bar{\bar{\Lambda}}_{1n}(1-\xi);\bar{\bar{\Lambda}}_{2n}\xi;\bar{\bar{\Lambda}}_{1n},\bar{\bar{\Lambda}}_{2n})d\xi = (-\bar{\bar{b}}_{1n},\bar{\bar{b}}_{2n},-\bar{\bar{b}}_{1n},\bar{\bar{b}}_{2n})$$

where $\bar{\bar{b}}'_{1n} = 6\bar{\bar{b}}_{1n}$; $\bar{\bar{b}}'_{2n} = 6\bar{\bar{b}}_{2n}$.

Since the $\bar{\bar{b}}'$ were arbitrary constants so are the $\bar{\bar{b}}$. The constraint term is now written as;

$$\Phi=\Delta x\Delta t((\bar{\bar{\beta}}_1\cdot(\dot{\bar{f}}_1+\frac{\bar{g}_2-\bar{g}_1}{\Delta x}))\cdot\bar{\lambda}_1+((\bar{\bar{1}}-\bar{\bar{\beta}}_{N-1})\cdot(\dot{\bar{f}}_{N-1}+\frac{\bar{g}_N-\bar{g}_{N-1}}{\Delta x}))\cdot\bar{\lambda}_{N-1}$$

$$+\sum_{n=2}^{N-1}((\bar{\bar{1}}-\bar{\bar{\beta}}_{n-1}+\bar{\bar{\beta}}_n)\cdot\dot{\bar{f}}_n+\bar{\bar{\beta}}_n\cdot(\frac{\bar{g}_{n+1}-\bar{g}_n}{\Delta x})+(\bar{\bar{1}}-\bar{\bar{\beta}}_{n-1})\cdot(\frac{\bar{g}_n-\bar{g}_{n-1}}{\Delta x}))\cdot\bar{\lambda}_n) \qquad (11)$$

where, in order to achieve a more recognizable form a substitution of $\bar{\bar{b}}_{2n} = (\bar{\bar{1}}-\bar{\bar{\beta}}_n)$; $\bar{\bar{b}}_{1n} = -\bar{\bar{\beta}}_n$ was made.

The variational statement of equation (6) becomes

$$S = \int_{\tau=0}^{\tau=1} \int_{v} \frac{\partial \rho s}{\partial \tau} dv d\tau + \Phi + \int_{\tau=0}^{\tau=1} \rho \bar{u} s \cdot d\bar{A} \Delta t d\tau \qquad (12)$$

Differentiation of equation (12) with respect to the nodal Lagrange multipliers yields the equations of constraint;

$$\frac{\partial \bar{S}}{\partial \lambda_1} = \bar{\bar{\beta}}_1 \cdot (\dot{\bar{f}}_1 + \frac{g_2 - g_1}{\Delta x}) = 0 \qquad (13a)$$

$$\frac{\partial \bar{S}}{\partial \lambda_N} = (\bar{\bar{1}} - \bar{\bar{\beta}}_{N-1}) \cdot (\dot{\bar{f}}_N + \frac{\bar{g}_N - \bar{g}_{N-1}}{\Delta x}) = 0 \qquad (13b)$$

$$\frac{\partial \bar{S}}{\partial \lambda_n} = (\bar{\bar{1}} - \bar{\bar{\beta}}_{n-1} + \bar{\bar{\beta}}_n) \cdot \dot{\bar{f}}_n + \bar{\bar{\beta}}_n \cdot (\frac{\bar{g}_{n+1} - \bar{g}_n}{\Delta x}) + (\bar{\bar{1}} - \bar{\bar{\beta}}_{n-1}) \cdot (\frac{\bar{g}_n - \bar{g}_{n-1}}{\Delta x}) = 0 \qquad (13c)$$

for $2 \leq n \leq N-1$

The above equations are an explicit numerical analog to the governing (or constraint) equations of motion. To determine the $\bar{f}_n$, however, the arbitrary parameters $\bar{\bar{\beta}}$ must be found. Let, for example, $\bar{\bar{\beta}}_n = \bar{\bar{0}}$ for all n. Then the interior nodal analog becomes;

$$\dot{\bar{f}}_n + \frac{\bar{g}_n - \bar{g}_{n-1}}{\Delta x} = 0 \qquad (14a)$$

while if $\bar{\bar{\beta}}_n = \bar{\bar{1}}$ we get;

$$\dot{\bar{f}}_n + \frac{\bar{g}_{n+1} - \bar{g}_n}{\Delta x} = 0 \qquad (14b)$$

which are backward and forward differencing schemes respectively. The $\bar{\bar{\beta}}_n$ therefore control the type of analog generated. It is also apparent that the $\bar{\bar{\beta}}_n$ control the portion of each element that is associated with the node. Figure 3 illustrates the point.

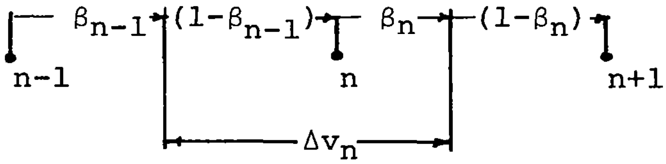

Figure 3 Effective control volume

The control volume is seen to be $\Delta v_n = \Delta x(1-\beta_{n-1}+\beta_n)$. Returning to the constrained equation (12) and performing the integration on the same control volume basis yields;

$$S=\Delta x\Delta t((\frac{\partial\overline{\rho s_1}}{\partial f}\cdot\bar{\bar{\beta}}_1-\frac{1}{2\Delta x}\frac{\partial\overline{\rho us_1}}{\partial f})\cdot\dot{\bar{f}}_1+(\frac{\partial\overline{\rho s_N}}{\partial f}\cdot(\bar{\bar{1}}-\bar{\bar{\beta}}_{N-1})+\frac{1}{2\Delta x}\frac{\partial\overline{\rho us_N}}{\partial f})\cdot\dot{\bar{f}}_N$$

$$+\sum_{n=2}^{N-1}\frac{\partial\overline{\rho s_n}}{\partial f}\cdot(\bar{\bar{1}}-\bar{\bar{\beta}}_{n-1}+\bar{\bar{\beta}}_n)\cdot\dot{\bar{f}}_n) + \Phi + (\rho us_N-\rho us_1)\Delta t \qquad (15)$$

where the flux term was expanded first order in time and integrated with respect to time. Differentiation of the above functional with respect to the $\dot{\bar{f}}_n$ at each node yields;

$$\frac{\partial\bar{S}}{\partial\dot{f}_1} = \Delta x\Delta t(\frac{\partial\overline{\rho s_1}}{\partial f}\cdot\bar{\bar{\beta}}_1-\frac{1}{2\Delta x}\frac{\partial\overline{\rho us_1}}{\partial f}+\bar{\bar{\beta}}_1\cdot\bar{\lambda}_1) = 0 \qquad (16a)$$

$$\frac{\partial\bar{S}}{\partial\dot{f}_N} = \Delta x\Delta t(\frac{\partial\overline{\rho s_N}}{\partial f}\cdot(\bar{\bar{1}}-\bar{\bar{\beta}}_{N-1})+\frac{1}{2\Delta x}\frac{\partial\overline{\rho us_N}}{\partial f}+(\bar{\bar{1}}-\bar{\bar{\beta}}_{N-1})\cdot\bar{\lambda}_N) = 0 \qquad (16b)$$

$$\frac{\partial\bar{S}}{\partial\dot{f}_n} = \Delta x\Delta t(\bar{\bar{1}}-\bar{\bar{\beta}}_{n-1}+\bar{\bar{\beta}}_n)\cdot(\frac{\partial\overline{\rho s_n}}{\partial f}+\bar{\lambda}_n) = 0 \qquad 2\leq n\leq N-1 \qquad (16c)$$

Equations (16) therefore define the Lagrange multipliers so that, for an interior node;

$$\bar{\lambda}_n = -\frac{\partial\overline{\rho s_n}}{\partial f} \qquad (17)$$

Finally, using the above results, the constrained functional is differentiated with respect to the β_n. The result is;

$$\frac{\partial \bar{S}}{\partial \beta_n} = \Delta x \Delta t \left(\left(\frac{\partial \overline{\overline{\rho s}}_{n+1}}{\partial f} - \frac{\partial \overline{\overline{\rho s}}_{n}}{\partial f} \right) \cdot (\bar{g}_{n+1} - \bar{g}_n) \right) \tag{18}$$

Equation (18) indicates that for this low order analysis it is not possible to find a stationary value of the functional. This is of course due to the fact that the functional is linear in β_n. What can be done is to determine the value of β_n which is in the direction of increasing system entropy. If β_n is viewed as an interpolant then it must have a value between zero and unity. The approach taken for the purposes of the following computations is to choose β_n equal to unity if the term in equations (18) is positive and equal to zero if the term is negative. In this fashion the differences become one-sided in the direction of maximum increase (or minimum decrease) of system entropy. It is also interesting to note that the boundary conditions naturally evolve from the analysis. Suppose that the left-most node remains at a fixed condition for all variables. In this case β_1 is not a variable and may not be determined by equation (18), rather it must be zero so that (13a) is removed from the equation list. In the diaphragm burst problem to be discussed later, the axial velocity must be fixed (zero) while density and energy are variable. Therefore the value of β_n for the momentum equation must be zero while the other two are determined by equation (18). It can be seen, therefore, that the analysis determines a differencing scheme for each equation at each node for each time step which simultaneously satisfies boundary conditions and the condition of maximum entropy increase. As will be seen, depending on the values of β_n any particular equation at any particular node may be differenced forward or backward or centered or unchanged.

Equations (13) may be solved for the $\dot{\bar{f}}$ at each node. This results in a nonconservative analog. If, however, equations (13) are solved in the following fashion;

$$\Delta x \bar{\bar{\beta}}_1 \cdot \dot{\bar{f}}_1 = -\bar{\bar{\beta}}_1 \cdot (\bar{g}_2 - \bar{g}_1) \tag{19a}$$

$$\Delta x (1 - \bar{\bar{\beta}}_{N-1}) \cdot \dot{\bar{f}}_N = -(1 - \bar{\bar{\beta}}_{N-1}) \cdot (\bar{g}_N - \bar{g}_{N-1}) \tag{19b}$$

$$\Delta x (1 - \bar{\bar{\beta}}_{n-1} + \bar{\bar{\beta}}_n) \cdot \dot{\bar{f}}_n = -\bar{\bar{\beta}}_n \cdot (\bar{g}_{n+1} - \bar{g}_n) - (1 - \bar{\bar{\beta}}_{n-1}) \cdot (\bar{g}_n - \bar{g}_{n-1}) \tag{19c}$$

then the result is absolutely conservative. To illustrate this, note that;

$$\int_V \dot{\bar{f}} \, dV = \sum_{n=1}^{N} \dot{\bar{f}}_n \Delta V_n = -(\bar{g}_N - \bar{g}_1) \qquad (20)$$

so that all the interior flux terms cancel and just the entering and exiting flux terms remain.

To summarize the computational procedure, having known values of $\bar{f}_n$ at a given time level, then

(1) compute $\bar{g}_n = \bar{g}_n(\bar{f}_n)$ for all nodes.

(2) compute $\partial \rho s/\partial f$ for all equations at all nodes.

(3) use equations (18) (and boundary conditions) to determine the β_n for each element.

(4) solve equations (19) for $(\dot{\bar{f}}_n \Delta V_n)$ at all nodes.

(5) integrate for next time level;

$$\bar{f}_n^{k+1} = \bar{f}_n^k + (\dot{\bar{f}}_n \Delta V_n)\Delta t/\Delta V$$

(6) repeat (1)-(5).

2.2 Results

The one-dimensional equations restrict the problems which can be solved to demonstrate the method. Two relatively difficult problems may be investigated, however. These are the shock tube and diaphragm burst. In the former case the boundary conditions dictate that $\bar{\beta}_1=(0,0,0)$ while $\bar{\beta}_{N-1}$ are free. In the latter case $\bar{\beta}_1=\bar{\beta}_{N-1}=(*,0,*)$ where the (*) indicates a free parameter. In all cases $\gamma=1.4$ and Z=1.

Figure 4 illustrates the behavior of the method for the shock tube conditions. The initial disturbance of the square wave has not yet washed out. This impulsive start typically gives rise to wavelets which migrate back and forth between the inlet and the traveling primary wave. If the solution domain were long enough a better description of the wave characteristics would result. In a higher spatial dimension analysis, however, economics prohibit the use of considerably more than the 40 points in a single direction. The traveling wave description shown in figure 4 is therefore typical of what would occur in a two-dimensional or three-dimensional analysis. The final velocity and pressure distributions are, of course, correct.

Figure 5 illustrates typical results on a diaphragm burst problem. The results shown occur just before the shock wave impinges on the downstream wall and just before the expansion wave reaches the upstream wall. Calculations have been run for many thousands of time steps in which the waves reflect many times from both ends. These results are not particularly interesting and in the interest of brevity are not shown here.

A typical time step is shown in figure 6. The rightmost three columns contain the values of beta for each equation at each node for this time step. These values of beta correspond to differencing schemes which are identified in the column headed by DIFF. The three letters at each node identify the scheme constructed for the three equations of motion. U means unchanged, B means backward, F means forward and C means centered. Time steps exceeding the CFL condition, as well as negative pressures and/or densities, are physically unrealistic. In the context of the variational approach they must be viewed as inequality constraints. Due to the difficulty of formally entering an inequality constraint into the functional definition, these constraints were handled in the following fashion: The time step was never allowed to exceed some predetermined fraction of the least local CFL and should a violation of the pressure or density inequality constraint occur then the time step was halved. Subsequent time steps were increased by 10 percent each step until the maximum time step is reached. It seems reasonable to expect that, particularly during initial transients, time steps may be attempted which would lead to negative pressures or densities. This should only be a temporary condition. Instability would be manifested by repeated attempts to achieve unrealistic values; fortunately this never occurred.

SHOCK TUBE ANALYSIS

Initial Conditions: p=1, ρ=1, u=0 (field); p=5, ρ=2.5, u=2 (inlet)

Boundary Conditions: fixed inlet(left end); free outlet

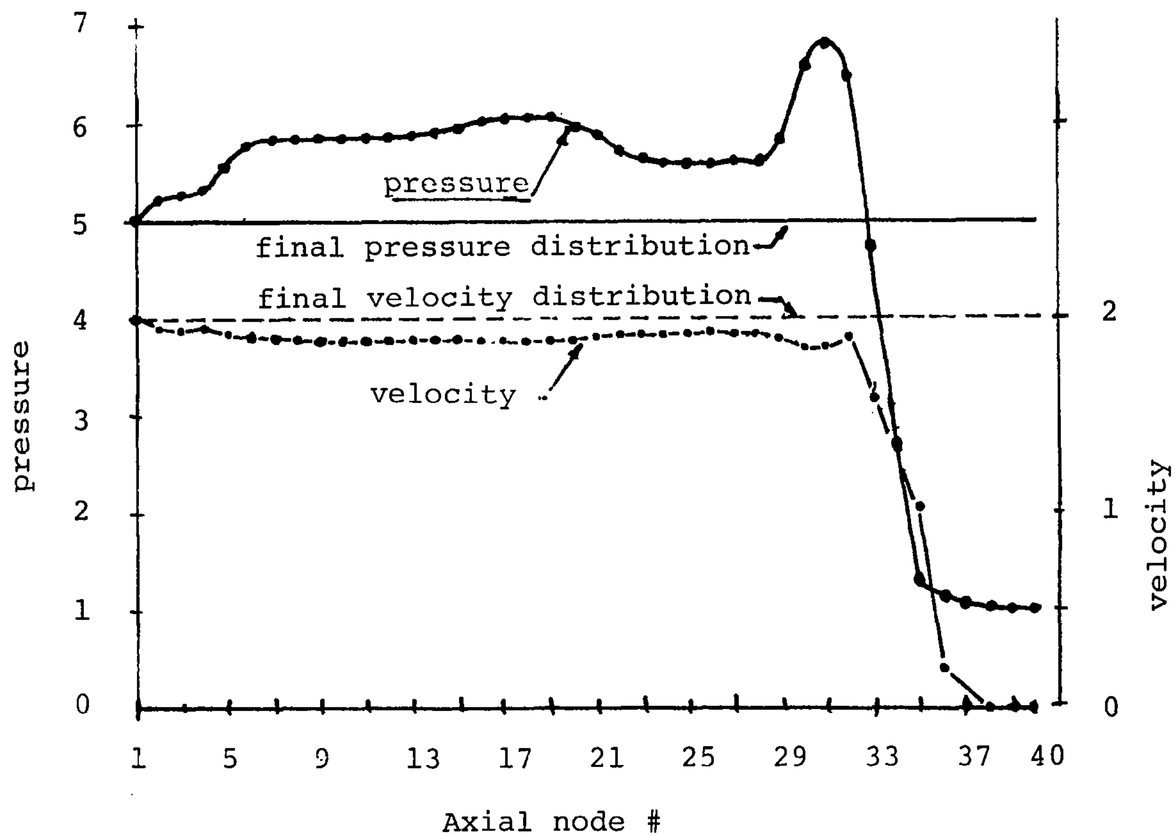

Figure 4 Typical shock tube solution

DIAPHRAGM BURST ANALYSIS

Initial Conditions: p=1, ρ=1, u=0; x>20   p=5, ρ=2.5, u=0; x<20

Boundary Conditions: ends closed

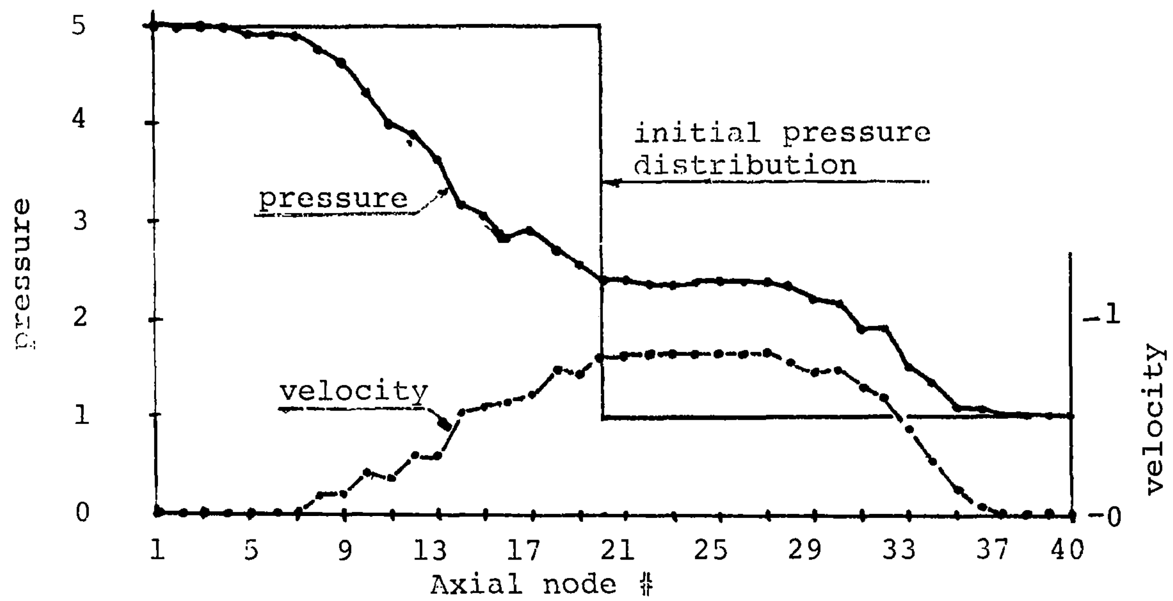

Figure 5 Typical diaphragm burst solution

RHO	U	P	S	DIFF	N	BETA		
						1	2	3
2.5	2	5	.326631	UUU	1	0	0	0
2.57916	1.94682	5.22646	.327287	BBB	2	0	0	0
2.70773	1.86161	5.60888	.329797	CBC	3	1	0	1
2.72572	1.84509	5.67329	.331944	UCU	4	0	1	0
2.74269	1.83781	5.73488	.334054	BUB	5	0	0	0
2.80334	1.79863	5.85965	.324955	BCB	6	0	1	0
2.81434	1.79491	5.88684	.324099	BFC	7	0	1	1
2.82569	1.79309	5.90675	.321843	BUF	8	0	0	1
2.82779	1.79735	5.89313	.318495	CBF	9	1	0	1
2.82664	1.80098	5.88075	.316962	FBF	10	1	0	1
2.80971	1.81649	5.80511	.312425	UBU	11	0	0	0
2.82753	1.81106	5.83201	.308195	BBB	12	0	0	0
2.81948	1.81693	5.7813	.303457	BCB	13	0	1	0
2.84409	1.80773	5.94022	.318407	CFB	14	1	1	0
2.83937	1.79687	5.87819	.310232	UFB	15	0	1	0
2.86766	1.78805	5.99697	.316359	BUB	16	0	0	0
3.13584	1.63467	6.40562	.257118	BBB	17	0	0	0
3.26656	1.64389	6.68209	.242198	CBC	18	1	0	1
3.10797	1.75955	6.14306	.227764	UBU	19	0	0	0
2.72106	1.9472	5.54265	.311042	BBB	20	0	0	0
2.83974	1.95249	5.30401	.207265	CBC	21	1	0	1
2.73827	1.70407	5.41724	.27933	FCU	22	1	1	0
1.91331	1.63961	2.53598	2.22153E-2	FUC	23	1	0	1
1.39086	.890265	2.07643	.268764	FBU	24	1	0	0
1.16036	.264713	1.2473	1.27515E-2	UBB	25	0	0	0
1.01275	7.62318E-2	1.08433	6.3226E-2	CBB	26	1	0	0
1.00341	4.62629E-3	1.0076	2.79814E-3	FBB	27	1	0	0
1.00033	2.55366E-3	1.00114	6.77699E-4	FBB	28	1	0	0
1.00015	1.38016E-4	1.00047	2.60028E-4	FBB	29	1	0	0
1.00001	6.17101E-5	1.00003	1.3826E-5	FBB	30	1	0	0

Figure 6 Illustration of differencing

3.0 CONCLUSIONS

In the preceding discussion it was proposed that the Second Law of Thermodynamics is a variational principle applicable to compressible gas dynamics. It was shown that the principle states that the system entropy must not decrease and that the equations of motion act as constraints to the entropy formation. It was further shown that, at least in an explicit formulation, arbitrary parameters exist which control or dictate the type of differencing scheme. The analysis then discusses how to select these arbitrary parameters such that the variational principle is satisfied while maintaining exact conservation.

The concept is demonstrated numerically for the shock tube and diaphragm burst situations. The success of these calculations demonstrates the validity of the original proposition, i.e., that the Second Law is indeed an applicable variational principle and furthermore demonstrates the validity of the calculational procedure derived from the stated principle.

A fundamental advance in the state of the art of computational fluid mechanics can be expected as a result of these findings.

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15. Supplementary Notes

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Interim Report

16. Abstract

A variational principle governing compressible fluid mechanics is introduced. A numerical analog based on this principle was devised and demonstrated for one-dimensional compressible flow in shock tube and diaphragm burst problems. The numerical behavior of the solution is excellent. The success of the numerical solution demonstrates the validity of the variational principle.

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