NASA
CR
3614
c.1

TECH LIBRARY KAFB, NM
0062121

NASA Contractor Report 3614

A Variational Principle for Compressible Fluid Mechanics

Discussion of the Multi-Dimensional Theory

LOAN COPY: RETURN TO
AFWL TECHNICAL LIBRARY
KIRTLAND AFB, N.M.

Robert Joel Prozan

CONTRACT NAS1-16646
OCTOBER 1982

NASA

TECH LIBRARY KAFB, NM

0062121

NASA Contractor Report 3614

A Variational Principle for Compressible Fluid Mechanics

Discussion of the Multi-Dimensional Theory

Robert Joel Prozan
Continuum, Inc.
Huntsville, Alabama

Prepared for
Langley Research Center
under Contract NAS1-16646

National Aeronautics
and Space Administration

Scientific and Technical
Information Branch

1982

FOREWORD AND ACKNOWLEDGEMENTS

The effort described herein was performed by Continuum, Inc., Huntsville, Alabama in support of the Supersonic Aerodynamics and the Performance Aerodynamics Branches of the High Speed Aerodynamics Division and the Computer Science and Applications Branch of the Analysis and Computation Division at the National Aeronautics and Space Administration's Langley Research Center. The technical monitors were Mr. James L. Hunt and Dr. Robert E. Smith, Jr.

1.0 SUMMARY AND INTRODUCTION

Although great strides have been made in the area of computational fluid mechanics in the past 40 years, it is probably fair to say that the progress has principally been due to enormous strides in the capacities of machinery rather than in the science of numerical methods. Problems of stability, conservation, and the treatment of corner flows inviscidly combined to restrict the ability of numericists to solve many problems of current interest.

In a previous discussion pertaining to one-dimensional compressible unsteady flow by Prozan[1], a variational principle for fluid mechanics was hypothesized. The excellent stability characteristics and absolutely conservative properties of that solution encouraged the extension of the investigation to multi-dimensional flow. The discussion in this report only deals with two-dimensional flow for square elements, but it is felt that the extension to three-dimensional flow and/or general element shapes presents no fundamental problems.

Introduction of the variational principle utilized herein indicates that the satisfaction of equations of motion which have been heretofore considered necessary and sufficient have only been necessary but not sufficient to guarantee a successful solution. Although successful solutions have been produced, they have been produced at the expense of conservation. Because (at least for explicit methods) absolutely conservative methods exhibit undesirable behavior with regards to stability, the conservative properties have been traded off against stability.

The key features of the methodology presented in the ensuing discussion are:

- absolutely conservative
- no explicit additions of artificial viscosity
- absolutely stable - stable time step internally controlled - operates near the CFL

- dynamically differences based on local conditions
- can be run with sparse grids for engineering or parametric solutions - can also be run with fine grid for more precise answers
- runs first time every time - no operator interaction nor special expertise is required.

In short, the methodology may be used to provide a quick response engineering analysis to whatever level of accuracy is required.

2.0 DISCUSSION

2.1 THE VARIATIONAL PRINCIPLES

For an unreacting, inviscid fluid, the Second Law of Thermodynamics states that

$$\int_V \left(\frac{\partial \rho s}{\partial t} + \nabla \cdot \rho \bar{q} s\right) dV \geq 0 \tag{1}$$

where ρ is the density, s is the intensive entropy, q is the velocity vector, and V is the volume of the domain. In the following discussion we will assume that the equations of motion are satisfied. Now equation (1) states that the internal entropy (extensive) production is greater than the net flux for <u>all</u> time. Since the production exceeds the flux then the accumulation of entropy must constantly increase. If we define the outer boundaries of the problem far enough away from the area of interest (or consider a closed system) then we can consider the inlet/outlet flux terms as constant. Rewriting equation (1);

$$\int_V \frac{\partial \rho s}{\partial t}\, dV - \int_{inlet} \rho \bar{q} s \cdot d\bar{A} + \int_{outlet} \rho \bar{q} s \cdot d\bar{A} \geq 0 \tag{2}$$

enables us to see that for an arbitrarily large time interval we have;

$$\int_V \frac{\partial \rho s}{\partial t}\, dV + C \geq 0 \tag{3}$$

where C is a constant (and is zero for a closed system).

It was previously stated that the entropy contained within the system must continually increase and since it cannot increase without limit then it must approach a maximum. Furthermore, since all unsteady fluctuations produce an entropy increase, however small, then the maximum entropy must occur at steady state.

If we view the numerical approximation as a process acting on the system we may conclude that the inexactitude of the approximation must be such that the predicted entropy is greater than or equal to the exact solution entropy in order to guarantee stability.

To clarify this conclusion we must state the equations of motion;

$$\frac{\partial e}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = D = 0 \tag{4}$$

where

$$e = (\rho,\ \rho u,\ \rho v,\ \rho E);$$
$$f = (\rho u,\ p+\rho u^2,\ \rho uv,\ \rho uH);$$
$$g = (\rho v,\ \rho uv,\ p+\rho v^2,\ \rho vH);$$

and D represents the continuity, axial momentum, lateral momentum, and energy equations, respectively, and where u is the axial velocity and v the lateral velocity.

Equation (1) may now be expanded as

$$\int_V Q_i D_i \, dV \geq 0 \quad (i=1,2,3,4) \tag{5}$$

where

$$Q_i = \frac{\partial \rho s}{\partial e_i}$$

Obviously, if the equations of motion are satisified everywhere within the system ($D_i = 0$), then equation (5) is satisfied. Under the numerical approximation, however, the equations of motion are not satisfied exactly but only in some approximate sense. Equation (5) may or may not be satisfied, therefore, even if the equations of motion are satisfied in the approximate sense.

Therefore, formulations which may be entirely acceptable in terms of the conservation equations may be unacceptable to (not satisfy) equation (5). It becomes clear then that satisfaction of the equations of motion is a necessary but not sufficient condition to satisfying the physical principles governing the motion.

It was earlier stated that the equations of motion would be assumed satisfied for discussion purposes. The approach taken to accomplish this will now be discussed.

The equations of motion act as equality constraints on the formation of extensive system entropy. Using the method of Lagrange to state the constrained functional yields;

$$S = \int_V \left(\frac{\partial \rho s}{\partial t} + \nabla \cdot \rho \bar{q} s\right) dV + \int_V \lambda_i D_i dV \geq 0 \tag{6}$$

where S is the constrained extensive system entropy production and λ_i are the Lagrange multipliers.

Differentiation of the constrained functional with respect to $\partial e_i/\partial t$ yields;

$$\frac{\partial S}{\partial\left(\frac{\partial e_i}{\partial t}\right)} = \int_V (Q_i + \lambda_i)\, dV \tag{7}$$

so that if the equality is chosen (exact solution) in equation (6) then we may conclude that the

$$\lambda_i = - Q_i \tag{8}$$

This, of course, is consistent with equation (5) which states that the constraints degenerate in the limit and that the Euler-Lagrange equations for the functional described in equation (1) are the equations of motion.

There could be, however, a whole class of functions which satisfy the above criterion (although only the one described above is embodied in a known principle of physics). In addition, we have no guarantee that a tractable solution can be devised, based on the principle, which offers a substantial advantage over current better known approaches. Of course, the success of the reference (1) solution for one-dimensional flow was an encouraging first step in the investigation.

Before proceeding with the numerical procedure which was developed to ascertain the applicability of the stated variational principle to numerical solutions in multi-dimensional flow, an interpretation of the Lagrange multipliers appearing in equation (6) is in order.

The integral constraint term of equation (6) looks exactly like a Method of Weighted Residuals statement and in point of fact enters into the problem formulation in an identical fashion as the quasi-variational definition of free parameters used by Oden[2] for the purpose of assembling finite elements into the entire computational domain.

Before concluding this section of the development it should be pointed out that for a closed system at constant temperature and pressure the principle stated does degenerate to Gibbs[3] criteria for equilibrium of a system of known energy. This observation suggests that the variational statement applies also to reacting flows. It further lends credence to a hypothesis by Prozan[4] which contends that there is a coupling between chemistry and flow that is not accounted for in the current usage of Gibbs free energy.

2.2 THE METHODOLOGY

2.2.1 Construction of the numerical model

Proceeding now with the construction of the model, we must first define

$$p = \frac{R}{c_v}\left\{\rho E - \frac{1}{2}(\rho u^2 + \rho v^2)\right\}, \quad H = E + \frac{p}{\rho}$$

and

$$s = c_v\,(\ln p - \gamma \ln \rho) \quad \text{where } p = \rho RT$$

Also,

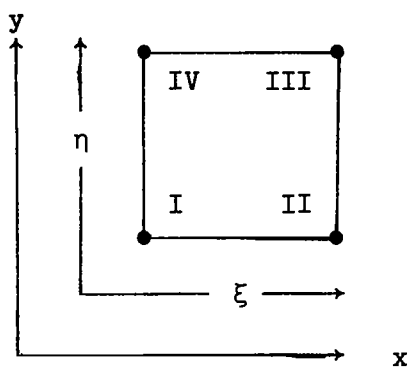
$$\frac{\partial \rho s}{\partial \rho} = (Ts - H + q^2)/T; \quad \frac{\partial \rho s}{\partial \rho u} = -u/T$$

$$\frac{\partial \rho s}{\partial \rho v} = -v/T; \quad \frac{\partial \rho s}{\partial \rho E} = 1/T$$

If the domain of interest is subdivided into a number of elements then we may write

$$S = \sum_{e=1}^{E} \int_{V_e} \left(\frac{\partial \rho s}{\partial t} + \frac{\partial \rho u s}{\partial x} + \frac{\partial \rho v s}{\partial y}\right) dV_e$$

$$+ \sum_{e=1}^{E} \int_{V_e} \lambda_i \left(\frac{\partial e_i}{\partial t} + \frac{\partial f_i}{\partial x} + \frac{\partial g_i}{\partial y}\right) dV_e \geq 0 \qquad (9)$$



Sketch 1 - Element Description

where the corners of the element are nodes in the assembled system. Due to the exploratory nature of this development, simplifying assumptions were made which greatly reduced the development lead time but must be removed before a general numerical model can be devised. Thus the element was assumed square with sides of length one. Therefore we transform;

$$x = x_I + \xi; \quad y = y_I + \eta \qquad (10)$$

The following shape functions were also assumed;

$$e = e_I(1-\xi)(1-\eta) + e_{II}\xi(1-\eta) + e_{III}\xi\eta + e_{IV}(1-\xi)\eta \qquad (11a)$$

$$f = f_I(1-\xi)(1-\eta) + f_{II}\xi(1-\eta) + f_{III}\xi\eta + f_{IV}(1-\xi)\eta \qquad (11b)$$

$$g = g_I(1-\xi)(1-\eta) + g_{II}\xi(1-\eta) + g_{III}\xi\eta + g_{IV}(1-\xi)\eta \qquad (11c)$$

$$\lambda = \lambda_I\Lambda_I(\xi,\eta)+\lambda_{II}\Lambda_{II}(\xi,\eta)+\lambda_{III}\Lambda_{III}(\xi,\eta)+\lambda_{IV}\Lambda_{IV}(\xi,\eta) \qquad (11d)$$

Notice that the "weight" functions Λ_I, Λ_{II}, Λ_{III}, Λ_{IV} have not been specified at this juncture.

Substitution of the above relations into a single element of the constraint terms of equation (9) yields, in general, an implicit analog. It is of interest, however, to create an explicit analog. If we choose the weight functions orthogonal to the shape functions, an explicit analog results.

$$\Lambda_I = b_I\left(\frac{2}{3} - \xi\right)\left(\frac{2}{3} - \eta\right) \tag{12a}$$

$$\Lambda_{II} = b_{II}\left(\frac{1}{3} - \xi\right)\left(\frac{2}{3} - \eta\right) \tag{12b}$$

$$\Lambda_{III} = b_{III}\left(\frac{1}{3} - \xi\right)\left(\frac{1}{3} - \eta\right) \tag{12c}$$

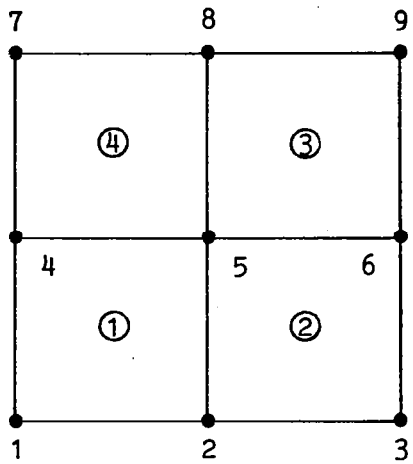
$$\Lambda_{IV} = b_{IV}\left(\frac{2}{3} - \xi\right)\left(\frac{1}{3} - \eta\right) \tag{12d}$$

(This orthogonality observation is the basis for the reference (5) analysis where a more complete discussion may be found). This step ("explicitizing" the solution) introduces undetermined coefficients b_I, b_{II}, b_{III}, b_{IV} which may be chosen in various ways and are therefore critical in controlling the solution behavior.

Substitution of the shape and weight functions into a single element integral of the constraint term in equation (9) yields, after integration,

$$\begin{aligned} C_{\textcircled{e}} = {} & \lambda_I b_{I_{\textcircled{e}}}(\dot{e}_I + f_{II} - f_I + g_{IV} - g_I) \\ & + \lambda_{II} b_{II_{\textcircled{e}}}(\dot{e}_{II} + f_{II} - f_I + g_{III} - g_{II}) \\ & + \lambda_{III} b_{III_{\textcircled{e}}}(\dot{e}_{III} + f_{III} - f_{IV} + g_{III} - g_{II}) \\ & + \lambda_{IV} b_{IV_{\textcircled{e}}}(\dot{e}_{IV} + f_{III} - f_{IV} + g_{IV} - g_I) \end{aligned} \tag{13}$$

The entire constraint term will now be formed. Consider a small subset of the assembled region.



Sketch 2 - Assembly Description

The constraint term integral becomes

$$
\begin{aligned}
&C_{①} + C_{②} + C_{③} + C_{④} + \cdots = \\
&\quad \lambda_1 b_{I_{①}}(\dot{e}_1 + f_2 - f_1 + g_4 - g_1) + \lambda_2 b_{II_{①}}(\dot{e}_2 + f_2 - f_1 + g_5 - g_2) \\
&+ \lambda_5 b_{III_{①}}(\dot{e}_5 + f_5 - f_4 + g_5 - g_2) + \lambda_4 b_{IV_{①}}(\dot{e}_4 + f_5 - f_4 + g_4 - g_1) \\
&+ \lambda_2 b_{I_{②}}(\dot{e}_2 + f_3 - f_2 + g_5 - g_2) + \lambda_3 b_{II_{②}}(\dot{e}_3 + f_3 - f_2 + g_6 - g_3) \\
&+ \lambda_6 b_{III_{②}}(\dot{e}_6 + f_6 - f_5 + g_6 - g_3) + \lambda_5 b_{IV_{②}}(\dot{e}_5 + f_6 - f_5 + g_5 - g_2) \\
&+ \lambda_5 b_{I_{③}}(\dot{e}_5 + f_6 - f_5 + g_8 - g_5) + \lambda_6 b_{II_{③}}(\dot{e}_6 + f_6 - f_5 + g_9 - g_6) \\
&+ \lambda_9 b_{III_{③}}(\dot{e}_9 + f_9 - f_8 + g_9 - g_6) + \lambda_8 b_{IV_{③}}(\dot{e}_8 + f_9 - f_8 + g_8 - g_5) \\
&+ \lambda_4 b_{I_{④}}(\dot{e}_4 + f_5 - f_4 + g_7 - g_4) + \lambda_5 b_{II_{④}}(\dot{e}_5 + f_5 - f_4 + g_8 - g_5) \\
&+ \lambda_8 b_{III_{④}}(\dot{e}_8 + f_8 - f_7 + g_8 - g_5) + \lambda_7 b_{IV_{④}}(\dot{e}_7 + f_8 - f_7 + g_7 - g_4) \\
&+ \ldots = 0
\end{aligned}
\tag{14}
$$

Notice that all terms with coefficients of λ_5 are explicitly present in equation (14). The same may or may not be true for the other values of $\lambda_1 - \lambda_9$ depending on whether or not they are on boundaries.

A digression from the element derivation is taken here to explicitly recreate the nodal analog. This step is not actually in the computation, but is undertaken at this point with the intention of clarifying the analog.

Collecting coefficients of λ_5 yields, for the constraint term,

$$\begin{aligned}\lambda_5\{&(b_{III_{①}} + b_{IV_{②}} + b_{I_{③}} + b_{II_{④}})\dot{e}_5 + b_{III_{①}}(f_5 - f_4 + g_5 - g_2)\\ &+ b_{IV_{②}}(f_6 - f_5 + g_5 - g_2) + b_{I_{③}}(f_6 - f_5 + g_8 - g_5)\\ &+ b_{II_{④}}(f_5 - f_4 + g_8 - g_5)\} + \ldots = 0 \qquad (15)\end{aligned}$$

In the quasi-variational formulation of Oden, λ_5 is considered an arbitrary parameter, therefore its coefficient must be zero. In this formulation, we recapture the constraint equation by differentiation with respect to the Lagrange multipliers. The result is the same for either interpretation; i.e.

$$\begin{aligned}&(b_{III_{①}} + b_{IV_{②}} + b_{I_{③}} + b_{II_{④}})\dot{e}_5 + b_{III_{①}}(f_5 - f_4 + g_5 - g_2)\\ &+ b_{IV_{②}}(f_6 - f_5 + g_5 - g_2) + b_{II_{③}}(f_6 - f_5 + g_8 - g_5)\\ &+ b_{II_{④}}(f_5 - f_4 + g_8 - g_5) = 0 \qquad (16)\end{aligned}$$

The above relation is the assembled nodal analog used for a general interior point. In the actual procedure this equation is not formulated and coded but rather is constructed as an assembly. Equation (16) is presented here, however, in its assembled form so that its features may be examined.

Now at this point all of the b factors appearing in equation (16) are arbitrary. Choosing all parameters equal to 1/4 creates a centered space

backward time analog. Other choices give other analogs (perhaps not all of which have been attempted by previous researchers).

Now that the analog has been explicitly illustrated, a return will be made to the element derivation.

Collecting all coefficients of f_5 and g_5 which will appear in a system volume integral results in

$$\int_V \frac{\partial e}{\partial t}\, dV + (b_{III_{①}} + b_{IV_{①}} - b_{III_{②}} - b_{IV_{②}} - b_{I_{③}} - b_{II_{③}} + b_{I_{④}} + b_{II_{④}})\, f_5$$
$$+ (b_{II_{①}} + b_{III_{①}} + b_{I_{②}} + b_{IV_{②}} - b_{I_{③}} - b_{IV_{③}} - b_{II_{④}} - b_{III_{④}})\, g_5$$
$$+ \ldots = 0 \qquad (17)$$

If the conservation equations are to apply over the entire domain, then the contribution of f_5 and g_5 must disappear. Therefore, for integral conservation, we have;

$$b_{III_{①}} + b_{IV_{①}} - b_{III_{②}} - b_{IV_{②}} - b_{I_{③}} - b_{II_{③}} + b_{I_{④}} + b_{II_{④}} = 0 \qquad (18a)$$

$$b_{II_{①}} + b_{III_{①}} + b_{I_{②}} + b_{IV_{②}} - b_{I_{③}} - b_{IV_{③}} - b_{II_{④}} - b_{III_{④}} = 0 \qquad (18b)$$

To preserve the volume of the system we must have (contributions of subvolume pieces add up to the system volume);

$$b_I + b_{II} + b_{III} + b_{IV} = 1 \qquad (18c)$$

It is desirable to have a scheme which defines the b parameters on an element level without regard to the surrounding elements. At least one such definition is, for each element,

$$b_I + b_{II} = \frac{1}{2}\ ; \quad b_{III} + b_{IV} = \frac{1}{2}\ ; \quad b_I = b_{III}\ ; \quad b_{II} = b_{IV} \qquad (19)$$

which leaves us with one free parameter per element. This selection is modified for boundary elements in such a fashion that all conservation requirements are met while exactly satisfying boundary conditions.

The definition of parameters found in equation (19) solves a wide range of very difficult problems but did exhibit instabilities at very high shock tube and diaphragm burst pressure ratios (1000/1). In view of the fact that the one-dimensional solution did successfully handle even higher pressure ratios (greater than 1000/1) it seemed that a superior technique could be created. Fortunately this was the case.

If the original differential equation is split

$$D = \frac{\partial e}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = \left(\frac{\partial e_x}{\partial t} + \frac{\partial f}{\partial x}\right) + \left(\frac{\partial e_y}{\partial t} + \frac{\partial g}{\partial y}\right) = 0 \tag{20}$$

and the identical derivation is followed, we find that the coefficients of f_5 and g_5 are;

$$\alpha_{III_{①}} + \alpha_{IV_{①}} - \alpha_{III_{②}} - \alpha_{IV_{②}} - \alpha_{I_{③}} - \alpha_{II_{③}} + \alpha_{I_{④}} + \alpha_{II_{④}} = 0 \tag{21a}$$

$$\beta_{II_{①}} + \beta_{III_{①}} + \beta_{I_{②}} + \beta_{IV_{②}} - \beta_{I_{③}} - \beta_{IV_{③}} - \beta_{II_{④}} - \beta_{III_{④}} = 0 \tag{21b}$$

where equation (21a) is identical to equation (18a) but with a substitution of α for b while equation (21b) is identical to equation (18b) with a substitution of β for b.

The system volume integral is preserved if

$$\alpha_I + \alpha_{II} + \alpha_{III} + \alpha_{IV} = 1 \tag{22a}$$

$$\beta_I + \beta_{II} + \beta_{III} + \beta_{IV} = 1 \tag{22b}$$

Equations (21) and (22) are satisfied if

$$\alpha_I + \alpha_{II} = \frac{1}{2}\ ; \quad \alpha_{III} + \alpha_{IV} = \frac{1}{2}\ ; \quad \beta_I + \beta_{IV} = \frac{1}{2}\ ; \quad \beta_{II} + \beta_{III} = \frac{1}{2} \tag{23}$$

Again, only for discussion purposes, we write the nodal analog.

$$(\dot{e}\Delta V)_5 = -\{(\alpha_{III_{①}} + \alpha_{II_{④}})(f_5 - f_4) + (\alpha_{IV_{②}} + \alpha_{I_{③}})(f_6 - f_5)$$

$$+ (\beta_{III_{①}} + \beta_{IV_{②}})(g_5 - g_2) + (\beta_{I_{③}} + \beta_{II_{④}})(g_8 - g_5)\} \qquad (24)$$

where

$$(\dot{e}\Delta V)_5 = (\alpha_{III_{①}} + \alpha_{IV_{②}} + \alpha_{I_{③}} + \alpha_{II_{④}})(\dot{e}_x)_5$$

$$+ (\beta_{III_{①}} + \beta_{IV_{②}} + \beta_{I_{③}} + \beta_{II_{④}})(\dot{e}_y)_5 \qquad (25)$$

Comparison of equations (24) and (25) with equation (16) shows that we have sacrificed nothing in the substitution of α and β for b. As we shall see later a great deal has been gained since the scheme based on α and β is much more powerful.

Inspection of equations (22) and (23) reveals that there are now four free parameters (instead of only one using equations (19)). If we define

$$\alpha_I = \frac{1}{2}\alpha_S \; ; \quad \alpha_{II} = \frac{1}{2}(1 - \alpha_S) \qquad (26a)$$

$$\alpha_{IV} = \frac{1}{2}\alpha_N \; ; \quad \alpha_{III} = \frac{1}{2}(1 - \alpha_N) \qquad (26b)$$

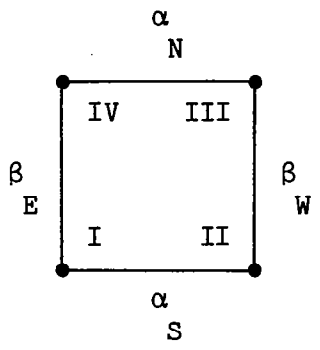
$$\beta_I = \frac{1}{2}\beta_W \; ; \quad \beta_{IV} = \frac{1}{2}(1 - \beta_W) \qquad (26c)$$

$$\beta_{II} = \frac{1}{2}\beta_E \; ; \quad \beta_{III} = \frac{1}{2}(1 - \beta_E) \qquad (26d)$$

where α_S, α_N, β_W, β_E may take on values between 0 and 1 (values less than zero or greater than one will generate negative volumes and are therefore avoided).

It is necessary at this time to introduce boundary conditions. The computer code which was produced under this effort utilized a scheme which will be explained here. Although the identification scheme is not central to the theory it will simplify the explanation of the necessary treatment.

At each node (corner of a square element) in the system, a boundary condition code word is input. This code word consists of four digits (0 or 1) where each digit corresponds to an independent variable. The variables are taken in the order ρ, ρu, ρv, and ρE. Zero means the parameter cannot change while one means that it is free. Thus 1011 identifies a tangency condition where ρu cannot change but ρv can while 1101 is an axial slip condition. A fixed inlet then is 0000. An interior node is 1111. Consider then the element shown below.



Sketch 3 - Free Parameters

Suppose now that the property at nodes I and II cannot change, i.e., $\dot{e}\Delta V = 0$. Unless this is a corner element then the element to the right and to the left will have the same condition. Further, let us assume that corner I is node 5 in equations (24,25). Obviously, regions ① and ② do not exist so that under those conditions equations (24,25) become,

$$(\dot{e}\Delta V)_5 = -\left\{\alpha_{II_{④}}(f_5 - f_4) + \alpha_{I_{③}}(f_6 - f_5) + (\beta_{I_{③}} + \beta_{II_{④}})(g_8 - g_5)\right\} \quad (27a)$$

where

$$(\dot{e}\Delta V)_5 = (\alpha_{I_{③}} + \alpha_{II_{④}})(\dot{e}_x)_5 + (\beta_{I_{③}} + \beta_{II_{④}})(\dot{e}_y)_5 \quad (27b)$$

Apparently

$$\alpha_{I_{③}} = \alpha_{II_{④}} = \beta_{I_{③}} = \beta_{II_{④}} = 0$$

for if they did not, $(\dot{e}\Delta V)_5$ would have a value and (e) would change. We can see that, within the element,

$$\alpha_I = \alpha_{II} = 0 \; ; \quad \alpha_{III} + \alpha_{IV} = 1$$

$$\beta_I = \beta_{II} = 0 \; ; \quad \beta_{III} = \beta_{IV} = \frac{1}{2}$$

while maintaining absolute conservation, that there is only one free parameter ($2\alpha_N$).

There are many other situations which can occur for corner nodes, nodes on left and right-hand walls. These situations may be derived by the interested reader but a treatment of each situation would considerably lengthen this discussion and is therefore omitted. The final scheme which treats all conditions is stated later.

It is now possible to discuss the selection of the values for α_S, α_N, β_W, and β_E, which control the stability of the solution. Since the constraint equations have been satisfied we may write, for the system entropy production,

$$S = \sum_{e=1}^{E} \int_{V_e} \frac{\partial \rho s}{\partial t} \, dV_e = \sum_{e=1}^{E} \{ Q_{I_i} (\mathring{e}\Delta V)_{I_i} + Q_{II_i} (\mathring{e}\Delta V)_{II_i}$$

$$+ Q_{III_i} (\mathring{e}\Delta V)_{III_i} + Q_{IV_i} (\mathring{e}\Delta V)_{IV_i} \}_e$$

where there is a contribution from each equation (i). Examining the contribution from a single equation within a typical element;

$$S_{ie} = - Q_I \{ \alpha_I (f_{II} - f_I) + \beta_I (g_{IV} - g_I) \} - Q_{II} \{ \alpha_{II} (f_{II} - f_I) + \beta_{II} (g_{III} - g_{II}) \}$$

$$- Q_{III} \{ \alpha_{III} (f_{III} - f_{IV}) + \beta_{III} (g_{III} - g_{II}) \} - Q_{IV} \{ \alpha_{IV} (f_{III} - f_{IV}) + \beta_{IV} (g_{IV} - g_I) \}$$

or

$$S_{ie} = \alpha_S (A_I - A_{II}) + \alpha_N (A_{IV} - A_{III}) + \beta_W (B_I - B_{IV})$$

$$+ \beta_E (B_{II} - B_{III}) + \frac{1}{2} (A_{II} + A_{III} + B_{IV} + B_{III})$$

where

$$A_I = - Q_I(f_{II} - f_I) \; ; \quad B_I = - Q_I(g_{IV} - g_I) \tag{28a}$$

$$A_{II} = - Q_{II}(f_{II} - f_I) \; ; \quad B_{II} = - Q_{II}(g_{III} - g_{II}) \tag{28b}$$

$$A_{III} = - Q_{III}(f_{III} - f_{IV}) \; ; \quad B_{III} = - Q_{III}(g_{III} - g_{II}) \tag{28c}$$

$$A_{IV} = - Q_{IV}(f_{III} - f_{IV}) \; ; \quad B_{IV} = - Q_{IV}(g_{IV} - g_I) \tag{28d}$$

$$\frac{\partial S_{ie}}{\partial \alpha_S} = A_I - A_{II} \; ; \quad \frac{\partial S_{ie}}{\partial \alpha_N} = A_{IV} - A_{III} \tag{29a,b}$$

$$\frac{\partial S_{ie}}{\partial \beta_W} = B_I - B_{IV} \; ; \quad \frac{\partial S_{ie}}{\partial \beta_E} = B_{II} - B_{III} \tag{29c,d}$$

The above equations (29) tell us how to change the free parameters in order to promote entropy production but give us no information on what value the parameters should have. Since the range of parameters is (0,1) we choose the parameters such that the most entropy is produced. Therefore, assuming that α_S, α_N, β_W, β_E are set to zero to begin with, then

$$A_I - A_{II} > 0 \rightarrow \alpha_S = 1 \tag{30a}$$

$$A_{IV} - A_{III} > 0 \rightarrow \alpha_N = 1 \tag{30b}$$

$$B_I - B_{IV} > 0 \rightarrow \beta_W = 1 \tag{30c}$$

$$B_{II} - B_{III} > 0 \rightarrow \beta_E = 1 \tag{30d}$$

Notice that there is no guarantee that the system entropy production will exceed the flux but that within the constraints of the equations of motion, boundary conditions, and element interactions that the production rate is maximized.

The corner node α,β are then computed from equations (26). The boundary condition digits for this particular equation are summed. If the sum equals four then all nodes are free. If the sum is two or one, an alteration of the α,β is required to satisfy boundary conditions.

If the sum is two, then

$$\left.\begin{array}{l}\alpha_j \leftarrow \frac{1}{2}\,\delta_j \\ \beta_j \leftarrow \delta_j\beta_j\end{array}\right\}\ \delta_{II} - \delta_I \neq 0 \tag{31a}$$

$$\left.\begin{array}{l}\alpha_j \leftarrow \delta_j\alpha_j \\ \beta_j \leftarrow \frac{1}{2}\,\delta_j\end{array}\right\}\ \delta_{II} - \delta_I = 0 \tag{31b}$$

while if the sum is one;

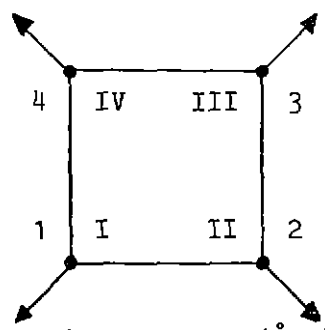
$$\alpha_j \leftarrow \delta_j\ ;\quad \beta_j \leftarrow \delta_j \tag{31c}$$

where δ is the (0,1) digit signifying free or fixed and j is the node (I,II,III,IV).

To assemble the element into the system the following procedure is used.

$$(\dot{e}\Delta V)_4' = (\dot{e}\Delta V)_4 - \alpha_{IV}(f_{III}-f_{IV}) - \beta_{IV}(g_{IV}-g_I)$$

$$(\dot{e}\Delta V)_3' = (\dot{e}\Delta V)_3 - \alpha_{III}(f_{III}-f_{IV}) - \beta_{III}(g_{III}-g_{II})$$



$$(\dot{e}\Delta V)_1' = (\dot{e}\Delta V)_1 - \alpha_I(f_{II}-f_I) - \beta_I(g_{IV}-g_I)$$

$$(\dot{e}\Delta V)_2' = (\dot{e}\Delta V)_2 - \alpha_{II}(f_{II}-f_I) - \beta_{II}(g_{III}-g_{II})$$

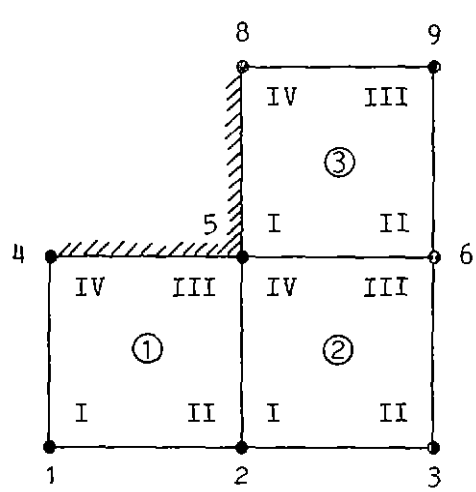
Sketch 4 - Derivative Assembly

In the diagram above, the nodes in the full domain numbering system are 1, 2, 3, and 4. At the beginning of each time step, the $(\dot{e}\Delta V)$ for each node are set to zero and a sweep through each element is made adding in contributions from each corner of the element. In this fashion, the explicit analog is constructed dynamically at each time step.

2.2.2 Expansion Corner Treatment

Another very important facet of the development was the expansion corner treatment. Due to the very simple nature of the element shape and time and core restraints on the machine, the following corner procedure was developed.

The element analog in the expansion corner region was assembled (on paper) and examined. Having only one node at a corner which was subject to axial slip on one side and lateral slip on the other, the only acceptable conclusion to satisfy both conditions was that the corner is a stagnation point. While this is certainly true in the real world, on the scale of the element sizes and nodal densities which we must accept in the development, a stagnation treatment was out of the question. A scheme was devised whereby special boundary conditions were enforced which allowed the corner to be treated as axial slip on one side, free at the corner, and lateral slip on the other. To clarify this, consider the assembly below.



Sketch 5 - Expansion Corner

Node 4 has boundary condition code of 1101 while node 8 is 1011 and node 5 is 1111. A special condition is introduced where node III of element ① is 1101 and node I of element ③ is 1011. Now if δ_u and δ_v are normally taken as unity for any node but are reset to the second and third digits of the special condition at node III of element ① and node I of element ③ then the corner satisfies slip on both sides and is absolutely conservative as long as we redefine

$$f = \delta_u \rho u,\ p + \delta_u \rho u^2,\ \delta_{uv} \rho uv,\ \delta_u \rho uH \tag{32a}$$

$$g = \delta_v \rho v,\ \delta_{uv} \rho uv,\ p + \delta_v \rho v^2,\ \delta_v \rho vH \tag{32b}$$

where $\delta_{uv} = 0$ at the corner (common) node.

Since the pressure is continuous at the corner, the treatment leaves something to be desired for supersonic flow but seems to be an excellent solution for subsonic flow.

To this point the solution has been first order time. A second order (or higher) method may be readily evolved. The statements in equations (1), (2) and (6) may also be made over an arbitrary time interval. For instance, equation (6) becomes

$$S(t_2) - S(t_1) = \int_{t_1}^{t_2} S\, dt \tag{33}$$

while our differential equation becomes

$$\int_{t_1}^{t_2} \left(\frac{\partial e}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right) dt = 0 \tag{34}$$

The second order time solution was effected by letting;

$$f = C_1 f_k - C_2 f_{k-1} \tag{35a}$$

$$g = C_1 g_k - C_2 g_{k-1} \tag{35b}$$

where

$$C_1 = 1 + \frac{1}{2}\frac{\Delta t_k}{\Delta t_{k-1}} \; ; \quad C_2 = \frac{1}{2}\frac{\Delta t_k}{\Delta t_{k-1}}$$

and understanding that $(\dot{e}\Delta V)$ is the average change over the time interval Δt_k.

To advance the assembled system nodal quantities one time step we let

$$e_{k+1} = e_k + (\dot{e}\Delta V)\Delta t_k/\Delta V \tag{36}$$

where ΔV is the assembled system volume associated with that node. To arrive at this system volume we associated 1/4 of each element surrounding the node with that node. A concave corner node for example has $\Delta V = 1/4$ while a wall node has $\Delta V = 1/2$ and an expansion corner has $\Delta V = 3/4$ and finally an interior node has $\Delta V = 1$.

2.3 THE COMPUTER PROGRAM

A computer program was written to test the new procedure on an Alpha-Micro 100 micro computer at Continuum. Due to severe storage limitations, the largest grid attainable was 13 x 13 nodes (12 x 12 elements). The computational sequence is

1. Given the current state of the system (ρ, ρu, ρv, ρE are known at all nodes) compute f, g, Q at each node. Null $\dot{e}\Delta V$ for all nodes.

2. Sweep through all elements performing the following steps for each element and each equation for that element

   - Compute $A_I,\ldots,A_{IV}$, $B_I,\ldots,B_{IV}$ using (28)
   - Compute α_S, α_N, β_W, β_E using (30)
   - Compute $\alpha_I,\ldots,\alpha_{IV}$, $\beta_I,\ldots,\beta_{IV}$ using (26)
   - Enforce boundary conditions using (31)
   - Assemble contribution into nodal system as in Sketch 4.

3. Step forward in time using (36).

4. Return to Step 1.

The CFL condition was used to compute the time step. An input quantity was used to define the maximum fraction of the CFL at which the solution was allowed to operate. The inequality constraint of non-zero and non-negative pressure and density was also enforced. If such a situation occurred, the time step was halved. For each successful time step, the time step was increased by 4 per cent (doubles every 20 steps) up to the limiting step.

Each node was supplied with a boundary condition code. This information was principally used to give tangency conditions but also was used on density and energy if it was desired, for example, to keep an inlet fixed.

An option was provided for first or second order time expansion. All results presented used second order time, but first order time also apparently works very well (this statement is qualified since not very many cases were run first order).

3.0 COMPUTATIONAL RESULTS

The first tests of the new computer program were one-dimensional shock tube and diaphragm burst problems. Due to the splitting technique outlined previously, the method degenerates exactly to one-dimensional flow formulation for these cases. Absolute conservation was achieved. The same results occurred whether the problems were run left to right, right to left, top to bottom, or bottom to top. No results are shown here since they were previously documented in reference (1).

Figure 1 illustrates the results of a problem which was run to determine corner conservation and long-term system entropy production. Absolute conservation was noted. The system extensive entropy did not monotonically increase but rather increased rapidly for the first 50 time steps and then oscillated with a general upward trend for the remainder of the problem.

Figure 2 shows the velocity vectors resulting from the impulsive start of a Mach 1.2 jet (γ = 1.4) exhausting into a quiescent background. The solution was run for 800 time steps at which time conditions were changing very slowly. The outflow boundaries of the problem were free. No instability occurred.

Figure 3 illustrates flow over a rear-facing step and the results are shown at 200 time steps. Once again we have a Mach 1.2 jet (γ = 1.4). This run was not an evolutionary run since the entire field was set to uniform parallel flow except at the back side of the step where the lateral slip condition was enforced. An inviscid recirculation cell has occurred along the back side of the step. No instabilities were noted (at least to this stage of the solution).

Figure 4 gives the results for a Mach 1.2 jet (γ = 1.4) into which a small high momentum jet is being injected. The Mach number of the secondary jet is 2.4 (γ = 1.4). The solution flow vectors may be found in the figure as well as pressure distributions on the upper and lower walls. A high pressure region occurs just upstream of the secondary jet and a very low pressure region occurs downstream. The high pressure region along the upper wall has a

peak shifted downstream of the secondary jet position. The solution seemed very well behaved and was changing only slowly at 100 time steps.

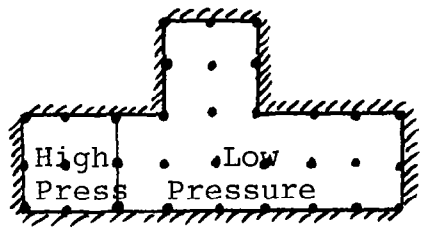
In general it can be stated that the method has demonstrated the following features:

- No instabilities have occurred.
- Absolute conservation, no matter what the complexity.
- Successfully handles implusive starts of 1000/1 pressure ratios for diaphragm burst and imposed jets.
- Stability for closed systems approaching or achieving steady state.

Due to the extremely long running time on this small machine, we cannot absolutely conclude that the solution is stable at very long run times when the solution approaches steady state. Problems of this nature must be investigated on a more powerful machine.

The number of operations per step should be typical of explicit finite difference operators such as MacCormack[6].

The entropy production shown in Figure 1 illustrates that this numerical approximation to the variational statement does not guarantee monotonically increasing entropy and therefore does not absolutely guarantee stability. It is possible, however, that with a small enough time step or a higher order in time solution that monotonicity could be achieved (for a given problem).



Diaphragm

High Press

$p=5, \rho=2$

Low Press

$p=1, \rho=1$

Final

$p=1.91, \rho=1.23$

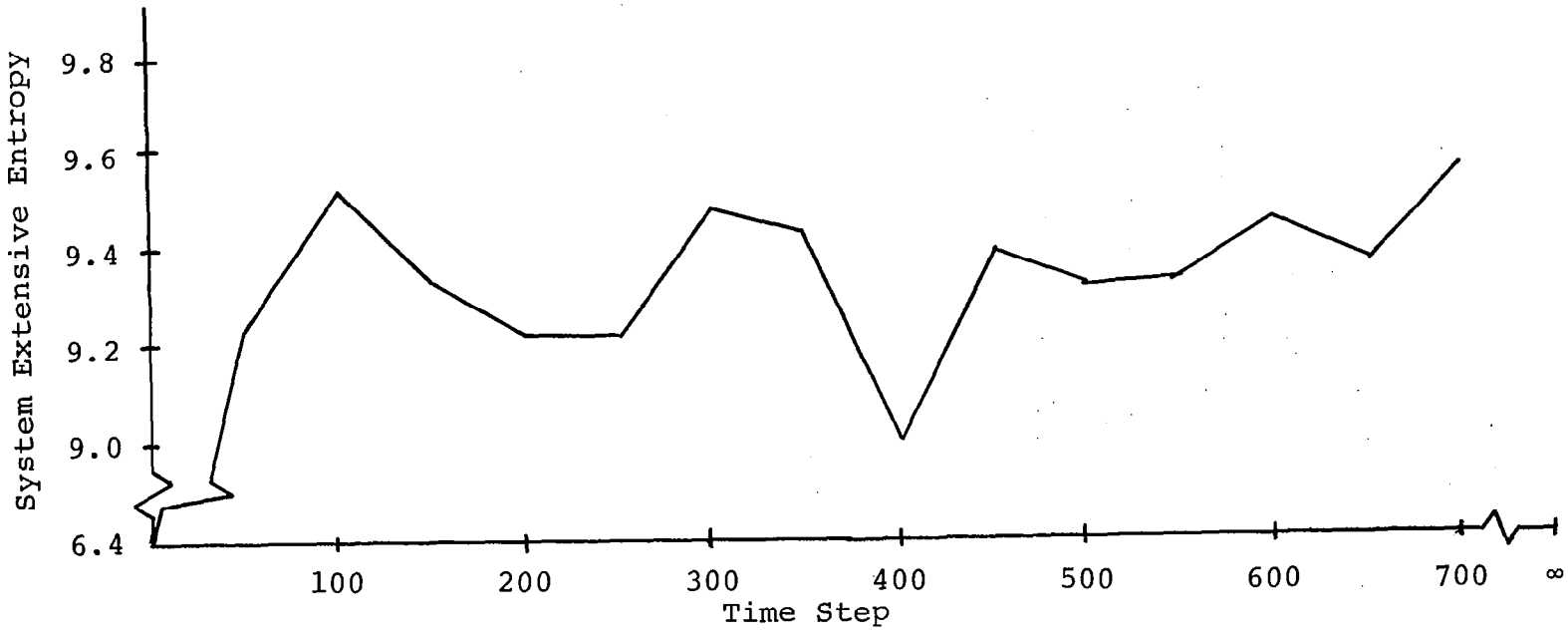


Figure 1.- Corner Conservation and Long Time Behavior.

RUN INFORMATION

Initial Conditions: $p=5, \rho=2.5, u=2, v=0$ (inlet)
$p=1, \rho=1, u=0, v=0$ (field)

Boundary Conditions: slip along walls, inlet fixed

Results plotted: 800 time steps

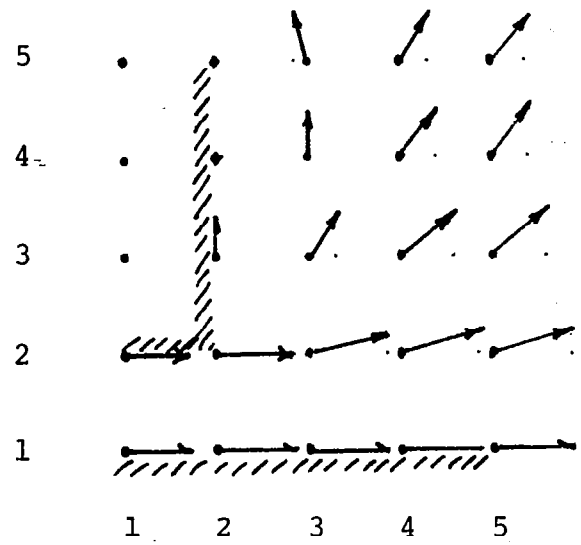


Figure 2.- Supersonic Jet

Exhausting into Quiescent Background.

RUN INFORMATION

Initial Conditions: $p=5, \rho=2.5, u=2, v=0$ (field)
$p=5, \rho=2.5, u=0, v=0$ (backside of step)

Boundary Conditions: slip along walls, inlet held fixed

Results plotted @ 200 time steps

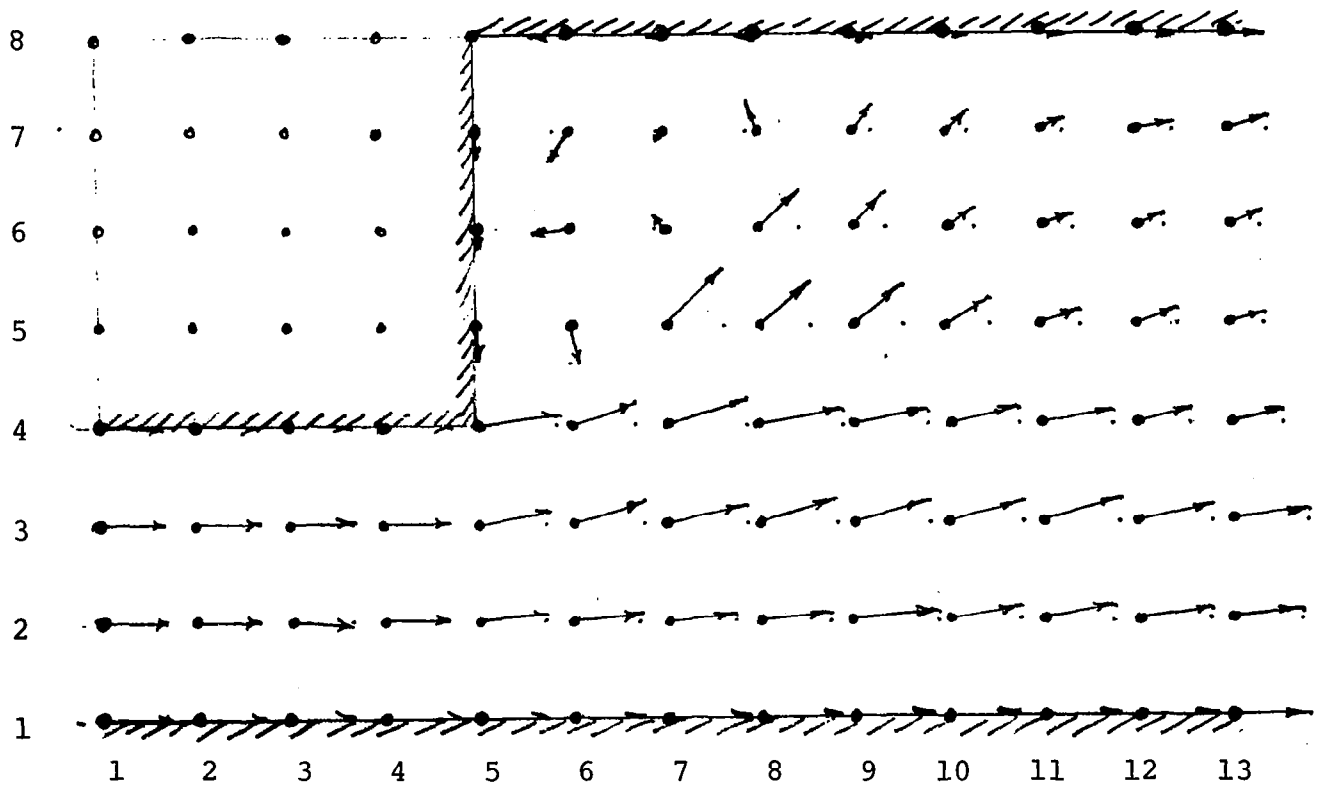


Figure 3. - Flow over a

Rear Facing Step.

RUN INFORMATION

Initial Conditions: p=5,ρ=2.5,u=2,v=0 (primary jet inlet and field)
p=3,ρ=2.5,u=0,v=4 (secondary jet inlet)

Boundary Conditions: slip along walls,inlets held fixed

Results plotted @ 100 time steps

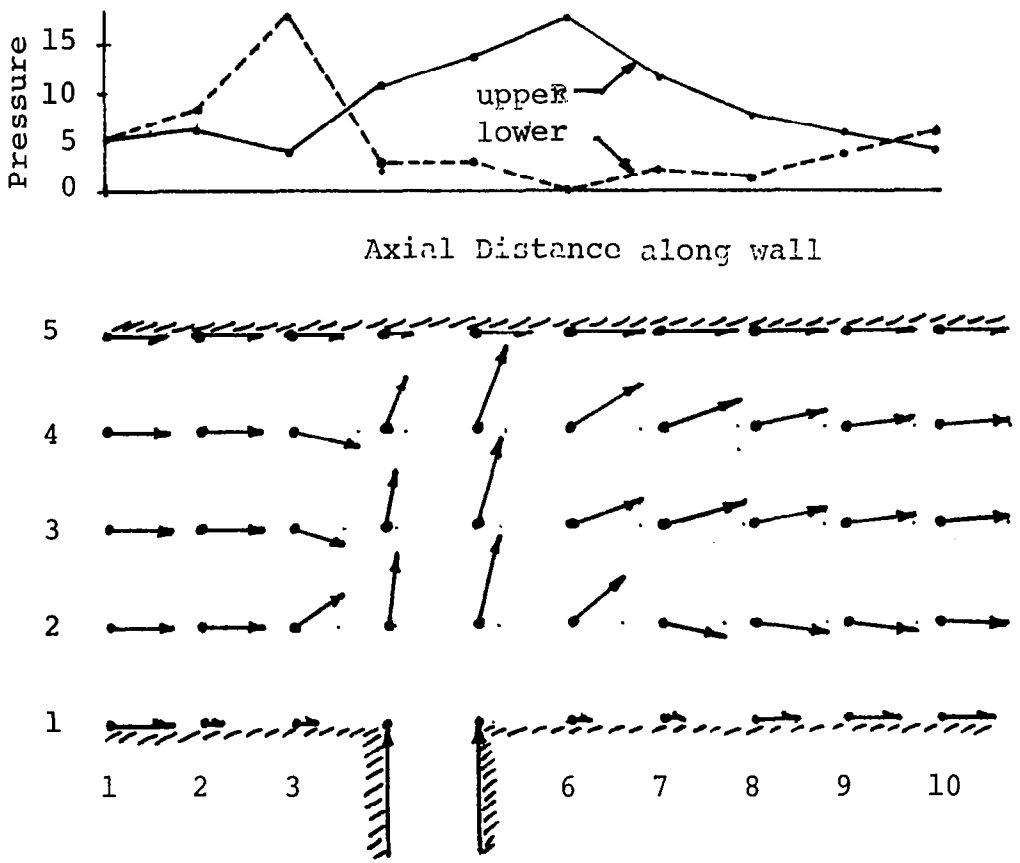


Figure 4.- Jet Interaction.

4.0 CONCLUSIONS

The foregoing discussion lends credence to the hypothesis that a variational principle for fluid mechanics does exist and that it can be utilized to create a powerful new approach to numerical solutions. The procedure developed here is applicable to problems of a complex yet practical nature which would be extremely difficult to solve by any other procedure.

To summarize the developments discussed earlier, an analog has been created which is:

- o absolutely conservative
- o absolutely stable
- o explicitly adds no artificial viscosity
- o dynamically differences based on local conditions
- o can provide inexpensive and quick response for engineering and/or parametric solutions to whatever level of sophistication is deemed reasonable by the user.

There is, of course, much more to be done to further verify the technique, investigate higher order solutions, and to extend it to general quadrilaterals, axisymmetric flows, three-dimensional flows, viscous flows, and reacting flows.

REFERENCES

1. Prozan, R.J., "A Variational Principle for Compressible Fluid Mechanics (Discussion of One-Dimensional Theory)," NASA CR 3526, April 1982.

2. Oden, J.T., "A General Theory of Finite Elements," International Journal of Numerical Methods in Engineering, Vol. I, pp. 205-221, 1969.

3. Gibbs, J.W. (Collected Works) 1928, Yale University Press.

4. Prozan, R.J., "Maximization of Entropy for Flowing Systems Subject to Downstream Boundary Conditions," Lockheed Missiles & Space Company, LMSC/HREC D149342, 1969.

5. Prozan, R.J., L.W. Spradley, P.G. Anderson, and M.L. Pearson, "The General Interpolants Method: A Procedure for Generating Numerical Analogs of the Conservation Laws," AIAA Paper 77-642, AIAA Third Computational Fluid Dynamics Conference, Albuquerque, NM, June 1977.

6. MacCormack, R.W., "The Effect of Viscosity in Hypervelocity Impact Cratering," AIAA Paper 69-354, Cincinnati, Ohio, May 1969.

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA CR- 3614		

4. Title and Subtitle	5. Report Date
A VARIATIONAL PRINCIPLE FOR COMPRESSIBLE FLUID MECHANICS - DISCUSSION OF THE MULTI-DIMENSIONAL THEORY	OCTOBER 1982
	6. Performing Organization Code
7. Author(s) Robert Joel Prozan	8. Performing Organization Report No. CI-TR-0062
	10. Work Unit No.
9. Performing Organization Name and Address Continuum, Inc. 4717 University Dr. (Suite 96) Huntsville, Alabama 35805	11. Contract or Grant No. NAS1-16646
	13. Type of Report and Period Covered Contractor Report
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, DC 20546	14. Sponsoring Agency Code 505-31-82-02 505-31-73-01

15. Supplementary Notes

Langley Technical Monitor: James L. Hunt
Interim Report

16. Abstract

The variational principle for compressible fluid mechanics previously introduced in NASA CR-3526 is extended to two-dimensional flow. The analysis is stable, exactly conservative, adaptable to coarse or fine grids, and very fast. Solutions for two-dimensional problems are included. The excellent behavior and results lend further credence to the variational concept and its applicability to the numerical analysis of complex flow fields.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Variational Principle Numerical Analysis Fluid Mechanics	Unclassified - Unlimited Subject Category 02

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified	32	A03

* For sale by the National Technical Information Service, Springfield, Virginia 22161

NASA-Langley, 1982