Journal of Engineering Mathematics, Vol. 15, No. 3, July 1981

Applications of a variational method for mixed differential equations*

P. K. KHOSLA and S. G. RUBIN

Department of Aerospace Engineering and Applied Mechanics, University of Cincinnati, Cincinnati, Ohio 45221, USA

(Received August 1, 1980 and in revised form October 28, 1980)

SUMMARY

Variational principles for elliptic boundary-value problems as well as linear initial-value problems have been derived by various investigators. For initial-value problems Tonti and Reddy have used a convolution type of bilinear form of the functional for the time-like coordinate. This introduces a certain amount of directionality thereby reflecting the initial-value nature of the problem. In the present investigation the methods of Tonti and Reddy are used to derive the appropriate variational formulation for the transonic flow problem. A number of linear and non-linear examples have been investigated. As a test for the existence of directionality, finite-differences are used to discretize the variational integral. For initial-value problems of wave equation and diffusion equation type, fully implicit finite-difference approximations are recovered. The small-disturbance transonic equation leads to the Murman and Cole differencing theory; when applied to the full potential-flow equations, the rotated difference scheme due to Jameson is obtained.

1. Introduction

The inviscid compressible-flow equations are of elliptic or hyperbolic type for sub- and supersonic flows, respectively. Transonic flow is characterized by both and therefore a mixed system must be considered. Two classes of numerical techniques have been proposed for the solution of mixed differential equations.

1. Based on the theory of positive symmetric partial differential equations, which are type independent, a well-developed theory for linear partial differential equations, due to Friedrichs [1], is available. The differential equation is first reduced to a general form, which is type independent; then, finite differences or finite-element discretization is used. Numerical computations for the two-dimensional Tricomi equation, using these methods, have been carried out by Katsanis [2], Lesaint [3] and Aziz and Leventhal [4]. The application to non-linear equations of mixed type does not appear to be straightforward.

2. The second approach is a finite-difference method. Two distinct procedures for differencing the derivatives are specified for the equations in the elliptic and hyperbolic regions. These difference techniques are consistent with the boundary and initial conditions, and take into consideration the proper domain of dependence in the hyperbolic region. The application to

* An extended version of this paper was first presented at the Bat-Sheva International Seminar on Finite Elements for Non-Elliptic Problems, Tel-Aviv, Israel, July 1977.

the Tricomi equation and more general linear partial differential equations of the mixed type have been considered by Filippov [5] and Ogawa [6], respectively. Successful application of this method to the solution of the non-linear equations governing transonic flow has been developed to a reasonable degree of sophistication in the work of Murman and Cole [7] and Jameson [8].

The inability to formulate a variational principle for initial-value problems is due to the lack of a self-adjoint property, (see [4]) and has been known for quite some time. Gurtin [9] was the first to successfully formulate a variational principle for the heat-conduction equation by the convolution method. Although this approach has the advantage of implicitly incorporating the initial conditions, the resulting Euler-Lagrange equation is an integro-differential equation and therefore remains quite complex. Tonti [10], by incorporating a convolution type bilinear form, derived a variational principle for the diffusion equation. His method has been further extended to more general parabolic and hyperbolic equations by Reddy [11]. These variational principles are derived only for linear equations, but they do prepare the way for incorporating the necessary directionality required for the solution of the transonic-flow equations.

For non-linear equations, the incorporation of the convolution-type bilinear form in the variational formulation leads to the inverse problem of the calculus of variations for initial-value problems. The problem of finding a variational principle for a given operator has been solved by Vainberg [12]. Recently, it has been further elucidated by Atherton and Homsy [13]. The operational formulas for an arbitrary number of non-linear differential equations have been derived to verify if a variational principle exists.

In the present investigation the methods of Tonti [10] and Reddy [11] are used to derive the appropriate composite variational formulation, or in effect Galerkin method, for the transonic-flow problem. A number of linear and non-linear examples are also described. As a test for the existence of directionality, finite differences are used to discretize the variational integral. For initial-value problems described by the wave equation and diffusion equation, fully-implicit finite-difference approximations are recovered. The small-disturbance transonic analysis leads to the Murman and Cole [7] differencing theory; when applied to the full potential-flow equations, the rotated difference scheme due to Jameson [8] is obtained.

In Section 2 a general summary of the inverse problem of the calculus of variations is given. Section 3 contains the application of these ideas to the wave equation and non-linear Burgers' equation. In Section 4 the application to the compressible-flow problem (small disturbance as well as full potential-flow equations) is presented. For additional examples and details, see [14].

2. General formulation

Let $L(u)$ be any operator. The inverse problem of variational calculus requires the construction of a functional F such that the linear Gateau differential of F, i.e., the general derivative $\delta F = 0$, leads to the Euler-Lagrange equations when $L(u) = 0$. This can be achieved, when it can be shown that $L(u)$ is a potential operator. Toward this end, Vainberg's [12] theorem provides, as the necessary and sufficient conditions for $L(u)$ to be a potential operator, that the linear Gateau differential $\delta L(u)$ be symmetric. Therefore, if (A, B) represents the appropriate scalar product, then for $L(u)$ to be a potential operator,

$$(\delta L(u, \Phi), \Psi) = (\delta L(u, \Psi), \Phi). \tag{1}$$

The functional $F(u)$ can be given by

$$F(u) = (u, \int_0^1 L(\lambda u) d\lambda) = \int u \int_0^1 L(\lambda u) d\lambda dV.$$

Following Atherton and Homsy [13], we assume that the linear Gateau differential is uniformly continuous; i.e., the Fréchet differential of the operator exists. Therefore,

$$\delta F = \frac{d}{d\epsilon} \int (u + \epsilon\Phi) \int_0^1 L[\lambda(u + \epsilon\Phi)] d\lambda dV \Big|_{\epsilon = 0}.$$

With the symmetry condition (1) and an integration by parts, we find

$$\delta F = \int L(u) \Phi dV,$$

Since,Φ is arbitrary, $\delta F = 0$ leads directly to

$$L(u) = 0,$$

as the Euler-Lagrange equation.

From (1), Atherton and Homsy [13] have developed a number of consistency requirements, which determine whether a given operator is in fact a potential operator. If the given operator is not a potential operator, Atherton and Homsy [13] have shown how a composite variational principle, or in effect a Galerkin method can be devised to provide $L(u) = 0$. The required functional $F(u, v)$ is formed by introducing the adjoint variable v as:

$$F(u, v) = (v, L(u)) = \int v L(u) dV.$$

Once again performing the operator derivative,

$$\delta F = \frac{d}{d\epsilon} \int (v + \epsilon\Psi) L(u + \epsilon\Phi) dV \Big|_{\epsilon = 0} = \int [\Psi L(u) + v \widetilde{L}_u^1(\Phi)] dV. \tag{2}$$

Integrating by parts, we obtain

$$\int v \widetilde{L}_u^1(\Phi) dV = \int \Phi \widetilde{L}_u^1(v) dV, \tag{3}$$

where $\widetilde{L}_u^1$ is the adjoint of the Fréchet derivative of $L(u)$. Since Φ and Ψ are arbitrary functions the equations (2) and (3), with $\delta F = 0$, lead to

$$L(u) = 0,$$

and

$$\widetilde{L}_u^1(v) = 0.$$

Therefore one of the Euler-Lagrange equations leads to $L(u) = 0$. Finlayson [15] has noted the equivalence of this derivation with Galerkin procedures. For finite-element methods the existence of a variational principle is not necessary; therefore, we will use the composite variational principle, with the appropriate integral formulation which leads to a finite-element treatment of the transonic- and supersonic-flow equations.

In the following discussion, we will examine several equations of practical interest. We shall determine whether potential operators exist with respect to either of two scalar products; viz,

$$(u,v) = \int_{\Omega}\int_{t^*}^{t_0} u(\mathrm{x},t)v(\mathrm{x},t)dtd\mathrm{x}, \tag{4}$$

and

$$(u,v) = \int_{\Omega}\int_{t^*}^{t_0} u(\mathrm{x},t)v(\mathrm{x},t_0 - t)dtd\mathrm{x}. \tag{5}$$

In boundary-value problems t denotes a space variable, while for initial-value problems t corresponds to either time or a 'time-like' coordinate. It is the second scalar product (5) that has enabled Tonti [10] and Reddy [11] to develop a consistent variational formulation for initial-value problems of heat-conduction or wave-propagation type. They only consider linear systems.

In the next section, we shall re-examine the variational principles for the wave, heat-conduction and non-linear Burgers' equations. We shall demonstrate that the proper formulation leads to the appropriate stable discrete forms of these equations in each case. The Fréchet derivative and its classical analogue, the ordinary derivative, will be used interchangeably. Finally, finite-difference equations are derived, in each case, directly from the variational integral. The domain-of-dependence principle is satisfied immediately when the scalar product (5) is assumed for the wave equation. This leads to the retarded differencing commonly applied for transonic flows. Detailed discussions for sub-, trans- and supersonic flows are presented in Section 4.

3. Examples

In this section we will illustrate some of the general ideas outlined previously and show how the second form of scalar product defined by equation (5) is important in properly formulating the variational principle for initial-value problems.

3.1 Wave equation

Let us examine the wave equation

$$\Phi_{tt} - c^2\Phi_{yy} = 0,$$

with respect to both scalar products (4, 5). It can be shown that the linear wave operator is a potential operator with respect to (4) and (5). Although, as pointed out by Reddy [11] and others, the initial conditions should be taken into account when formulating the functional. We shall ignore the contribution from initial as well as boundary conditions in the present discussion. The functionals corresponding to (4) and (5) are, respectively,

$$F_1 = \iint (\Phi_t^2 - c^2 \Phi_y^2) dt dy, \tag{6a}$$

and

$$F_2 = \iint_0^{t_0} [\Phi_t \Phi_\tau + c^2 \Phi_y(t,y) \Phi_y(\tau,y)] dt dy, \tag{6b}$$

where $\tau = t_0 - t$.

If we replace Φ by $\Phi + \epsilon u$, where u is some arbitrary function, the Fréchet derivative, after integration by parts, leads to

$$\delta F_1 = 2 \iint u(t,y) [\Phi_{tt} - c^2 \Phi_{yy}] dt dy,$$

and

$$\delta F_2 = \iint \{u(t,y)[\Phi_{\tau\tau}(\tau,y) - c^2 \Phi_{yy}(\tau,y)] + u(\tau,y)[\Phi_{tt}(t,y) - c^2 \Phi_{yy}(t,y)]\} dt dy.$$

Since u is arbitrary, the Euler-Lagrange equation for both cases is given by

$$\Phi_{tt} - c^2 \Phi_{yy} = 0. \tag{7}$$

We see that a variational principle exists for both scalar products; for the latter (6b) the concept of domain of dependence is implicitly taken into account.

If we consider a finite-difference discretization for the functionals F_1 and F_2, in lieu of the usual discretization for the governing second-order wave equation (7), some interesting results are obtained. Let

$$\Phi_t = \frac{\Phi_{i,j} - \Phi_{i-1,j}}{\Delta t}; \Phi_y = \frac{\Phi_{i,j} - \Phi_{i,j-1}}{\Delta y}, \tag{8a}$$

where $\tau = t_0 - t$; $\Delta\tau = -\Delta t$; i, j are the t- and y-grid indices, respectively, and $t_0 = N\Delta t$. Then

$$\Phi_\tau = \frac{\Phi(\tau + \Delta\tau) - \Phi(\tau)}{\Delta\tau} = \frac{\Phi_{N-(i+1)} - \Phi_{N-i}}{-\Delta t} = \frac{\Phi_{N-i} - \Phi_{N-i-1}}{\Delta t},$$

$$F_1 = \sum_{ij}\sum \left[\left(\frac{\Phi_{i,j} - \Phi_{i-1,j}}{\Delta t} \right)^2 - c^2 \left(\frac{\Phi_{i,j} - \Phi_{i,j-1}}{\Delta y} \right)^2 \right] \Delta t \Delta y, \tag{8b}$$

$$F_2 = \sum_{ij}\sum \left[\frac{\Phi_{i,j} - \Phi_{i-1,j}}{\Delta t} \frac{\Phi_{N-i,j} - \Phi_{N-i-1,j}}{\Delta t} \right. \tag{8c}$$

$$\left. + c^2 \frac{\Phi_{i,j} - \Phi_{i,j-1}}{\Delta y} \frac{\Phi_{N-i,j} - \Phi_{N-i,j-1}}{\Delta t} \right] \Delta t \Delta y.$$

If we now formally evaluate the Fréchet derivative with respect to the discretized variable Φ_{ij}, i.e., evaluate $\partial F_{1,2}/\partial\Phi_{ij}$, and if we define

$$F_1 = \sum_{ij}\sum J_{1ij}\,\Delta y\Delta t\;; F_2 = \sum_{ij}\sum J_{2ij}\,\Delta y\Delta t,$$

then

$$\frac{\partial F_1}{\partial\Phi_{i,j}} = \frac{\partial J_{1ij}}{\partial\Phi_{i,j}}\,\delta^{ij}_{i,j} + \frac{\partial J_{1ij}}{\partial\Phi_{i-1,j}}\,\delta^{ij}_{i-1,j} + \frac{\partial J_{1ij}}{\partial\Phi_{i,j-1}}\,\delta^{ij}_{i,j-1},$$

or

$$\frac{\partial F_1}{\partial\Phi_{i,j}} = -\frac{\Phi_{i+1,j}-2\,\Phi_{i,j}+\Phi_{i-1,j}}{\Delta t^2} + c^2\,\frac{\Phi_{i,j+1}-2\,\Phi_{i,j}+\Phi_{i,j-1}}{\Delta y^2}.$$

Similarly,

$$\frac{\partial F_2}{\partial\Phi_{k,j}} = 2\left[\frac{\Phi_{N-k,j}-2\,\Phi_{N-k-1,j}+\Phi_{N-k-2,j}}{\Delta t^2} - c^2\,\frac{\Phi_{N-k,j+1}-2\,\Phi_{N-k,j}+\Phi_{N-k,j-1}}{\Delta y^2}\right].$$

If we redefine $N-k = i$, then $\partial F_1/\partial\Phi_{i,j}= 0$ and $\partial F_2/\partial\Phi_{i,j}= 0$ lead to

$$\frac{\Phi_{i+1,j}-2\,\Phi_{i,j}+\Phi_{i-1,j}}{\Delta t^2} - c^2\,\frac{\Phi_{i,j+1}-2\,\Phi_{i,j}+\Phi_{i,j-1}}{\Delta y^2} = 0, \tag{9}$$

and

$$\frac{\Phi_{i,j}-2\,\Phi_{i-1,j}+\Phi_{i-2,j}}{\Delta t^2} - c^2\,\frac{\Phi_{i,j+1}-2\,\Phi_{i,j}+\Phi_{i,j-1}}{\Delta y^2} = 0, \tag{10}$$

respectively. Equation (9) is the central-difference analogue of the wave equation, while equation (10) corresponds to a retarded differencing in the time direction. Equation (9) represents an explicit scheme, that is restricted by the CFL stability requirement, $c\Delta t/\Delta y \leqq 1$. Equation (10) is an implicit finite-difference form of the wave equation and is unconditionally stable. The proper domain of dependence is automatically taken into account. It should be noted that the stable implicit scheme is a direct consequence of the scalar product (5) which provides the necessary directional property for the hyperbolic equations. It is also interesting that proper directionality is obtained by discretizing the functionals and then applying the differentiation. In this way, it is necessary to prescribe only the first-derivative difference approximations (8a). For more complex gas dynamic equations, this is a significant simplification.

3.2 Burgers' equation

The simplest model of a non-linear equation with diffusion and convection is given by Burgers' equation. It has been shown by Atherton and Homsy [13] that this equation does not satisfy the requirements of a potential operator. Thus a true variational formulation is not possible. However, one can use the composite variational principle, see Section 2. An appropriate functional which leads to

$$\Phi_t + ½(\Phi^2)_x = \nu\Phi_{xx} \tag{11}$$

as one of the Euler-Lagrange equations of the composite variational principle can be defined by

$$F(u, \Phi) = \iint \left(u(\tau, x)\, \Phi_t - \frac{\Phi^2}{2} u_x + \nu \Phi_x u_x \right) dt dx, \tag{12}$$

where u is an adjoint variable. With the difference equations (8), we have $F = \sum\sum_{ij} J_{ij} \Delta t \Delta x$, where

$$J_{ij} = u_{N-i,j} \frac{\Phi_{i,j} - \Phi_{i-1,j}}{\Delta t} - \frac{\Phi_{i,j}^2}{2} \frac{u_{N-i,j} - u_{N-i,j-1}}{\Delta x}$$

$$+ \nu \frac{\Phi_{i,j} - \Phi_{i,j-1}}{\Delta x} \frac{u_{N-i,j} - u_{N-i,j-1}}{\Delta x} .$$

As we are interested in the discretized form of the Burgers' equation, the Fréchet derivative with respect to u is required. This leads to

$$\delta F = \sum\sum_{kj} u_{N-k,j} \left[\frac{\Phi_{k,j} - \Phi_{k-1,j}}{\Delta t} + \frac{\Phi_{k,j+1}^2 - \Phi_{k,j}^2}{2\Delta x} \right.$$

$$\left. - \nu \frac{\Phi_{k,j+1} - 2\Phi_{k,j} + \Phi_{k,j-1}}{\Delta x^2} \right]$$

Since u is arbitrary, we have

$$\frac{\Phi_{k,j} - \Phi_{k-1,j}}{\Delta t} + \frac{\Phi_{k,j+1}^2 - \Phi_{k,j}^2}{2\Delta x} = \nu \frac{\Phi_{k,j+1} - 2\Phi_{k,j} + \Phi_{k,j-1}}{\Delta x^2} . \tag{13}$$

Equation (13) is the familiar implicit finite-difference form of Burgers' equation. It can be seen that the convective term is only first-order accurate, although second-order accuracy is achieved for the diffusion derivative.

At this stage, it should be noted that the differencing of the space derivative is not unique and as an alternative to the backward difference (8), we could specify the forward spatial approximation

$$\Phi_x = \frac{\Phi_{i,j+1} - \Phi_{i,j}}{\Delta x} . \tag{14}$$

This flexibility is not available with the other coordinate (t) because of its time-like character; only, backward differencing is physically acceptable. One can apply either type of differencing for multiple spatial coordinates as in elliptic equations. The use of equation (14) instead of the one given in (8) does not alter the final result for either the wave- or diffusion equations. However, Burgers' equation (13) becomes

$$\frac{\Phi_{k,j} - \Phi_{k-1,j}}{\Delta t} + \frac{\Phi_{k,j}^2 - \Phi_{k,j-1}^2}{2\Delta x} = \nu \frac{\Phi_{k,j+1} - 2\Phi_{k,j+1} + \Phi_{k,j-1}}{\Delta x^2} . \tag{15}$$

By averaging (13) and (15) we recover the conservative central-difference form of Burgers' equation. This is second-order accurate in space for both diffusion and convection. Uniform second-order accuracy in space and time can also be achieved by centering all terms in F at $(i - ½, j - ½)$, see [16].

4. Transonic small-disturbance equations

Steady transonic small-disturbance theory is governed by the equation

$$[K - (\gamma + 1)\,\Phi_x]\Phi_{xx} + \Phi_{yy} = 0, \tag{16}$$

where γ is the ratio of the specific heats and K is the transonic similarity parameter. For supercritical flows, local regions of supersonic flow with $K < (\gamma + 1)\,\Phi_x$ are created, thereby making equation (16) locally hyperbolic. Everywhere the problem is boundary-value in character, except in the supersonic bubble where it is initial-value like. Any discretization must take into account the directionality associated with the supersonic region, i.e., whenever, $K < (\gamma + 1)\,\Phi_x$. We shall use the variational formulations previously described to discretize equation (16) in both subsonic and supersonic regions.

4.1 Subsonic region

It can be shown that the operator (16) is potential and the appropriate functional is given as:

$$F = \iint\int_0^1 \Phi L(\lambda\Phi)d\lambda dxdy,$$

or

$$F = -\tfrac{1}{2}\iint[K\Phi_x^2 - \frac{\gamma + 1}{3}\,\Phi_x^3 + \Phi_y^2]dxdy . \tag{17}$$

Recently, Geffen [17] has derived a similar variational principal in terms of the velocities $u = \Phi_x$ and $v = \Phi_y$. From (17), the Euler-Lagrange equation (16) can easily be obtained.
Now let

$$\Phi_x = \frac{\Phi_{i,j} - \Phi_{i-1,j}}{\Delta x}; \quad \Phi_y = \frac{\Phi_{i,j} - \Phi_{i,j-1}}{\Delta y} . \tag{18}$$

Substituting in (17), we obtain

$$F = -\frac{1}{2}\sum_i\sum_j\left[\left(K - \frac{\gamma+1}{3}\,\frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}\right)\left(\frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}\right)^2 + \left(\frac{\Phi_{i,j}-\Phi_{i,j-1}}{\Delta y}\right)^2\right]\Delta x \Delta y.$$

Now $\delta F = 0$ leads to

$$\left[K - (\gamma+1)\,\frac{\Phi_{i+1,j}-\Phi_{i-1,j}}{2\Delta x}\right]\frac{\Phi_{i+1,j}-2\Phi_{i,j}+\Phi_{i-1,j}}{\Delta x^2} + \frac{\Phi_{i,j+1}-2\Phi_{i,j}+\Phi_{i,j-1}}{\Delta y^2} = 0. \tag{19}$$

If, instead of (18), we had used backward differences to approximate Φ_x and/or Φ_y, equation (19) will remain unchanged. This is the central-difference form of equation (16).

4.2 Supersonic region

In this case, we are required to use the scalar product of the type given in equation (5). The operator (16) is not a potential operator. The composite variational principle can be easily established. If we define ω as an adjoint variable, the appropriate functional is then given by

$$F(\omega, \Phi) = \int_{-\infty}^{\infty}\int^{x_0}\left[[K\,\Phi_x\omega_\tau - \frac{\gamma+1}{2}\,\omega_\tau(\Phi_x^2) - \omega_y\Phi_y\right]dxdy, \tag{20}$$

where $\tau = x_0 - x$ and x_0 is representative of the length of the supersonic region. Because of the time-like character of the coordinate x, Φ_x must be differenced in the backward direction. For Φ_y one can use either forward or backward differences. Thus

$$\begin{aligned}
\Phi_x &= \frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}\ ;\ \omega_\tau = \frac{\omega_{N-i,j}-\omega_{N-i-1,j}}{\Delta x}\ ;\\
\Phi_y &= \frac{\Phi_{i,j}-\Phi_{i,j-1}}{\Delta y}\ \text{ or }\ \Phi_y = \frac{\Phi_{i,j+1}-\Phi_{i,j}}{\Delta y}\ ;\\
\omega_y &= \frac{\omega_{N-i,j}-\omega_{N-i,j-1}}{\Delta y}\ \text{ or }\ \omega_y = \frac{\omega_{N-i,j+1}-\omega_{N-i,j}}{\Delta y}.
\end{aligned} \tag{21}$$

Substituting from equation (21) into equation (20) we obtain

$$F = \sum_i\sum_j\left[K\,\frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}\,\frac{\omega_{N-i,j}-\omega_{N-i-1,j}}{\Delta x} - \frac{\gamma+1}{2}\left\{\frac{\omega_{N-i,j}-\omega_{N-i-1,j}}{\Delta x}\times\left(\frac{\Phi_{i,j}-\Phi_{i-1,j}}{\Delta x}\right)^2\right\} - \frac{\Phi_{i,j}-\Phi_{i,j-1}}{\Delta y}\,\frac{\omega_{N-i,j}-\omega_{N-i,j-1}}{\Delta y}\right]\Delta x\Delta y.$$

The derivative $\partial F/\partial \omega_{N-k,j} = 0$ leads to

$$\left[K - \frac{\gamma+1}{2}\frac{\Phi_{k,j} - \Phi_{k-2,j}}{\Delta x}\right]\frac{\Phi_{k,j} - 2\Phi_{k-1,j} + \Phi_{k-2,j}}{\Delta x^2}$$

$$+ \frac{\Phi_{k,j+1} - 2\Phi_{k,j} + \Phi_{k,j-1}}{\Delta y^2} = 0. \tag{22}$$

This is the retarded difference form of equation (16). Equations (19) and (22) were first proposed by Murman and Cole [7]. These equations are implicit and unconditionally stable. They are generally solved by relaxation methods.

4.3 Complete compressible potential flow equations

Although Bateman [18] and Lush and Cherry [19] have presented general variational formulations for potential flows, the composite variational principle dealing directly with the potential flow equation will achieve the same results. Greenspan and Jain [20] and Rasmussen and Heys [16] have obtained the discretized form of the potential-flow equations from the variational principle. The relationship of these results with central finite-differences appears to have been overlooked by these authors. It will be shown here that for subsonic flows, the discretized equations derived either from Bateman's principle or the composite variational principle are in fact identical. For supersonic flows with the composite variational formulation, the retarded difference formulas, obtained previously for the transonic small-disturbance equation, will be recovered for the full compressible-flow equations.

Subsonic flow

Bateman's principle states that minimizing the pressure $p(q^2)$ with the functional

$$F = \iint p(q^2)\,dx\,dy \tag{23}$$

leads to the general potential equation of gas dynamics,

$$(a^2 - u^2)\,\Phi_{xx} - 2uv\Phi_{xy} + (a^2 - v^2)\,\Phi_{yy} = 0, \tag{24}$$

where $q^2 = u^2 + v^2$; $u = \Phi_x$, $v = \Phi_y$, and a is the sound speed. We follow Greenspan and Jain [20] and discretize the equation (23). Let

$$\Phi_x = \frac{\Phi_{i+1,j} - \Phi_{i,j}}{\Delta x}\,;\ \Phi_y = \frac{\Phi_{i,j+1} - \Phi_{i,j}}{\Delta y}. \tag{25}$$

Then

$$F = \sum_i\sum_j p\left[\left(\frac{\Phi_{i+1,j} - \Phi_{i,j}}{\Delta x}\right)^2 + \left(\frac{\Phi_{i,j+1} - \Phi_{i,j}}{\Delta y}\right)^2\right]\Delta x\Delta y,$$

and $\partial f/\partial\Phi_{k,j} = 0$ leads to

$$\frac{(p_u)_{k,j} - (p_u)_{k-1,j}}{\Delta x} + \frac{(p_v)_{k,j} - (p_v)_{k,j-1}}{\Delta y} = 0. \tag{26}$$

In order to show that equation (26) is equivalent to the central-difference form of equation (24), we will use certain results from the calculus of difference operators. Let

$$D_x^+ f = \frac{f_{i+1,j} - f_{i,j}}{\Delta x}\ ;\ D_y^+ f = \frac{f_{i,j+1} - f_{i,j}}{\Delta y}\ ;$$

$$D_x^- f = \frac{f_{i,j} - f_{i-1,j}}{\Delta x}\ ;\ D_y^- f = \frac{f_{i,j} - f_{i,j-1}}{\Delta y}\ ;$$

$$D_x^- D_x^+ f = (f_{i+1,j} - 2f_{i,j} + f_{i-1,j})/\Delta x^2\ .$$

Equation (25) is then equivalent to

$$u_{i,j} = D_x^+\Phi;\ \ v_{i,j} = D_y^+\Phi.$$

Equation (26) can now be written as:

$$D_x^-(p_u)_{k,j} + D_y^-(p_v)_{k,j} = 0. \tag{27}$$

Now $(p_u)_{k,j} = (p_q q_u)_{k,j} = (p_q)_{k,j}\,(q_u)_{k,j} = -(\rho)_{k,j}\,u_{k,j}$, and $(p_v)_{k,j} = -(\rho)_{k,j}\,v_{k,j}$, where the following relationship for a perfect adiabatic gas has been applied

$$p_q = \frac{\gamma p}{\rho}\,\rho_q = -\rho q.$$

Equation (27) then reduces to

$$D_x^-(\rho_{k,j}u_{k,j}) + D_y^-(\rho_{k,j}v_{k,j}) = 0,$$

or

$$D_x^-(\rho_{k,j}D_x^+\Phi_{k,j}) + D_y^-(\rho_{k,j}D_y^+\Phi_{k,j}) = 0. \tag{28}$$

It is easy to prove that (see Miller [21])

$$\begin{aligned} D^-(f_i g_i) &= f_i D^- g_i + g_{i-1} D^- f_i, \\ D^+(f_i q_i) &= f_i D^+ g_i + g_{i+1} D^+ f_i. \end{aligned} \tag{29}$$

With (29), equation (28) can be written as:

$$\rho_{k,j}D_x^- D_x^+ \Phi_{k,j}(D_x^+\Phi)_{k-1,j}(D_x^- \rho_{k,j}) + \rho_{k,j}(D_y^- D_y^+ \Phi_{k,j})(D_y^+\Phi)_{k,j-1}(D_y^- \rho_{k,j}) = 0. \tag{30}$$

Also

$$\begin{aligned} &(D_x^+\Phi)_{k-1,j} = (D_x^-\Phi)_{k,j}, \quad (D_y^+\Phi)_{k,j-1} = (D_y^-\Phi)_{k,j},\\ &(D_x^-\rho)_{k,j} = (\rho_u)_{k,j}D_x^- u_{k,j} + (\rho_v)_{k,j}D_x^- v_{k,j},\\ &(D_y^-\rho)_{k,j} = (\rho_u)_{k,j}D_y^- u_{k,j} + (\rho_v)_{k,j}D_y^- v_{k,j},\\ &(\rho_u)_{k,j} = -\left(\frac{\rho_u}{a^2}\right)_{k,j}; \quad (\rho_v)_{k,j} = -\left(\frac{\rho_v}{a^2}\right)_{k,j}. \end{aligned} \tag{31}$$

Substituting from equation (31) into (30), we obtain

$$\rho_{k,j}\left[\left(1 - \frac{u_{k,j}u_{k-1,j}}{a_{k,j}^2}\right) D_x^- D_x^+ \Phi_{k,j} - \left(\frac{u_{k-1,j}v_{k,j}}{a_{k,j}^2} D_x^- D_y^+ \Phi_{k,j} + \frac{u_{k,j}v_{k,j-1}}{a_{k,j}^2} D_y^- D_x^+ \Phi_{k,j}\right) + \left(1 - \frac{v_{k,j}v_{k,j-1}}{a_{k,j}^2}\right) D_y^- D_y^+ \Phi_{k,j}\right] = 0. \tag{32}$$

The implicit nature (from the point of view of unconditional stability) and the central-difference form of the second derivatives is clear. The cross derivative is less accurate than its central-difference form. The over-all accuracy of scheme (32) is less than its central-difference counterpart due to the lower accuracy of the first derivatives. As shown for Burgers' equation, mid-point differencing will provide second-order accuracy for all derivatives.

As an alternate derivation, in lieu of Bateman's variational principle, we apply the composite variational principle to the continuity equation. The functional F is defined as

$$F = \iint [\rho u \,\omega_x + \rho v \,\omega_y]\,dxdy,$$

where ω is the adjoint variable. The differentiation $\partial F/\partial\omega_{k,j} = 0$ leads to

$$D_x^-(\rho_{k,j}u_{k,j}) + D_y^-(\rho_{k,j}v_{k,j}) = 0.$$

This is precisely equation (28).

On the other hand, if we use the following functional, derivable from equation (24),

$$F = -\iint \left\{\Phi_x\left[(1 - \frac{u^2}{a^2})\,\omega\right]_x - \Phi_x\left[\frac{uv}{a^2}\,\omega\right]_y - \left[\frac{uv}{a^2}\,\omega\right]_x\Phi_y + \Phi_y\left[(1 - \frac{v^2}{a^2})\,\omega\right]_y\right\} dxdy,$$

the resulting difference equation will be given as

$$\left(1-\frac{u_{k,j}^2}{a_{k,j}^2}\right)D_x^-D_x^+\Phi_{k,j}-\frac{u_{k,j}v_{k,j}}{a_{k,j}^2}\left(D_x^-D_y^+\Phi_{k,j}+D_y^-D_x^+\Phi_{k,j}\right)$$

$$+\left(1-\frac{v_{k,j}^2}{a_{k,j}^2}\right)D_y^-D_y^+\Phi_{k,j}=0$$

This is similar to the final result (32) obtained from the Bateman variational principle.

Supersonic flow

In this case the flow is not aligned with any particular coordinate direction. The time-like direction, characteristic of this initial-value problem, follows the stream line. A variational formulation in the natural coordinates is preferable. Once again a composite variational principle can be devised and a retarded-difference scheme in the natural coordinates is recovered. We shall use the relationships between the natural and cartesian coordinates to derive the difference form of the continuity equation in cartesian coordinates. The functional is given by,

$$F=\iint[-\rho q\omega_\tau+\theta(\rho q\omega)_n]\,ds\,dn \tag{34}$$

where $\tau = s_0 - s$, ρ is the density, q the speed, s is the arc length along the stream line, n is the arc length normal to the stream line, θ is the angle that the stream line makes with the x-axis, and $\omega(\rho, n)$ is the adjoint variable. The Euler-Lagrange equation is given by

$$(\rho q)_s+\rho q\theta_n=0, \tag{35}$$

i.e., the continuity equation [22] in natural coordinates. The relationships between the cartesian and natural coordinates are as follows:

$$\frac{\partial}{\partial s}=\frac{u}{q}\frac{\partial}{\partial x}+\frac{v}{q}\frac{\partial}{\partial y}, \quad \theta_n=\left(\frac{u}{q}\right)_x+\left(\frac{v}{q}\right)_y .$$

These relations can be derived geometrically or by comparing the cartesian continuity equation with (35).

Since s is the time-like direction, we approximate

$$\omega_\tau=\frac{\omega_{N-i,j}-\omega_{N-i-1,j}}{\Delta x}, \tag{36}$$

$$(\rho q\omega)_n=\frac{\rho_{i,j}q_{i,j}\omega_{N-i,j}-\rho_{i,j-1}q_{i,j-1}\,\omega_{N-i,j-1}}{\Delta y}.$$

Substituting from equation (36) in (34) and setting $\partial F/\partial \omega_{N-k,j} = 0$ we obtain

$$\frac{(\rho q)_{k,j} - (\rho q)_{k-1,j}}{\Delta s} + \rho_{k,j} q_{k,j} \frac{\theta_{k,j+1} - \theta_{k,j}}{\Delta n} = 0,$$

or (37)

$$D_s^- [(\rho q)_{k,j}] + (\rho q)_{k,j} D_n^+ \theta_{k,j} = 0.$$

With the discretized version of (35) or from geometric considerations, it can be shown that

$$D_s^- f_{k,j} = \left(\frac{u}{q}\right)_{k,j} D_x^- f_{k,j} + \left(\frac{v}{q}\right)_{k,j} D_y^- f_{k,j}$$

and

$$D_n^+ \theta_{k,j} = D_x^+ \left(\frac{u}{q}\right)_{k,j} + D_y^+ \left(\frac{v}{q}\right)_{k,j} .$$

Substituting these relations in (37) we obtain

$$\left(\frac{u}{q}\right)_{k,j} D_x^- (\rho q)_{k,j} + \left(\frac{v}{q}\right)_{k,j} D_y^- (\rho q)_{k,j} + (\rho q)_{k,j} \left[D_x^+ \left(\frac{u}{q}\right)_{k,j} + D_y^+ \left(\frac{v}{q}\right)_{k,j}\right] = 0. \tag{38}$$

Finally, using solutions (29) in (38), we see that

$$\begin{aligned}
&\left(\frac{u}{q}\right)_{k,j} \left(1 - \frac{q_{k,j} q_{k-1,j}}{a_{k,j}^2}\right) D_x^- u_{k,j} + \left(\frac{v}{q}\right)_{k,j} \left(1 - \frac{q_{k,j} q_{k-1,j}}{a_{k,j}^2}\right) D_x^- v_{k,j} \\
&+ \left(\frac{u}{q}\right)_{k,j} \left(1 - \frac{q_{k,j} q_{k,j-1}}{a_{k,j}^2}\right) D_y^- u_{k,j} + \left(\frac{v}{q}\right)_{k,j} \left(1 - \frac{q_{k,j} q_{k,j+1}}{a_{k,j}^2}\right) D_y^- v_{k,j} \\
&+ \left(1 - \frac{u_{k,j} u_{k+1,j}}{q_{k,j}^2}\right) D_x^+ u_{k,j} - \frac{v_{k,j} u_{k+1,j}}{q_{k,j}^2} D_x^+ v_{k,j} - \frac{v_{k,j+1} u_{k,j}}{q_{k,j}^2} D_y^+ u_{k,j} \\
&+ \left(1 - \frac{v_{k,j} v_{k,j+1}}{q_{k,j}^2}\right) D_y^+ v_{k,j} = 0.
\end{aligned} \tag{39}$$

Apart from the first-order accuracy of the first-derivative coefficients in equation (39), the relationship with Jameson's rotated difference scheme is apparent. The present variational formulation can be used to discretize mixed-type equations for more general element shapes. Although

Apart from the first-order accuracy of the first-derivative coefficients in equation (39), the relationship with Jameson's rotated difference scheme is apparent. The present variational formulation can be used to discretize mixed-type equations for more general element shapes. Although this has not been carried out in the present paper, there does not seem to be any obvious difficulty in extending the procedure to more general element shapes.

5. Summary

1. A proper variational formulation can provide the appropriate implicit-difference equations for initial-value problems.

2. The relationship of the discrete equations, as obtained from Bateman's principle, with those of central finite-difference theory can be established; the lower-order accuracy of Greenspan and Jain's results has been noted, and the use of averaging to improve the accuracy has been demonstrated.

3. With the proper variational formulation for the initial-value problem, the small-disturbance transonic formulation leads to the Cole and Murman retarded-difference approximation.

4. For the full potential-flow equations, Jameson's rotated difference scheme is recovered for supersonic flows, and the equivalence of Bateman's true variational principle with the composite (Galerkin) variational formulation for subsonic flows has been demonstrated.

5. The Murman-Cole or Jameson retarded-difference methods can be made second-order accurate by appropriate mid-point differencing of the first-derivatives in the functional. The resulting equations for transonic small-disturbance theory have been derived previously, with an alternate procedure, in reference (23).

6. If Jameson's unsteady equations are considered, the present discretization procedure, with the appropriate composite variational principle, still applies. More desirable stability properties for the iterative process result. Midpoint differencing in artificial or iterative time would increase the temporal accuracy and should effect the convergence rate.

REFERENCES

[1] Friedrichs, K. O., Symmetric positive linear differential equations, *Comm. Pure Appl. Math.* 11 (1958) 333-418.
[2] Katsanis, T., Numerical solution of symmetric positive differential equations, *Math. Comp.* 22 (1968) 763-783.
[3] Lesaint, P., Finite element methods for symmetric hyperbolic equations, *Numer. Math.* 21 (1973) 244-255.
[4] Aziz, A. K. and Leventhal, S. H., Numerical solutions of equations of hyperbolic-elliptic type, (1974) *Naval Ordnance Laboratory NOLTR* 74-144.
[5] Filippov, A., On difference methods for the solution of the Tricomi problem, *Izv. Acad. Nauk SSR. Ser. Mat.* 2 (1957) 73-88.
[6] Ogawa, H., On difference methods for the solution of a Tricomi problem, *Trans. Amer. Math. Soc.* 100 (1961) 404-424.
[7] Murman, E. M. and Cole, J. D., Calculation of plane steady transonic flows, *AIAA J.* 9 (1971) 114-121.
[8] Jameson, A., Numerical calculation of three-dimensional transonic flow over a yawed wing, *Proceedings of AIAA Computational Fluid Dynamics Conference*, Palm Springs, Calif. (1973) 18-26.
[9] Gurtin, M. E., Variational principles for linear initial-value problems, *Quart. Appl. Math.* 22 (1964) 252-256.
[10] Tonti, E., *Annal. Mat. Pura Appl.* 95 (1973) 331-359.
[11] Reddy, J. N., A note of mixed variational principles for initial-value problems, *Quart. J. Mech. Appl. Math.* 28 (1975) 123-132.
[12] Vainberg, M. M., *Variational methods for the study of non-linear operators*, translated by A. Feinstein; Holden-Day, San Fransisco (1964).
[13] Atherton, R. W. and Homsy, G. M., On the existence and formulation of variational principles for non-linear differential equations, *Studies in Appl. Mathematics* 54 (1975) 31-60.

[14] Khosla, P. K. and Rubin, S. G., Applications of a variational method for mixed differential equations, (1980), *University of Cincinnati Report No. AFL* 80-10-55.
[15] Finlayson, B. A., *The method of weighted residuals and variational principles*, Academic Press, New York (1972).
[16] Rasmussen, H., Applications of variational methods in compressible flow calculations, *Progress in Aerospace Sciences* 15 (1974) 1-35; Edited by Küchemann, Pergamon Press.
[17] Geffen, N., Yaniv, S, A note on the variational formulation of quasi-linear initial-value problems, *ZAMP* 27 (1976) 833-838.
[18] Bateman, H., Irrotational motion of a compressible inviscid fluid, *Proc. Nat. Acad. Sci.* 16 (1930) 816-825.
[19] Lush, P. E. and Cherry, T. M., The variational method in hydrodynamics. *Quart. J. Mech. Appl. Math.* 9 (1956) 6-21.
[20] Greenspan, D. and Jain, P., Application of a method for approximating extremals of functionals to compressible subsonic fluid flows, *J. Math. Anal. Appl.* 19 (1967) 85-111.
[21] Miller, K. S., *An introduction to the calculus of finite differences and difference equations*, Henry Holt and Company, New York (1960).
[22] von Mises, R., *Mathematical theory of compressible fluid flow*, Academic Press, New York (1958).
[23] Rubin, S. G. and Khosla, P. K., An integral spline method for boundary-layer equations, *Polytechnic Institute of New York Report* No. POLY M/AE 77-12, July (1977).