FINITE ELEMENT METHOD FOR INVISCID COMPRESSIBLE FLUID USING CLEBSH VARIABLES.

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ABSTRACT

The Finite Element Method for compressible inviscid fluid is developed. It is based on the variational principle using Clebsch variables. The variational principle gives not only equations of motion but also conservation laws hence it can be used to describe shocks. It is shown that the same equations can be used for both supersonic and subsonic flow without the aid of added dissipation. In order to study the accuracy of the method the one-dimensional steady flow is calculated. The iterative procedure adopted here results quite naturally in a marching algorithm for supersonic flow and an "elliptic" algorithm for subsonic flow.

1. Introduction

The aim of this paper is to describe a Finite Element Method (F.E.M.) for solving ideal compressible inviscid fluid flows. Any such method consists of three parts: (a) choosing a variational principle, which adequately describes the flow, (b) choosing finite elements to approximate the solution and (c) a method of solving the resulting non-linear equations. These three parts are not entirely independent since the choice of variational principle to some extent predetermines the choice of finite elements and the method of solving the non-linear equations thus obtained.

It is, of course, possible to adopt a different strategy when the variational principle for the problem is known, namely, first to obtain the equations of motion and conservation laws and then to approximate these equations either by finite differences or by finite elements (the weak form of the differential equations - Petrov-Galerkin method). This strategy does not in fact require knowledge of the variational principle - it is enough to know the equations of motion to proceed with the solution. A disadvantage of this strategy is that the choice of a test space for non-self-adjoint or non-linear equations is not clear.

The method proposed here is based on the variational principle derived by Detyna (1981). It is a physical variational principle, therefore it can be approximated by the Galerkin method and minimalization procedure can be understood in terms of physical quantities.

A simplified form of this variational principle for irrotational flow - Bateman's principle, Bateman (1929), has already been used successfully by many authors, e.g. Jameson (1981), Williams (1979). The resulting algorithms are fast and accurate. It is perhaps worth pointing out here that the mathematical structure of potential equations is simpler than that of Euler's irrotational equations: transonic potential equations are mixed elliptic-hyperbolic while Euler's irrotational equations are mixed hybrid-hyperbolic.

Unfortunately, the potential equations cannot describe shocks since the latter generate vorticity. Even if shocks are weak or absent the assumption of irrotationality cannot be valid in many practical flows. The proposed variational method should overcome these difficulties.

It is preferable to have a physical variational principle since then a Hamiltonian H can also be calculated. A Hamiltonian H depends on conjugate pairs of variables: potentials q_α and their conjugate momenta p_α, $\alpha = 1, 2, \ldots N$. In that formulation, the equations of motion are

$$\frac{\partial}{\partial t} p_\alpha = - \frac{\partial H}{\partial q_\alpha} \quad ,$$

$$\frac{\partial}{\partial t} q_\alpha = \frac{\partial H}{\partial p_\alpha} \quad .$$

In other words, equations of motion resulting from a physical variational principle can be cast in pairs such that variation with respect to q_α results in an equation describing the evolution of p_α and vice versa. From the point of view of F.E.M. one could say that trial functions for q_α are test functions for p_α and vice versa. This symmetry can be exploited in numerical schemes. Buneman (1980) pointed out that if Hamilton equations exist they can always be approximated by a finite difference leapfrog scheme, a method with well understood stability and accuracy. The method proposed here is a F.E.M. exploiting the same symmetry of the above equations.

The variational principle and resulting equations are described in the next section, and discontinuous solutions are dealt with in Section 3. In the final part of this paper a F.E.M. solution for one-dimensional steady flow is given. Although the problem itself is trivial, the method of solution has all the main features of the solution of the more general problem and provides the basis for solving two and three-dimensional problems.

2. Variational Principle

2.1 Introduction

It has been shown, Detyna (1981), that the evolution of an inviscid ideal fluid without spin can be described by the variational principle

$$\delta A \equiv \delta \int dt \int_\Omega d_3x \; L = 0 \qquad (2.1)$$

where the Lagrangian L is

$$L = -\rho\left[\tfrac{1}{2}(\underline{\nabla}\phi + \alpha\underline{\nabla}\beta + S\underline{\nabla}\lambda)^2 + E\right] + \rho\left(\partial_t\phi + \alpha\partial_t\beta + S\partial_t\lambda\right), \qquad (2.2)$$

where ϕ, α, β and λ are certain "potential" functions with no particular physical meaning, ρ and S are the fluid density and entropy respectively and $E \equiv E(\rho, S)$ is the internal energy.

It is noticeable that the Lagrangian (2.2) does not depend on the velocity $\underline{v}$, pressure p or other familiar functions commonly used for describing fluids. We shall deal with this problem in Section 2.3 but it is useful to define the velocity $\underline{v}$ now in order to simplify notation.

The momentum of a fluid is $\underline{m} = \rho\underline{v}$ but, on the other hand, it is defined by the invariance of L under translations of co-ordinates as

$$\underline{m} = - \frac{\partial L}{\partial(\partial_t y_A)} \underline{\nabla} y_A$$

where y_A, $A = 1,2,\ldots,6$, stands for α, β, S, λ, ρ and ϕ. (Repeated indices imply summation over the whole range of the indices). With the aid of (2.2) we get

$$\underline{m} = - \rho(\underline{\nabla}\phi + S\underline{\nabla}\lambda + \alpha\underline{\nabla}\beta)$$

hence we can identify velocity as

$$\underline{v} = - (\underline{\nabla}\phi + S\underline{\nabla}\lambda + \alpha\underline{\nabla}\beta) \tag{2.3}$$

2.2 Equations of motion

By seeking the stationary value of the action A in (2.1) with the Lagrangian (2.2) we get the equations of motion:

$$\delta\phi: \quad \partial_t\rho + \underline{\nabla}\cdot(\rho\underline{v}) = 0 \tag{2.4}$$

$$\delta\lambda: \quad \partial_t(\rho S) + \underline{\nabla}\cdot(\rho S\underline{v}) = 0 \tag{2.5}$$

$$\delta\beta: \quad \partial_t(\rho\alpha) + \underline{\nabla}\cdot(\rho\alpha\underline{v}) = 0 \tag{2.6}$$

$$\delta\rho: \quad \partial_t\phi + \alpha\partial_t\beta + S\partial_t\lambda = \tfrac{1}{2}\underline{v}^2 + h \tag{2.7}$$

$$\delta S: \quad \partial_t\lambda + \underline{v}\cdot\underline{\nabla}\lambda = T \tag{2.8}$$

$$\delta\alpha: \quad \partial_t\beta + \underline{v}\cdot\underline{\nabla}\beta = 0 \tag{2.9}$$

where $\underline{v}$ is defined by (2.3) and specific enthalpy h and temperature T are defined by $h = \partial_\rho(\rho E)$ and $T = \partial_S E$. The equation (2.7) can be modified by subtracting from it the last two equations multiplied by S and α respectively

$$\partial_t\phi + \underline{v}\cdot\underline{\nabla}\phi = h - ST - \tfrac{1}{2}\underline{v}^2 \ . \tag{2.7a}$$

The equations (2.4) to (2.9) can be divided into two groups: the first three equations (2.4) to (2.6) describe conservation of mass, entropy and function α respectively, while the last three equations (2.7) to (2.9) describe the evolution of potentials ϕ, λ and β: they are all in the form $(\partial_t + \underline{v}\cdot\underline{\nabla})f =$ r.h.s. But from the point of view of F.E.M. it is more interesting to note that these equations form three pairs: variation with respect to λ gives

the equation for S and vice versa - equations (2.5) and (2.8); the same applies to the pair α and β - equations (2.6) and (2.9). The third pair of equations (2.4) and (2.7) does not lend itself to the same interpretation unless we use equations (2.8) and (2.9) to obtain equation (2.7a) which clearly describes the evolution of ϕ while (2.4) is the equation for ρ. The lack of symmetry between equations (2.4) and (2.7) is due to the use of S and α as independent variables rather than $S^* = \rho S$ and $\alpha^* = \rho\alpha$ which are clearly the conjugate momenta to λ and β. If S^* and α^* were used as independent variables the symmetry of the Hamiltonian equations would be preserved, Detyna 1981, but the Lagrangian L would contain terms of the type S^*/ρ and α^*/ρ which might prove cumbersome in F.E. approximation unless only piece-wise constants were used for trial functions for ρ.

2.3 Conservation laws

It has been shown, Detyna (1981), that the Lagrangian (2.2) is invariant under translation of space and time co-ordinates. The first invariance induces the momentum conservation law

$$\partial_t m_i + \nabla_j T_{ij} = 0, \tag{2.10}$$

where

$$m_i = -\frac{\partial L}{\partial(\partial_t y_A)} \nabla_i y_A = \rho v_i$$

and

$$T_{ij} = -\frac{\partial L}{\partial(\nabla_j y_A)} \nabla_i y_A + \delta_{ij} L = \rho v_i v_j + \delta_{ij} p.$$

In the last formula it is noted that L by virtue of equation (2.7) is

$$L = -\rho(\tfrac{1}{2}\underline{v}^2 + E) + \rho(\tfrac{1}{2}\underline{v}^2 + h) = \rho(h-E) = p .$$

Therefore the pressure p is identified as the Lagrangian itself.

The second invariance induces the energy conservation law

$$\partial_t e + \underline{\nabla}\cdot\underline{Q} = 0 \tag{2.11}$$

where the energy density e and its flux $\underline{Q}$ are

$$e = \frac{\partial L}{\partial(\partial_t y_A)} \partial_t y_A - L = \rho(\tfrac{1}{2}\underline{v}^2 + E)$$

$$\underline{Q} = \frac{\partial L}{\partial(\underline{\nabla} y_A)} \partial_t y_A = \rho\underline{v}(\tfrac{1}{2}\underline{v}^2 + h)$$

The Lagrangian (2.2) is also gauge invariant with respect to ϕ, λ and β since it only depends on their derivatives. This induces three conservation laws of mass, entropy and the function α. The form of these laws is identical to that of the equations (2.4) to (2.6). It should be noted that all the

conservation laws (2.10), (2.11) and (2.4) to (2.6), with the exception of the last one, are expressed in terms of physically observable quantities - density, velocity, etc. The equation (2.6) is exceptional due to the simplifying assumption made in the derivation of the function α (spinless fluid).

We shall return to the discussion of the relationship between equations of motion and conservation laws in Section 3 when we shall deal with discontinuities.

2.4 Steady flow

The physical observables (density, velocity, etc.) are time independent in steady flow. The same cannot be said for the potentials ϕ, λ and β - they may depend on time as long as they form time independent observables. It was shown, Detyna (1981), that a particularly simple linear time dependence

$$\phi(\underline{x},t) \to \phi(\underline{x})$$

$$\beta(\underline{x},t) \to \beta(\underline{x}) + t$$

$$\lambda(\underline{x},t) \to \lambda(\underline{x})$$

results in identification of variable α with the total enthalpy H. The above choice is, of course, not unique.

The variational principle is now

$$\delta \int_{\Omega} \rho[H - \tfrac{1}{2}(\nabla\phi + S\nabla\lambda + H\nabla\beta)^2 - E(\rho,S)]\, d_3x = 0 \qquad (2.12)$$

and the equations of motion obtained from this principle are the same as (2.4) to (2.9) provided that all the time derivatives are neglected (with the exception $\partial_t\beta$ which is replaced by unity):

$$\underline{\nabla}\cdot(\rho\underline{v}) = 0 \qquad (2.13)$$

$$\underline{\nabla}\cdot(\rho S\underline{v}) = 0 \qquad (2.14)$$

$$\underline{\nabla}\cdot(\rho H\underline{v}) = 0 \qquad (2.15)$$

$$\tfrac{1}{2}\underline{v}^2 + h = H \qquad (2.16)$$

$$\underline{v}\cdot\underline{\nabla}\lambda = T \qquad (2.17)$$

$$\underline{v}\cdot\underline{\nabla}\beta = 0 \qquad (2.18)$$

where H, the total enthalpy, replaces α. This definition is justified by equation (2.16).

The conservation laws follow in the same manner as in the general case but we do not have conservation of energy. Instead there is the conservation law of total enthalpy H due to the gauge invariance of β, equation (2.15).

Thus although we have one fewer conservation law in steady state than in the time dependent problem, the same physical quantities are conserved in both cases.

For homenergic flow, $H = H_0 = \text{const}$, one can introduce a new potential

$$\phi^* = \phi - H_0\beta \tag{2.19}$$

in the equation (2.12):

$$\delta \int \rho[H_0 - \tfrac{1}{2}(\underline{\nabla}\phi + S\underline{\nabla}\lambda)^2 - E(\rho,S)]d_3x = 0 \tag{2.20}$$

which removes the term $H\nabla\beta$. In consequence we do not have equations (2.15) and (2.18) any longer.

If the flow is also isentropic $S = S_0 = \text{const}$ then the transformation

$$\phi^{**} = \phi^* - S_0\lambda \tag{2.21}$$

also removes the $S\nabla\lambda$ term from (2.20) which becomes

$$\delta \int_\Omega [H_0 - \tfrac{1}{2}\underline{\nabla}\phi\cdot\underline{\nabla}\phi - E(\rho)]d_3x = 0 \tag{2.22}$$

This is Bateman's variational principle for potential flow. The resulting equations are just (2.13) and (2.16). (Superscripts * are omitted in 2.20 and 2.22).

3. Boundary conditions and discontinuities

3.1 Boundary conditions

It was shown in the previous section that the solution of a flow problem is determined by six equations of motion (2.4) to (2.9), subject to appropriate boundary conditions. The number of unknowns is also six: ρ, S, α, ϕ, λ and β. When these have been solved, the five physical functions required to describe the flow are then determined uniquely: ρ and S are part of the solution and $\underline{v}$ is calculated from equation (2.3). The boundary conditions are, of course, given in terms of physical variables ρ, S and $\underline{v}$, hence in order to apply them they have to be translated into boundary conditions for our original six variables. The problem is somewhat complicated by the existence of function α - although it is not a physical variable it is conserved, see equation (2.6), and therefore plays the role of a physical variable. Strictly speaking it should be said that there are six physical variables ρ, S, $\underline{v}$ and α with the appropriate boundary conditions given for all of them. But since α is not required in the final description of the flow, an arbitrary boundary condition can be imposed on it. This complication is absent in steady flow where α becomes a truly physical quantity - total enthalpy H.

Since the boundary conditions for three functions ρ, S and α (or H) are given, the remaining three conditions for ϕ, β, and λ can be calculated from equation (2.3)

$$\underline{\nabla}\phi + S\underline{\nabla}\lambda + \alpha\underline{\nabla}\beta = -\underline{v} \tag{3.1}$$

for given $\underline{v}$ on the boundary. It is clear that the potentials ϕ, λ and β are not determined uniquely by this equation but only up to an arbitrary constant. This, of course, does not affect the solution since only derivatives of these potentials are required.

3.2 Discontinuities

If boundary conditions are not smooth or flow is supersonic in some region, discontinuities may develop. In order to find a unique solution a method of relating values of all variables on both sides of a discontinuity (jump conditions) has to be established. This is achieved with the aid of the conservation laws. For the general flow there are seven conservation laws - four scalar equations (2.4), (2.5), (2.6) and (2.11) and one vector equation (2.10). In steady flow the number is limited to six since there is no energy equation (2.11). Integrating these equations over a slim volume enclosing a discontinuity, the relationships between variables on both sides of this discontinuity are obtained. We note that in the general case there are six and in steady flow five independent variables: ρ, S, $\underline{v}$ and α' (in general case only). The total enthalpy H is not an independent variable, see equation (2.16). Since there is one more equation than unknowns a solution may not exist. Since in nature a solution always exists our description must be inadequate: if the discontinuity is a shock the process is irreversible hence entropy cannot be conserved. For physical reasons the entropy conservation equation (2.5) is replaced by

$$[S] \geq 0 \tag{3.2}$$

where $[f]$ stands for the jump in value of quantity f across the shock. Now the number of equations and unknowns is the same and if more than one solution exists the condition (3.2) selects the physical solution. These jump conditions are the well known Rankine-Hugoniot relations. But these relations describe the jump in physical variables only and the jump conditions for potentials ϕ, λ and β are still unknown. In order to calculate these relations we shall study the two different types of discontinuities in more detail.

3.2.1 Contact discontinuity

A contact discontinuity is a discontinuity which does not cross stream lines, or in other words, no matter flows across it. It is seen that all the equations of motion (2.4) to (2.9) are of the form

$$\frac{d}{ds}\, y_A = \text{r.h.s.} \tag{3.3}$$

where y_A stands for any of the variables ($A = 1, 2, \ldots, 6$) and d/ds is the total derivative along the stream line. Since no stream lines cross the discontinuity all the variables y_A are continuous functions of s and their values on either side of the contact discontinuity are determined solely by the external or internal boundary conditions.

3.2.2 Shocks

A shock is a discontinuity which crosses stream lines hence, according to equation (3.3), relationships between all y_A's on either side of the shock are needed.

From momentum conservation equation (2.10) we can deduce that the velocity vector $\underline{v}_{\parallel}$ tangent to the shock surface is continuous. On the other hand the equation (2.3) for velocity is

$$\underline{v}_{\parallel} = -(\underline{\nabla}_{\parallel}\, \phi + S\underline{\nabla}_{\parallel}\, \lambda + \alpha\underline{\nabla}_{\parallel}\, \beta) \tag{3.4}$$

where $\underline{\nabla}_{\parallel}$ stands for the gradient tangent to the shock surface. Since, according to the equation (2.6) the function α is continuous, the functions ϕ, λ and β can be continuous only if S is continuous. Thus the shock surface with $[S] > 0$ has to be treated as an internal boundary and the potentials ϕ, λ and β behind the shock have to be recalculated from physical variables, which are given by Rankine-Hugoniot relations. This is not surprising since the variational principle (2.1) is contradicted by the entropy condition (3.2) on the shock surface. Consequently the equations of motion on the shock surface are not valid.

The details of calculations of the potentials from physical variables will be given when numerical schemes are developed.

3.3 Dissipation

The method of dealing with shocks described above should prove adequate numerically. A different approach, not used in this paper, can also be applied. The conservation law of entropy, equation (2.5), is due to the gauge invariance of the Lagrangian (2.2) with respect to λ. Since shocks do not conserve entropy we could break that invariance by adding an ad hoc term $L_1 = \lambda f(\cdot)$ to the Lagrangian (2.2), where f is some function of the physical variables. The

total Lagrangian $L + L_1$ is not gauge invariant with respect to λ and, consequently, there is no entropy conservation law. The equation (2.5) is now replaced by

$$\partial_t(\rho S) + \underline{\nabla}\cdot(\rho S\underline{v}) = f \ . \qquad (3.5)$$

If, for instance, we chose

$$f = k\nabla^2 T/T$$

where k is a coefficient of heat conduction the equation (3.5) is just the heat balance equation. Since the temperature T is a function of ρ and S the equations (2.7) and (2.8) would also be modified appropriately. The equation (3.5) is dissipative and the solutions are shock free (at small Mach numbers) but the flow is no longer described by Euler's equations. One could choose k to be very small so the term L_1 is insignificant in most of the region. But in that case there will be layers where temperature varies rapidly and $\nabla^2 T$ is very large thus making L_1 large. These layers are the "dissipated shocks" since they contain regions where, according to equation (3.5), the entropy is rapidly produced. One suspects that they would be more difficult to handle numerically than the original equations (2.4) to (2.9) which admit discontinuities.

4. Finite Element Calculations

4.1 Introduction

The numerical calculations based on the variational principle (2.1) can be divided into two parts. Firstly, the spaces of trial functions approximating each of the variables in equation (2.2) have to be chosen; seeking the minimum with respect to arbitrary parameters (nodal values) results in a set of non-linear equations. Secondly, the non-linear equations are solved by an appropriate iterative procedure. A simple example of one dimensional steady flow calculation is given in this section. The non-linear set of equations approximating the flow is obtained in the next paragraph and the remainder of this section is devoted to solving these equations for various types of flow. Since the aim of this paper is to develop a general method of calculating complicated flows, a deliberate effort has been made in this example not to exploit the simplicity of one-dimensional steady flow. That is to say, some of the equations here could have been solved much more simply but then a similar simplification would not be available in two or three dimensional flow calculations.

Since one-dimensional flow is necessarily homenergetic, the Lagrangian is given by equation (2.20) with all the variables depending only on one co-ordinate; hence the integration over the other two co-ordinates can be performed trivially. Depending on the co-ordinate system used a flow in a uniform pipe, a section of cylinder or a cone can be described by

$$\delta \int F(x)\rho[\tfrac{1}{2}(\phi_x + S\lambda_x)^2 + E(\rho,S) - H_0]dx = 0 , \qquad (4.1)$$

where x is the independent co-ordinate, subscript x stands for a derivative with respect to x and function $F(x)$ is related to the Jacobian of transformation. For linear, cylindrical or conical flow $A(x) = 1$, x or x^2 respectively. Sometimes a more general flow in a pipe with an arbitrarily varying cross-section is studied in the literature, see for example Courant and Friedrich (1976). Such a pipe is approximated by pieces of cones joined together so that $F(x)$ approximates the area of cross-section as a function of the length of the pipe. Such an approximation cannot be treated rigorously with the variational principle since it requires different momentum equations in different parts of the pipe. Although valuable practical results can be obtained by skilful use of this approximation, it will not be studied here since our aim is to develop a method of solving exact equations for two or three dimensional flow rather than to find a good one-dimensional approximation to them.

Since the one-dimensional flows in a uniform pipe, a section of cylinder or a cone are very similar from a numerical point of view, only the case $A(x) = 1$ is calculated in this section.

4.2 Finite element approximation

Let the flow take place between $x = x_0$ and $x = x_N$ and let this region be divided into N elements: (x_0,x_1), (x_1,x_2), ..., (x_{N-1},x_N), where x_i is a position of the i-th node.

The Lagrangian (4.1) depends on functions ρ and S and on first derivatives of functions ϕ and λ, therefore the simplest F.E. that can approximate these functions consistently are piece-wise constants for ρ and S and piece-wise linear functions for ϕ and λ;

$$\rho(x) = \sum_{i=1}^{N} \rho_i \, C_i(x) \qquad (4.2)$$

$$\phi(x) = \sum_{i=0}^{N} \phi_i \, \theta_i(x) \qquad (4.3)$$

$$S(x) = \sum_{i=1}^{N} S_i C_i(x) \; ; \; \lambda(x) = \sum_{i=0}^{N} \lambda_i \theta_i(x) \qquad (4.4)$$

where ρ_i, S_i and ϕ_i, λ_i are nodal values while $C_i(x)$ and $\theta_i(x)$ are piecewise constants and piecewise linear respectively.

$$C_i(x) = \begin{cases} 1 \\ 0 \end{cases} \quad \text{for} \quad \begin{cases} x_{i-1} \le x < x_i \\ x > x_i \quad \text{or} \quad x < x_{i-1} \end{cases} \tag{4.5}$$

$$\theta_i(x) = \begin{cases} \dfrac{x - x_{i-1}}{x_i - x_{i-1}} \\ \dfrac{x_{i+1} - x}{x_{i+1} - x_i} \\ 0 \end{cases} \quad \text{for} \quad \begin{cases} x_{i-1} \le x \le x_i \\ x_i \le x \le x_{i+1} \\ x < x_{i-1} \quad \text{or} \quad x > x_i \end{cases} \tag{4.6}$$

The approximations for $S(x)$ and $\lambda(x)$ are identical to those for $\rho(x)$ and $\phi(x)$, equation (4.4). It is seen that ϕ_i (or λ_i) is the value of $\phi(x)$ (or $\lambda(x)$) at the point $x = x_i$; whereas ρ_i (or S_i) is the value of $\rho(x)$ (or $S(x)$) between $x = x_{i-1}$ and $x = x_i$. For that reason there are N values of ρ_i or S_i but $N + 1$ values of ϕ_i or λ_i.

Introducing (4.2) to (4.4) into the Lagrangian (4.1) and integrating over x we get the action A:

$$A = \int_{x_0}^{x_N} L \, dx = \sum_{i=1}^{N} \rho_i [H_0 - \tfrac{1}{2} v_i^2 - E(\rho_i, S_i)] \Delta x_i, \tag{4.7}$$

where v_i stands for

$$v_i = (\phi_i - \phi_{i-1} + S_i(\lambda_i - \lambda_{i-1}))/\Delta x_i \tag{4.8}$$

and $\Delta x_i = x_i - x_{i-1}$.

Now the approximate equations of motion can be obtained by finding a stationary value of the sum (4.7):

$$\frac{\partial A}{\partial \rho_i} = H_0 - \tfrac{1}{2} v_i^2 - h_i = 0 \tag{4.9}$$

$$\frac{\partial A}{\partial \phi_{i-1}} = \rho_{i-1} v_{i-1} - \rho_i v_i = 0 \tag{4.10}$$

$$\frac{\partial A}{\partial S_i} = \rho_i [v_i(\lambda_i - \lambda_{i-1}) - T_i \Delta x_i] = 0 \tag{4.11}$$

$$\frac{\partial A}{\partial \lambda_{i-1}} = \rho_{i-1} S_{i-1} v_{i-1} - \rho_i v_i S_i = 0 \tag{4.12}$$

where h_i and T_i are the local enthalpy and temperature respectively:

$$h_i = \frac{\partial}{\partial \rho_i} \rho_i E(\rho_i, S_i) = \frac{\gamma}{\gamma-1} \rho_i^{\gamma-1} e^{S_i/c_v} \tag{4.13}$$

$$T_i = \frac{\partial}{\partial S_i} E(\rho_i, S_i) = \frac{1}{c_v(\gamma-1)} \rho_i^{\gamma-1} e^{S_i/c_v} \tag{4.14}$$

It is seen that equation (4.12) by virtue of equation (4.10) reduces to

$$S_i = S_{i-1} \tag{4.12a}$$

in the absence of shocks.

In the remainder of this section methods of solving the above equations for subsonic, supersonic and transonic flows are given.

4.3 Solutions of equations of motion

The equations (4.9) to (4.12) are non-linear hence an iterative method of solution is required. We shall adopt simple sequential Newton iterations although a higher order method could be used, but then it would be difficult to extend such a method to two- or three-dimensional flow. We shall adopt different strategies for subsonic and supersonic flows in order to use the boundary conditions in each case in a natural way.

4.3.1 Supersonic flow

It has been noted earlier that the equation (4.9), which is the finite element approximation of the equation (2.7), can be regarded as an equation for the potential ϕ. Therefore if a trial solution ϕ_i, ρ_i, S_i and λ_i is given the next approximation for ϕ can be obtained by introducing

$$\phi^i = \phi_i + \delta\phi_i \tag{4.15}$$

into equation (4.9) and calculating $\delta\phi_i$. (The usual notation of subscript denoting the old and superscript denoting the new values is adopted here).

Neglecting terms nonlinear in $\delta\phi$ we get

$$v_i(\delta\phi_i - \delta\phi_{i-1}) = (\tfrac{1}{2}v_i^2 + h_i - H_0)\Delta x_i \equiv R_i \tag{4.16}$$

If the value ϕ_0 on the boundary is given then equation (4.16) can be solved by the marching procedure:

$$\delta\phi_i = \delta\phi_{i-1} + R_i/v_i \tag{4.17}$$

Alternatively, with the aid of equations (4.11) and (4.15), we get

$$v_i(\phi^i - \phi^{i-1}) = (-\tfrac{1}{2}v_i + h_i - S_iT_i - H_0)\Delta x_i \tag{4.18}$$

which is an equation for the new values of ϕ. We note that the above equation is just the finite element approximation to the equation (2.7a) which described the evolution of ϕ along streamlines.

The remaining equations (4.10) to (4.12) treated in the same manner give

$$\rho^i v_i - \rho^{i-1} v_{i-1} = 0 \tag{4.19}$$

$$v_i(\lambda^i - \lambda^{i-1}) = T_i \Delta x_i \tag{4.20}$$

$$S^i - S^{i-1} = 0 \tag{4.21}$$

All the equations (4.18) to (4.21) can be solved by marching provided that the boundary values ϕ_0, ρ_1, λ_0 and S_1 are given. The potentials ϕ and λ are determined up to arbitrary constants which can be taken to be ϕ_0 and λ_0. As is well known the three boundary values ρ_1, S_1 and v_1 ensure existence and uniqueness of the solution for supersonic flow. The third boundary value is necessary to determine the total enthalpy

$$H_0 = \tfrac{1}{2}v_1^2 + h_1(\rho_1, S_1) \quad .$$

Having solved equations (4.18) to (4.21) the iteration is repeated until the desired accuracy is obtained.

4.3.2 Subsonic flow

For subsonic flow we adopt a different iterative procedure in order to suit the different natural boundary conditions. We note that the equation (4.9) depends on a single value of ρ_i while the equation (4.10) depends on three consecutive values of ϕ: ϕ_{i-2}, ϕ_{i-1} and ϕ_i. Therefore they can be solved as follows:

$$\rho^i = \left\{\frac{\gamma-1}{\gamma}(H_0 - \tfrac{1}{2}v_i^2)e^{-S_i/c_v}\right\}^{1/(\gamma-1)} \tag{4.22}$$

$$\frac{\rho_{i-1}}{\Delta x_{i-1}}\phi^{i-2} - \left(\frac{\rho_{i-1}}{\Delta x_{i-1}} + \frac{\rho_i}{\Delta x_i}\right)\phi^{i-1} + \frac{\rho_i}{\Delta x_i}\phi^i = \tag{4.23}$$

$$= \rho_{i-1} S_{i-1} T_{i-1}/v_{i-1} - \rho_i S_i T_i / v_i$$

where in the last equation use of equation (4.11) has been made again.

The equation (4.22) is an algebraic equation and equation (4.23) is a three point "elliptic" equation requiring Dirichlet or Newman boundary conditions for uniqueness. These are natural conditions for subsonic flow. The remaining equations (4.11) and (4.12) for λ and S are solved in the same manner as in the supersonic case, i.e. using equations (4.20) and (4.21), for the following reason: the potential λ is given up to an arbitrary constant which can be taken to be λ_0; the entropy S is also given at the inflow as S_1. Therefore the natural boundary conditions are for λ and S both given at the inflow. Dirichlet boundary conditions for entropy S (or equivalently for λ), given at S_1 and S_N, are not physically admissible since the subsonic flow may contain a supersonic region which generates entropy, thus S_N is not known a priori. (This does not occur in one-dimensional flow but cannot be excluded in two- or three-dimensional flow).

4.3.3 Transonic flow

Let us suppose the flow between x_0 and x_j is supersonic and between x_j and x_N subsonic. We note that an equation (4.9) is obtained by variation with respect to ρ_i. This equation is then used in the supersonic case for obtaining a new value for ϕ_i, equation (4.18), or in the subsonic case for a new value ρ_i, equation (4.22). This can be shown graphically, Fig. 1, by drawing an arrow from point ρ_i ("x" on the top line) to ϕ_i or ρ_i ("x" or "0" on the bottom line). The top line here shows which variation was used for obtaining an equation and the bottom line which variable was calculated from that equation. Potential ϕ is represented by "0" at nodal points and density ρ by "x" between them.

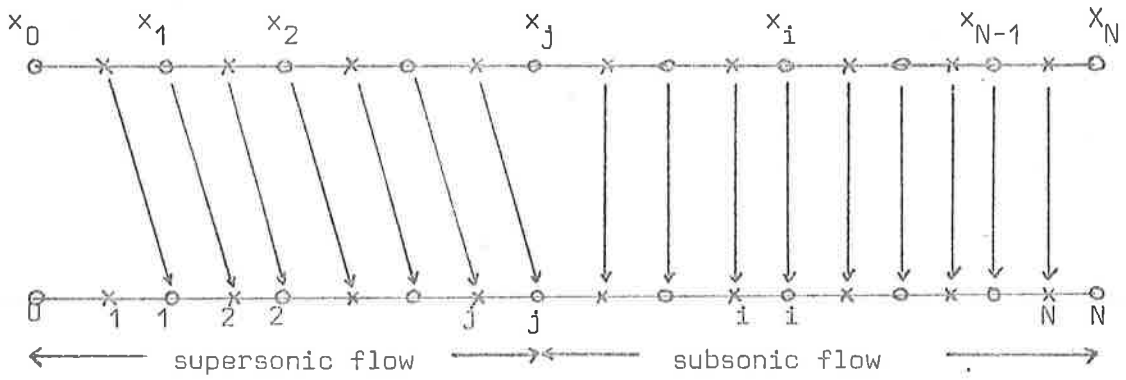

Fig. 1 - Graphical description of the equations used for transonic flow. The potentials ϕ_i and λ_i are at the nodal points x_i (marked with symbol "0"); density ρ_i and entropy S_i are between nodal points (marked "x"). The values at x_0 are given (ϕ_0, λ_0, ρ_1, and S_1).

The equation (4.23) for ϕ^{i-2}, ϕ^{i-1} and ϕ^{i} is obtained from (4.10) by taking a variation with respect to ϕ^{i-1}. Although it is a three point formula it can be regarded as an equation for ϕ_{i-1} as it is a central variable in an elliptic operator. For that reason the arrow from ϕ_i in Fig. 1 points at ϕ_i solution in the subsonic region. It is seen that the equation (4.10) at point x_j, where flow changes from supersonic to subsonic, is not used. On the other hand the equation for ϕ_N is missing since (4.23) could only be used if a boundary condition were known. This is not the case as the flow started as supersonic hence Cauchy conditions are used at the $x = x_0$ boundary alone. But the mass is conserved by virtue of equation (4.10) hence the spare equation at $x = x_j$ can be used for calculation of ϕ_N:

$$\rho_j v_j - \rho_N v_N = 0$$

or after expanding

$$\frac{\rho j}{\Delta x_j}(\phi^{j-1} - \phi^{j}) - \frac{\rho N}{\Delta x_N}(\phi^{N-1} - \phi^{N}) = \tag{4.24}$$

$$= \rho_j S_j T_j / v_j - \rho_N S_N T_N / v_N$$

The values ϕ_0 and ρ_1 are given as boundary conditions hence we have a complete set of equations for all values of ϕ and ρ. The solution for S_i and λ_i is obtained from (4.20) and (4.21) regardless of the type of flow. But if the flow changes at $x = x_j$ from supersonic to subsonic a shock may be present at that point. In that case the entropy is not conserved and its increase can be calculated from conservation laws.

A simple formula in terms of density alone is

$$S^{j+1} - S^{j} = \Delta S_{j+1} \equiv C_v \ln \frac{R - \mu^2}{1 - R\mu^2} - C_p \ln R \tag{4.25}$$

where $R = \rho_{j+1}/\rho_j$ and $\mu^2 = (\gamma - 1)/(\gamma + 1)$.

This formula is used at the shock point $i = j$ instead of the conservation law (4.21). We note that according to (4.25)

$$\Delta S_{j+1} \gtrless 0 \qquad \text{for} \qquad \rho_{j+1} \gtrless \rho_j \tag{4.26}$$

and since the entropy cannot decrease across the shock the density cannot decrease either. Therefore if we replace the equation (4.25) by

$$\begin{aligned} &S^{j+1} - S^{j} = \Delta S_{j+1} \quad \text{for} \quad \Delta S_{j+1} \geq 0 \\ &\rho^{j+1} = \rho^{j}, \; S^{j+1} = S^{j} \quad \text{for} \quad \Delta S_{j+1} < 0 \end{aligned} \tag{4.27}$$

we ensure that the solution does not admit expansion shocks.

4.3.4 Shocks in transonic flow

The choice of finite elements, equations (4.2) to (4.6) is such that if a discontinuity in density or velocity is present it must coincide with one of the nodal points x_i. Since the position of a shock in one dimensional flow is not determined by the flow itself we shall add a supplementary condition to the equations (4.9) to (4.12) in order to fix the shock position. Such a condition can, for instance, be the requirement that the total mass in the flow does not change. That is to say

$$\sum_{i=1}^{N} \rho_i \Delta x_i = m \quad . \tag{4.28}$$

for all levels of iterations.

Let us suppose that after one iteration we have a new density distribution ρ^{*i} such that

$$\sum_{i} \rho^{*i} \Delta x_i = m_* = m + \Delta m \tag{4.29}$$

The excess mass Δm has to be subtracted from the distribution ρ^{*i} in order to satisfy the equation (4.28). For positive Δm it is subtracted from ρ^{*j+1} and for negative Δm we add $-\Delta m$ to ρ^{*j} where j is the last supersonic element. This procedure ensures that the total mass is conserved, equation (4.28), and for large enough $|\Delta m|$ the sonic point x_j is moved to x_{j-1} or x_{j+1} depending on the sign of Δm. At the end of the iterations (when sufficient accuracy has been obtained) the solution will converge to the exact one everywhere except on element j where the density ρ_j and consequently all other variables have an artificial value due to condition (4.28). This is because the shock point lies inside the element j (or $j + 1$), see Fig. 2, and the flow is a mixture of supersonic and subsonic flow. In order to obtain a simple solution a shock fitting procedure is used: the sonic point x_j in Fig. 2 is moved to a new position x_*. This new position $x^j = x_*$ is calculated assuming that the total mass m remains the same and the new density ρ^j in Fig. 2a (or ρ^{j+1} in Fig. 2b) is the same as in neighbouring element $j - 1$ (or $j + 2$). This procedure "divides" the hybrid element into its supersonic and subsonic part. After the shift of point x_j to its new position all other variables are recalculated in that element.

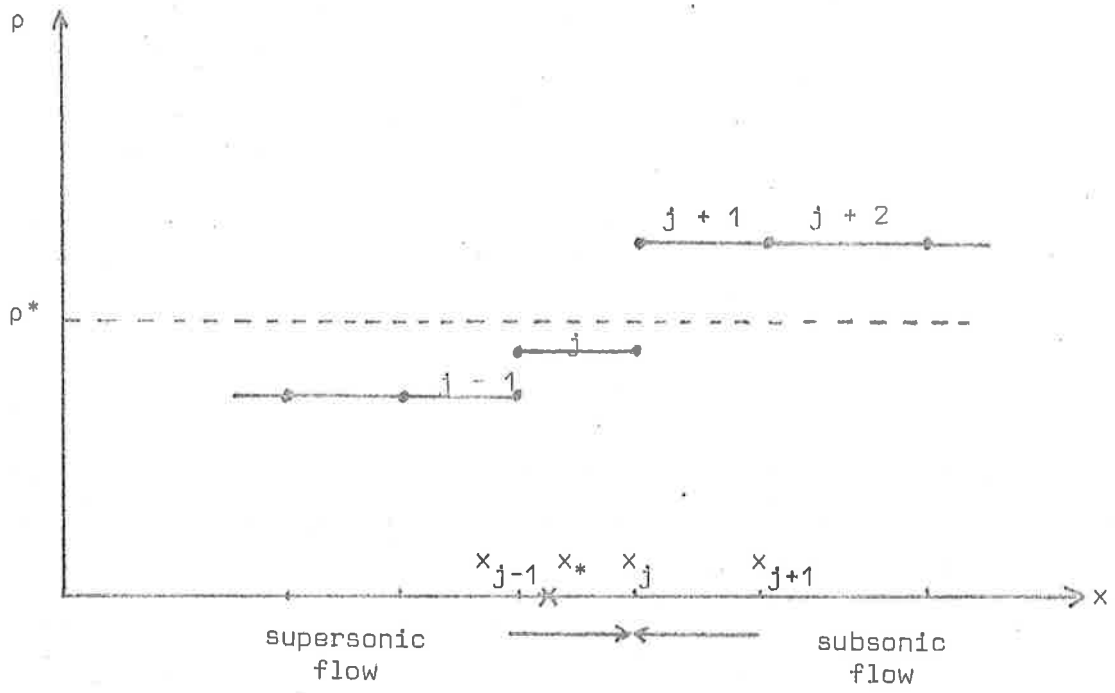

Fig. 2a

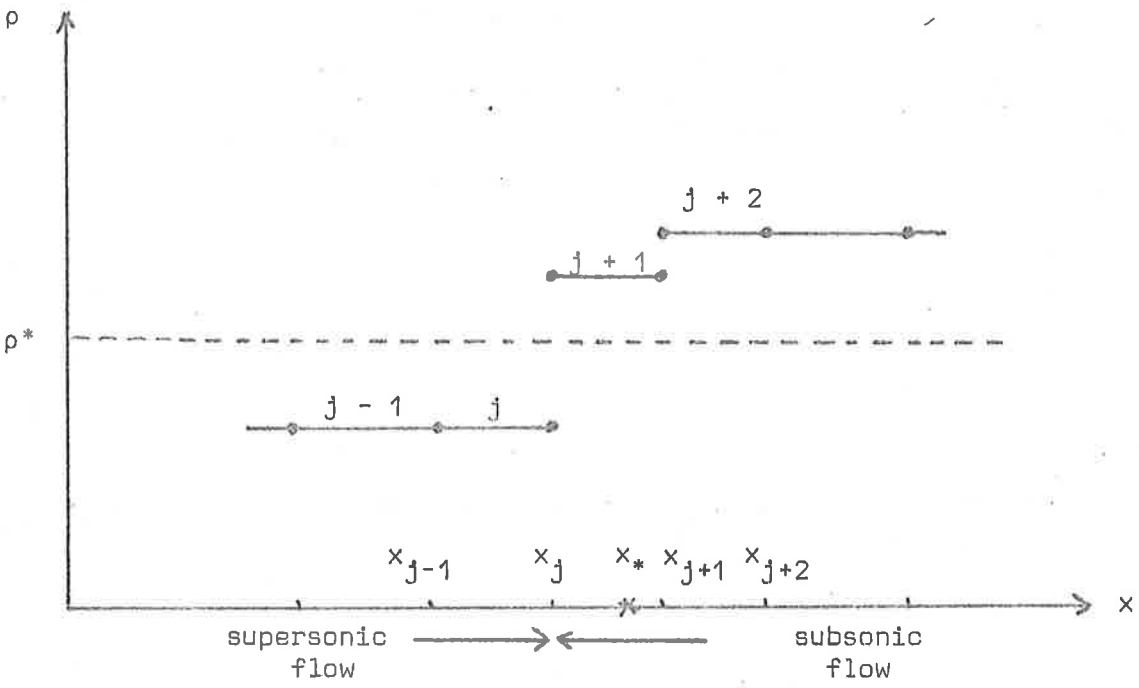

Fig. 2b

Fig. 2 Details of flow at sonic point.
x_* - position of shock, ρ^* - sonic density.

4.4 Numerical results

A Fortran program based on the above method has been used to study the speed and convergence of the algorithm.

Firstly the program was run without the condition (4.28) with initial distributions of density, velocity and entropy

$$\rho_i = \rho_1(1 + \alpha\, x_{i-1}^2) \qquad (4.30)$$

$$v_i = v_1\rho_1/\rho_i$$

$$S_i = 0 \qquad i = 1, 2, \ldots, N$$

and various Mach numbers greater than unity. α was chosen in such a way that for $i > j$ ρ_i represented subsonic flow (that is to say for $i > j$ the sound speed C_i calculated from ρ_i is greater than the critical speed $C_* = \sqrt{2\mu^2 H_0}$). This ensures the flow is transonic and the shock point is at $x = x_j$. A typical convergence speed is shown on Fig. 4 where ϵ is the maximum error in the total enthalpy

$$\epsilon = \left|\tfrac{1}{2}v^2 + h - H_0\right|$$

as a function of the number of iterations J. The straight line on Fig. 3 is at

$$\epsilon \tilde{=} 10^{-0.375J} \tilde{=} 2.37^{-J}$$

The linear convergence rate is typical for sequential Newton methods and in this case the error is about halved at each iteration.

In order to study the shock capture and fitting procedure the same initial distributions (4.30) were used but the iterations were subjected to the condition (4.28) of the total mass conservation.

The density distributions $\rho(x)$ for each iteration are shown on Fig. 4. The initial distribution is shown on the first graph marked "0". The nodal points are distributed randomly between $x_0 = 0$ and $x_{12} = 12.81$. The position of shock is moved during iterations 1 to 7 from element 9 to element 6, see Table I third column. The shock fitting procedure of the last paragraph is not used until the average velocity error ϵ

$$\epsilon = \sqrt{\sum_i (v^i - v_i)^2/N}$$

is less than 10^{-2}. In this case this occurs at iteration 7, see Table I, and the nodal point x_6 is moved to a new position at iteration 8. The "hybrid" element containing shock is found by seeking an element with the largest error in mass, i.e. the element i for which

$$\left|\rho_i v_i - \rho_1 v_1\right|$$

is largest. The last graph on Fig. 4 shows the density distribution after the first shock fitting. The error in the shock position is then $1.9\ 10^{-3}$, see Table I.

The convergence rate is also shown on Fig. 5. It is seen that ϵ diminishes slowly until the shock fitting procedure is used at iteration 8. At subsequent iterations the error diminishes roughly linearly.

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References

Bateman, H., 1929, Proc. Roy. Soc., A125, p. 598.

Buneman, O., 1980, Phys. Fluids, 23, p. 1716.

Courant, R., and Friedrichs, K.O., 1976, Supersonic Flow and Shock Waves, Springer-Verlag, New York.

Detyna, E., 1981, Variational principle and gauge theory. An application to continuous media, Fluid Dynamics Report 2/81, Reading University.

Jameson, A., 1981, in "Proceedings of Conference on Numerical Methods in Fluid Dynamics",(ed. P.L. Roe), Reading, (to be published).

Williams, B., 1979, An investigation of the flow around multiple-element wings by the finite element method, Ph.D. thesis, Reading.

TABLE I

Average errors in velocity distribution and errors in shock position at different iterations.

Number of iterations	Average velocity error	Error in shock position
1	1.2	3.0
2	$8.8\ 10^{-2}$	1.9
3	$2.2\ 10^{-1}$	.87
4	$9.4\ 10^{-2}$	.87
5	$3.8\ 10^{-2}$	.87
6	$7.7\ 10^{-2}$	-.22
7	$4.0\ 10^{-3}$	-.22
8	$2.1\ 10^{-2}$	$1.9\ 10^{-3}$
9	$7.7\ 10^{-4}$	$1.9\ 10^{-3}$
10	$1.2\ 10^{-4}$	$1.9\ 10^{-3}$
11	$9.7\ 10^{-5}$	$-6.2\ 10^{-5}$
12	$6.4\ 10^{-6}$	$5.2\ 10^{-5}$
13	$2.7\ 10^{-6}$	$1.0\ 10^{-6}$

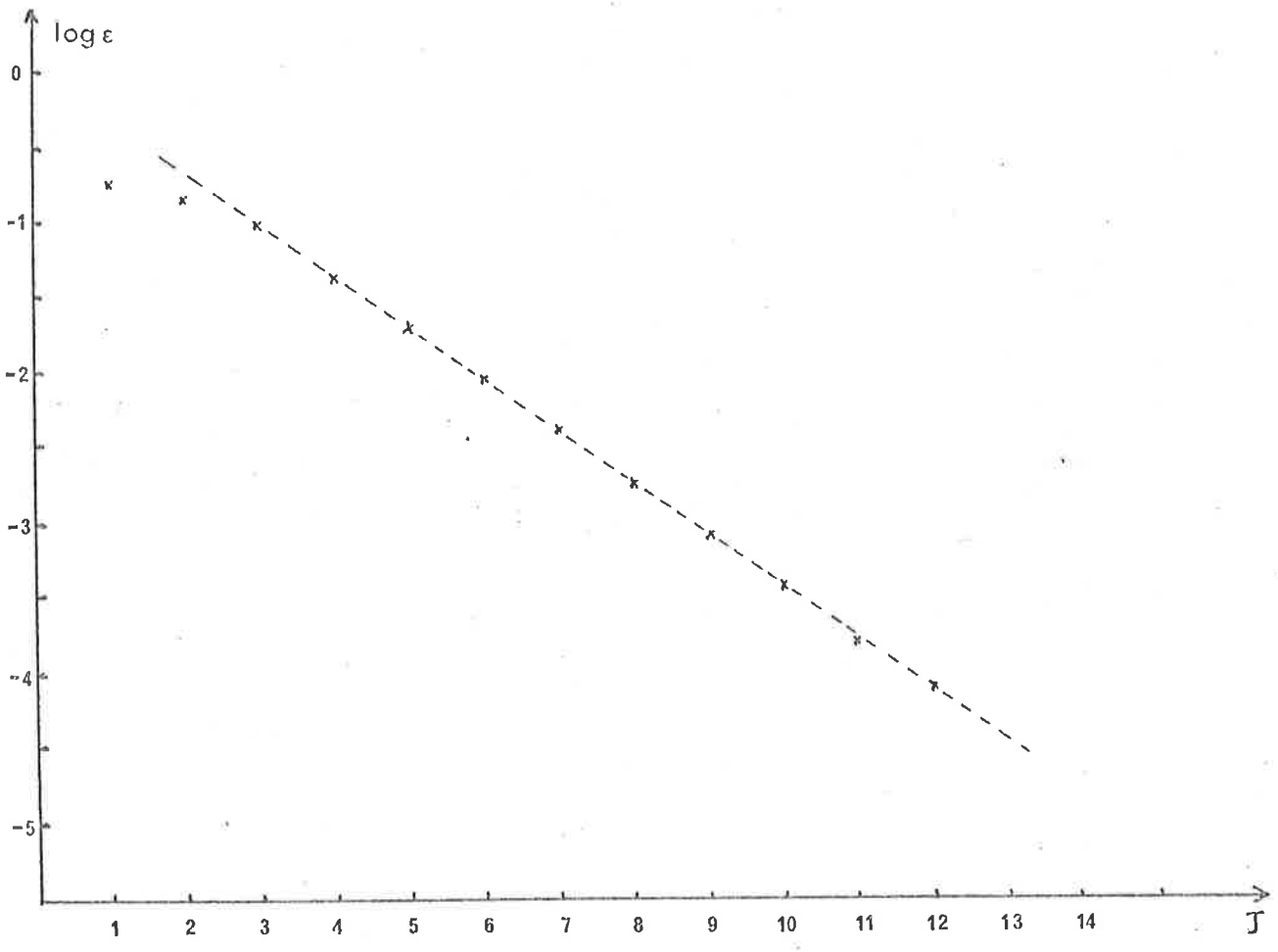

Fig. 3 Maximum error ϵ in velocity as a function of the number of iterations J.

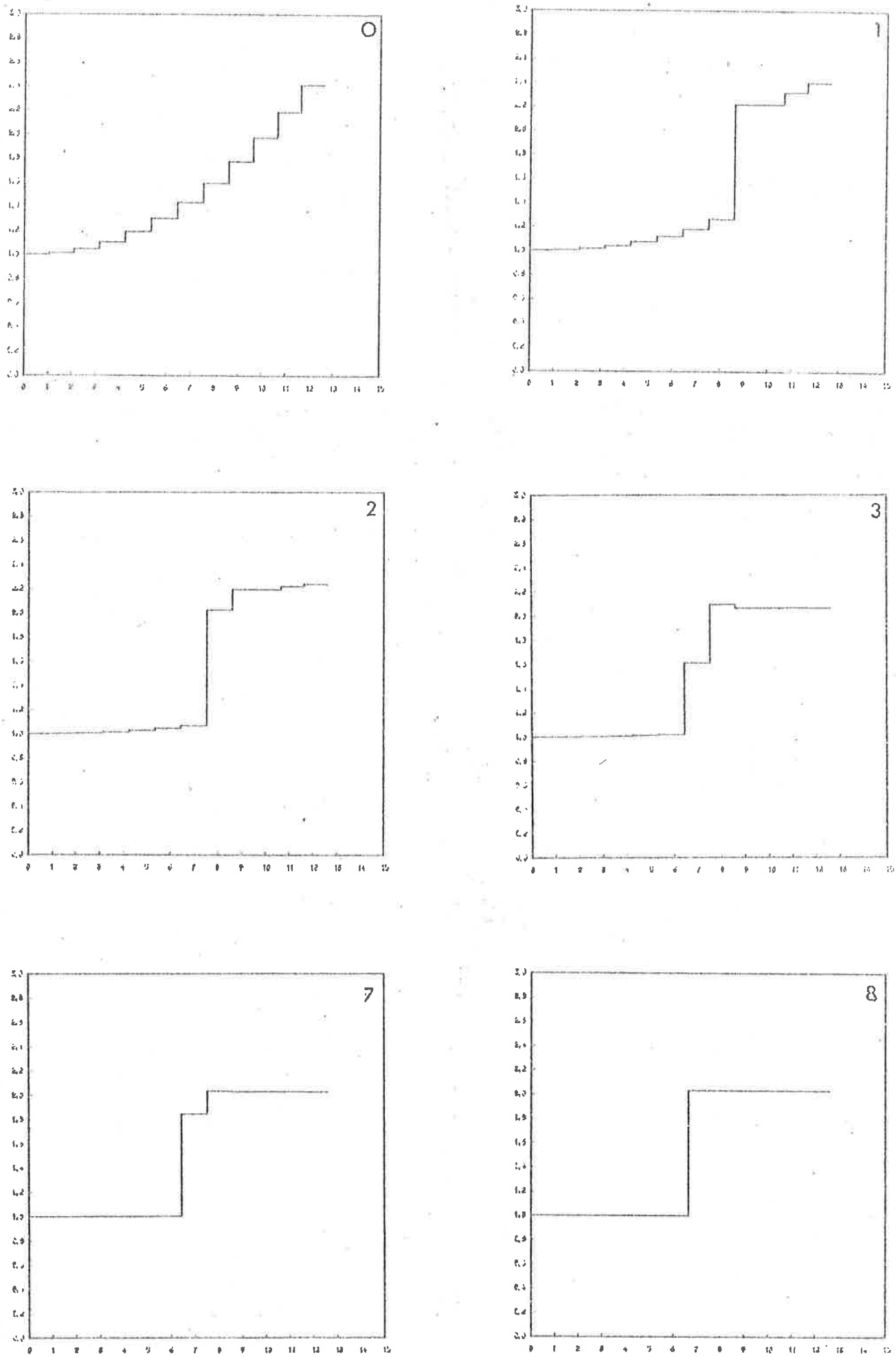

Fig. 4 Density distributions $\rho(x)$ at different iterations. Iteration number is in the top right corner.

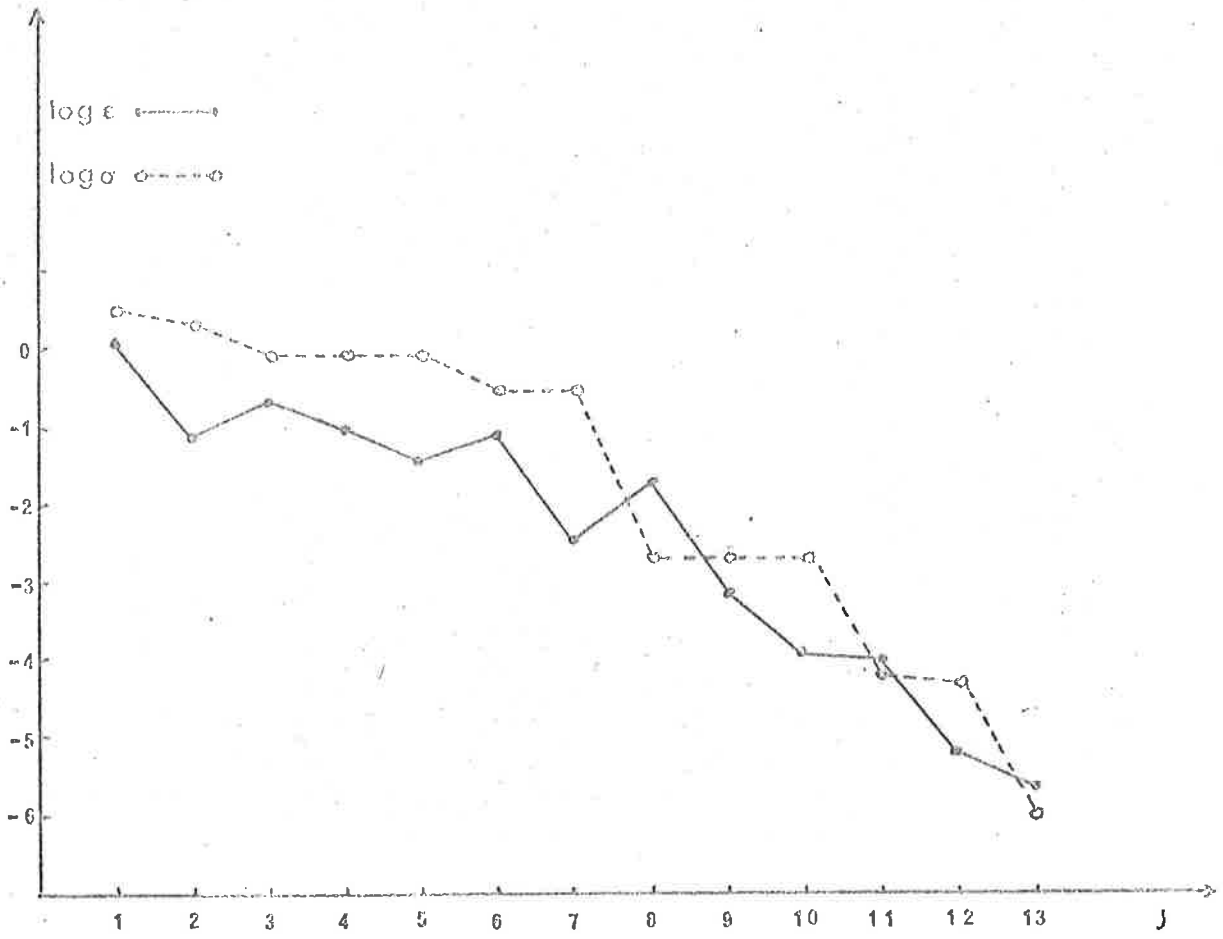

Fig. 5 Average error ϵ in velocity distribution and error in shock position σ as a function of iteration number J. The shock fitting procedure is applied from iteration 8 onwards.