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A MODIFIED LEAST SQUARES FORMULATION FOR A SYSTEM
OF FIRST ORDER EQUATIONS

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A MODIFIED LEAST SQUARES FORMULATION FOR A SYSTEM OF FIRST-ORDER EQUATIONS

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Abstract

Second-order equations in terms of auxiliary variables similar to potential and stream functions are obtained by applying a weighted least squares formulation to a first-order system. The additional boundary conditions which are necessary to solve the higher order equations are determined and numerical results are presented for the Cauchy-Riemann equations.

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INTRODUCTION

Least squares methods are often used to solve systems of first-order equations. Classical discretization and iterative procedures can then be applied to the resulting system of second-order equations. Simply differentiating the equations, however, may lead to difficulties particularly if the nonhomogeneous terms are not regular. In this paper the least squares method is modified and a system of second-order equations is obtained without the need to differentiate the nonhomogeneous terms. Numerical examples are presented and the advantages of the present formulation are discussed.

In Section 2 the classical least squares method is reviewed. The modified least squares method is introduced in Section 3. Section 4 gives some numerical details on the application of the two methods and in Section 5 we summarize our main results.

2. LEAST SQUARES METHOD FOR A SYSTEM OF FIRST-ORDER EQUATIONS

For illustrative purposes we consider the equations which describe the flow in a straight channel with a circular arc airfoil mounted on its lower wall. The governing equations are those of continuity and vorticity:

$$(\rho u)_x + (\rho v)_y = s, \tag{1}$$

$$u_y - v_x = -\omega, \tag{2}$$

where ρ is the density, and u and v are the components of velocity in the x and y directions, respectively. The nonhomogeneous terms s and ω represent some given source and vorticity distributions in the field. The linearized boundary conditions associated with this problem are

$$u = u_0 \qquad \text{along} \quad x = 0 \quad \text{and} \quad x = \ell, \tag{3}$$

$$v = v_0 \qquad \text{along} \quad y = 0 \quad \text{and} \quad y = h, \tag{4}$$

where ℓ and h are respectively the length and height of the channel. We shall refer to the boundary value problem (1), (2) with boundary conditions (3), (4) as Problem I. This problem is depicted in Figure 1.

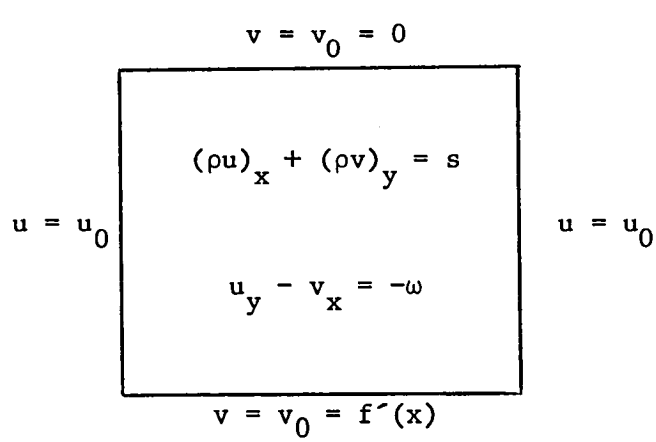

Figure 1. Pictorial Representation of Problem I

Let Ω denote the domain $\{(x,y) : 0 < x < \ell,\ 0 < y < h\}$ and $\partial\Omega$ its boundary. Applying Gauss' theorem to the divergence form of the first equation yields

$$\iint_{\Omega} \nabla\cdot(\rho\underline{q})dA = \oint_{\partial\Omega} \rho(\underline{q}\cdot\underline{n})ds, \tag{5}$$

where $\underline{q} = (u,v)$ and $\underline{n}$ is the unit outward drawn normal to the boundary.

Alternatively, if the tangential velocity is specified along the boundary a different compatability relation should be satisfied, in terms of the vorticity. Suppose that, in this case, the boundary conditions are given by

$$\begin{aligned} u &= g_1(x) \qquad \text{along} \quad y = 0 \\ u &= g_2(x) \qquad \text{along} \quad y = h \end{aligned} \tag{6}$$

$$v = v_0 = 0 \quad \text{along} \quad x = 0 \quad \text{and} \quad x = \ell. \tag{7}$$

We shall refer to the boundary value problem (1), (2) with boundary conditions (6), (7) as Problem II. This problem is depicted in Figure 2.

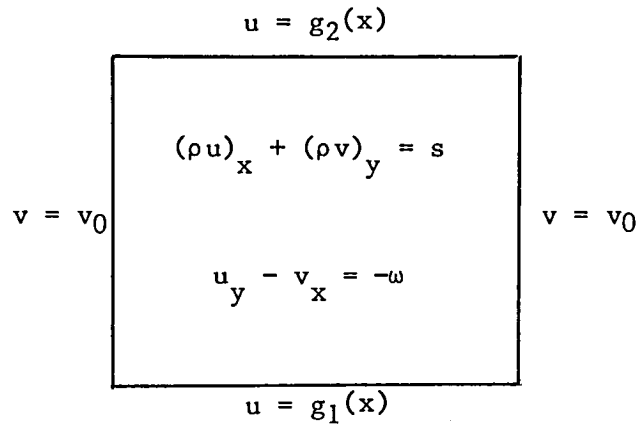

Figure 2. Pictorial Representation of Problem II

According to Stokes' theorem, the vorticity and the circulation are related as follows

$$\iint_{\Omega} \omega \, dA = \oint_{\partial\Omega} \underline{q} \cdot \underline{s} \, ds, \tag{8}$$

where $\underline{s}$ is a unit vector tangent to the boundary $\partial\Omega$ and the line integral is taken in the anti-clockwise direction.

An application of the least squares method to Problem I leads to the the following minimization problem:

Find the functions u,v which minimize the functional $I(u,v)$ over all functions belonging to some admissible class where

$$I(u,v) = \iint_{\Omega} \{[(\rho u)_x + (\rho v)_y - s]^2 + \alpha_0[u_y - v_x + \omega]^2\} \, dxdy$$

$$+ \alpha_1 \int (u - u_0)^2 \, dy + \alpha_2 \int (v - v_0)^2 \, dx, \tag{9}$$

and α_0, α_1 and α_2 are some Lagrange multipliers.

Suppose that $I(u,v)$ attains its minimum value for $u = u^*$ and $v = v^*$. In Eq. (9), ρ, s and ω are assumed to be known functions. If ρ is a positive function of x and y, then the original system (1) is elliptic. In the nonlinear case, when ρ depends on the solution u and v through Bernoulli's equation, the system is of mixed elliptic-hyperbolic type.

We choose as our admissible class of functions those which satisfy the given boundary conditions and are twice differentiable. Let $\tilde{u} = u^* + \varepsilon_1 \eta_1$ and $\tilde{v} = v^* + \varepsilon_2 \eta_2$, then

$$\frac{1}{2}[I(\tilde{u},\tilde{v}) - I(u^*,v^*)]$$

$$= - \iint_\Omega \varepsilon_1 \eta_1 \{\rho[(\rho u^*)_{xx} + (\rho v^*)_{xy} - s_x] + \alpha_0[u^*_{yy} - v^*_{xy} + \omega_y]\}dxdy$$

$$- \iint_\Omega \varepsilon_2 \eta_2 \{\rho[(\rho u^*)_{xy} + (\rho v^*)_{yy} - s_y] + \alpha_0[v^*_{xx} - u^*_{yx} - \omega_x]\}dxdy$$

$$+ \int \varepsilon_1 \eta_1 \{\rho[(\rho u^*)_x + (\rho v^*)_y - s] + \alpha_1(u^* - u_0)\}dy$$

$$+ \int \varepsilon_2 \eta_2 \{\rho[(\rho u^*)_x + (\rho v^*)_y - s] + \alpha_2(v^* - v_0)\}dx$$

$$+ \alpha_0 \int \varepsilon_1 \eta_1 [u^*_y - v^*_x + \omega]dx$$

$$- \alpha_0 \int \varepsilon_2 \eta_2 [u^*_y - v^*_x + \omega]dy + O(\varepsilon_1^2) + O(\varepsilon_2^2). \tag{10}$$

Since, by definition, η_1 vanishes along $x = 0$ and $x = \ell$ and η_2 vanishes along $y = 0$ and $y = h$, the third and fourth integrals in (10) are

identically zero. Following standard minimization arguments we can show that the functions u^*, v^* which minimize $I(u,v)$ are the solutions of the boundary value problems shown in Figure 3 and 4, taking $\alpha_0 = 1$.

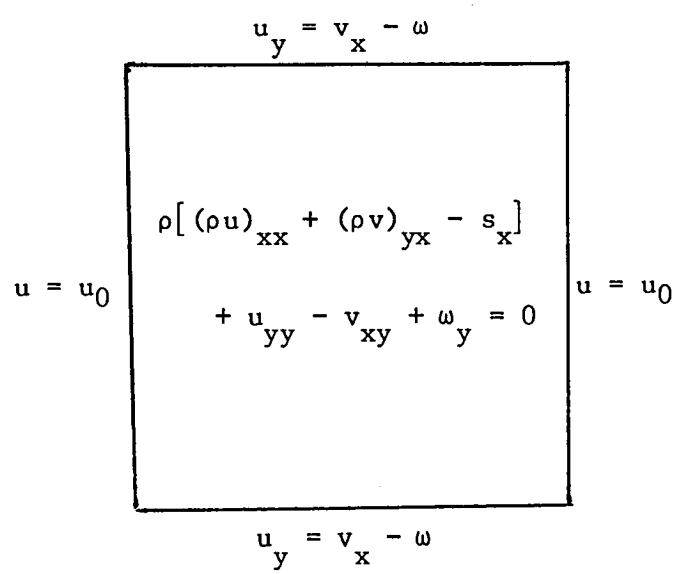

Figure 3. Pictorial Representation of the u Problem (Problem I)

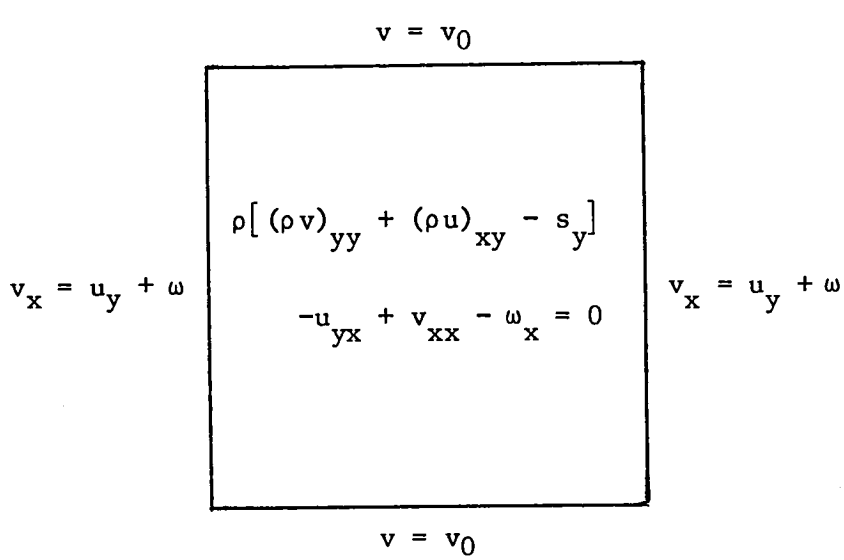

Figure 4. Pictorial Representation of the v Problem (Problem I)

Phillips [3] shows that when $\rho = 1$ the least squares formulation has a unique solution. Moreover, this solution satisfies the original problem.

In an iterative procedure it is natural to use the problems defined in Figures 3 and 4 to solve for u and v, respectively. There are many ways in which iterative methods can be implemented to solve such a coupled system of equations.

For Problem II, where the tangential rather than the normal component of the velocity is specified around the boundary, the functional we need to minimize takes the form

$$J(u,v) = \iint_{\Omega} \{[(\rho u)_x + (\rho v)_y - s]^2 + \alpha_0[u_y - v_x + \omega]^2\}dxdy$$
$$+ \alpha_1 \int (v - v_0)^2\, dy + \alpha_2 \int (u - u_0)^2\, dx. \qquad (11)$$

In a similar fashion we can proceed to show that the functions u^*, v^* that minimize $J(u,v)$ over all admissible functions must solve the boundary value problems, shown in Figures 5 and 6, again taking $\alpha_0 = 1$.

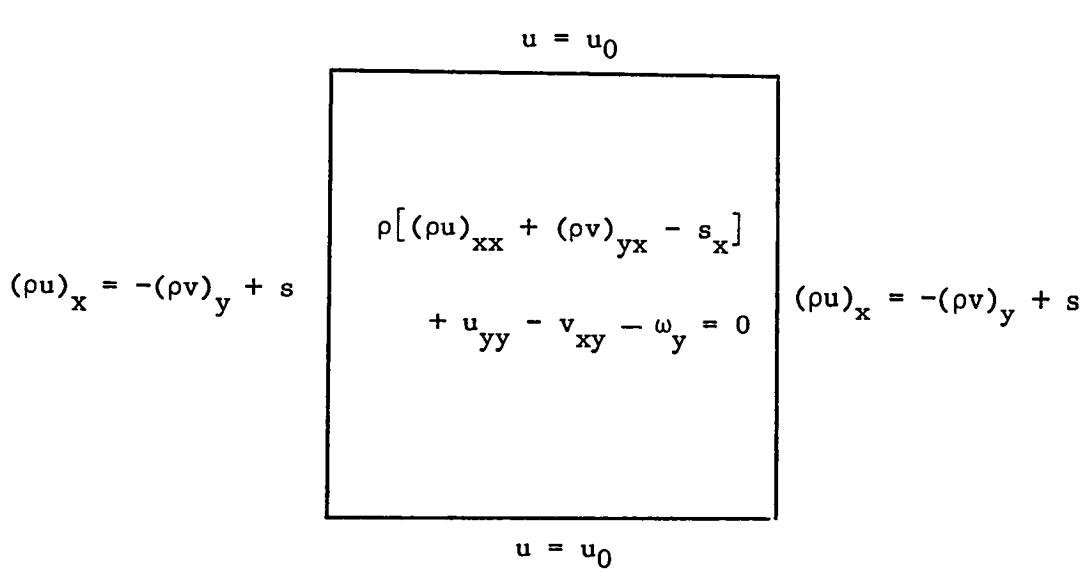

Figure 5. Pictorial Representation of the u Problem (Problem II)

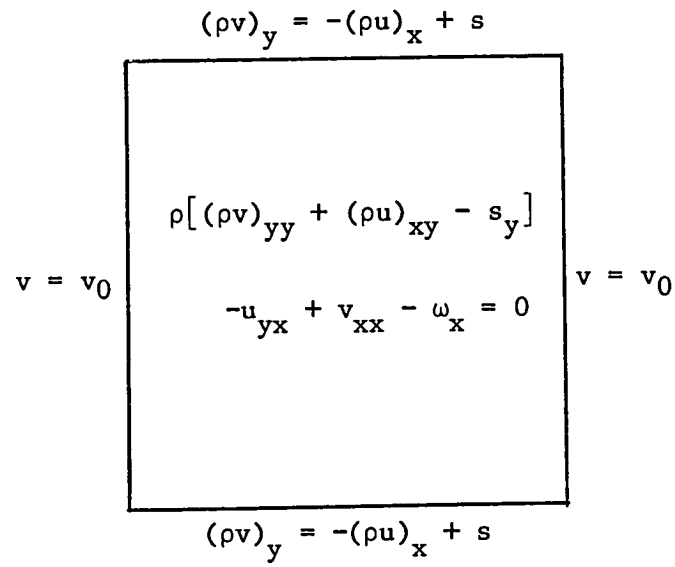

Figure 6. Pictorial Representation of the v Problem (Problem II)

3. MODIFIED LEAST SQUARES METHOD

If the original system is written in the form

$$DU = B \tag{12}$$

where

$$D = \begin{pmatrix} \partial_x \rho & \partial_y \\ \partial_y \rho & -\partial_x \end{pmatrix} ,$$

$$U = \begin{pmatrix} u \\ v \end{pmatrix} , \qquad B = \begin{pmatrix} s \\ -\omega \end{pmatrix} ,$$

then the above classical least squares formulation leads to a system which can be represented symbolically by

$$EDU = EB, \tag{13}$$

where

$$E = \begin{pmatrix} \rho\,\partial_x & \partial_y \\ \rho\,\partial_y & -\partial_x \end{pmatrix}.$$

To avoid the need for differentiation, a new variable V is introduced through the relationship

$$EV = U. \tag{14}$$

Hence, Eq. (12) becomes

$$DEV = B. \tag{15}$$

This choice is equivalent to applying a weighted least squares to the system (12) where the weight is related to

$$R = (DE)^{-1}.$$

The system of equations (15) is similar to the system (13) with one exception; the nonhomogeneous terms are not differentiated. With reference to Hafez [2], a positive weighting function Q may be introduced and Eq. (15) is slightly modified to read

$$DQEV = B. \tag{16}$$

In the particular example under consideration, Q is chosen to be

$$Q = \begin{pmatrix} 1/\rho & 0 \\ 0 & 1/\rho \end{pmatrix},$$

and so V can be identified in terms of potential and stream functions. More precisely, we have

$$DQE = \begin{pmatrix} \partial_x(\rho\ \partial_x) + \partial_y(\rho\ \partial_y) & 0 \\ 0 & \partial_x(1/\rho\ \partial_x) + \partial_y(1/\rho\ \partial_y) \end{pmatrix}.$$

Also, if $V^T = (\phi,\psi)$, then Eq. (14) can be written in the following component form to express u and v in terms of ϕ and ψ:

$$\begin{aligned} \phi_x + 1/\rho\ \psi_y &= u \\ \phi_y - 1/\rho\ \psi_x &= v. \end{aligned} \tag{17}$$

For the case in which ω vanishes identically, the boundary conditions on ϕ and ψ can be chosen so that ψ vanishes identically and Eq. (16) reduces to

$$(\rho\ \phi_x)_x + (\rho\ \phi_y)_y = s. \tag{18}$$

With the associated Neumann boundary conditions for Problem I or Dirichlet boundary conditions for Problem II, the formulation is complete.

Alternatively, if s vanishes identically, the boundary conditions on ϕ and ψ can be chosen so that ϕ vanishes identically in Ω and Eq. (16) reduces to

$$(\psi_x/\rho)_x + (\psi_y/\rho)_y = -\omega, \tag{19}$$

and together with Dirichlet boundary conditions for Problem I or Neumann boundary conditions for Problem II, the formulation of this problem is complete.

In the general case when neither s nor ω vanish identically in Ω the governing equations are (18) and (19). We note that the problems for ϕ and ψ decouple except for the boundary conditions.

This modified formulation is related to the Helmholtz theorem (see [2]) which allows a vector to be decomposed into two vectors, the first of which is curl free while the second is divergence free, i.e.,

$$\underline{q} = \nabla\phi + \nabla \times \underline{A}. \tag{20}$$

For two-dimensional flows, the vector $\underline{A}$ can be represented by one component, while for three-dimensional flows, at least two components of $\underline{A}$ are needed.

With the present method, s and ω (or both) can be discontinuous. In such a case, unlike u and v, ϕ and ψ remain continuous. Their derivatives, of course, are not continuous.

The jump conditions of a weak solution of Eqs. (18) and (19) are (assuming s and ω are integrable),

$$[\rho\phi_x] - \left(\frac{dx}{dy}\right)_D [\rho\phi_y] = 0 \tag{21}$$

and

$$[\psi_x/\rho] - \left(\frac{dx}{dy}\right)_D [\psi_y/\rho] = 0, \tag{22}$$

and since it is assumed that $\phi_{xy} = \phi_{yx}$ and $\psi_{xy} = \psi_{yx}$, across a discontinuity D, the following relations hold

$$[\phi_y] + \left(\frac{dx}{dy}\right)_D [\phi_x] = 0 \tag{23}$$

and

$$[\psi_y] + \left(\frac{dx}{dy}\right)_D [\psi_x] = 0. \tag{24}$$

It is obvious then, that a linear combination of Eqs. (21), (22), (23), and (24) satisfy the jump conditions admitted by Eqs. (1), namely,

$$[\rho u] - \left(\frac{dx}{dy}\right)_D [\rho v] = 0 \tag{25}$$

and

$$[v] + \left(\frac{dx}{dy}\right)_D [u] = 0. \tag{26}$$

In a sense, ϕ and ψ are integrals of u and v and thus a second-order system can be constructed without differentiation.

4. NUMERICAL RESULTS

We present results for the case in which $\rho = 1$, i.e., Eqs. (1) and (2) are the Cauchy-Riemann equations. Equations (18) and (19) can be discretized using finite difference or finite element methods and the resulting algebraic

system may be solved using SOR, ADI, conjugate gradient or multigrid techniques, for example.

The system of Eqs. (18) and (19) represents two Poisson equations, one for ϕ and one for ψ, when $\rho = 1$. Many of the standard iterative methods may be used to yield a solution to these equations. We have chosen to use the multigrid method since such methods are fast and efficient for these problems.

The domain Ω is covered with a square grid of mesh length $h = 1/N$ where N is a positive integer. Each of the Poisson equations:

$$\begin{aligned} \nabla^2 \phi &= s, \\ \nabla^2 \psi &= -\omega, \end{aligned} \tag{27}$$

is discretized using standard second-order central difference approximations. We restrict ourselves to Problem I in which the normal component of the velocity is specified around the boundary. We consider three types of problem and associated with each one will be different boundary conditions:

(a) $s \equiv 0$. In this case the boundary conditions can be chosen so that ϕ vanishes identically. The resulting problem for ψ is one in which Dirichlet conditions are given on the boundary. These are obtained by integrating the given velocity boundary conditions around $\partial\Omega$.

(b) $\omega \equiv 0$. In this case the boundary conditions can be chosen so that ψ vanishes identically. The resulting problem for ϕ is one in which Neumann conditions are given on the boundary. Here we require that the compatibility condition be satisfied in order for a unique solution to exist.

(c) $s \not\equiv 0$, $\omega \not\equiv 0$. This is the general case where we need to solve for both ϕ and ψ. The treatment of the boundary conditions in this case must be consistent with Eqs. (5) and (8).

We consider a multigrid method of solution to these problems using the correction storage algorithm of Brandt [1]. Let $G_1,\cdots,G_m$ be a sequence of grids approximating the domain Ω with corresponding mesh sizes $h_1,\cdots,h_m$. Let $h_k = 2h_{k+1}$ for $k = 1,\cdots,m-1$. The problem is discretized on each grid G_k as described above. We use the same components in the multigrid procedure as those chosen by Phillips [3]. Very briefly these are pointwise Gauss-Seidel with the points ordered in the checkerboard manner for relaxation, half-weighting to transfer the residuals to the coarser grid and bilinear interpolation to transfer the correction to the fine grid.

We consider three test problems defined in the unit square and characterized as follows:

(i) $s = 0$, $\qquad \omega = \left(\frac{\pi}{m}\right)(m^2 + n^2)\sin(n\pi x)\sin(m\pi y)$,

$u = \sin(n\pi x)\cos(m\pi y)$, $\quad v = -\left(\frac{n}{m}\right)\cos(n\pi x)\sin(m\pi y)$,

$\phi = 0$, $\qquad \psi = -\left(\frac{1}{m\pi}\right)\sin(n\pi x)\sin(m\pi y)$;

(ii) $s = (m^2 + n^2)\left(\frac{\pi}{n}\right)\cos(n\pi x)\cos(m\pi y)$, $\quad \omega = 0$,

$u = \sin(n\pi x)\cos(m\pi y)$, $\qquad v = \left(\frac{m}{n}\right)\cos(n\pi x)\sin(m\pi y)$,

$$\phi = -\left(\frac{1}{n\pi}\right) \cos(n\pi x) \cos(m\pi y), \qquad \psi = 0;$$

(iii) $s = (m+n)\pi \cos(n\pi x) \cos(m\pi y), \qquad \omega = (m-n)\pi \sin(n\pi x) \sin(m\pi y),$

$$u = \sin(n\pi x) \cos(m\pi y), \qquad v = \cos(n\pi x) \sin(m\pi y),$$

$$\phi = \frac{-(m+n)}{(m^2+n^2)\pi} \cos(n\pi x) \cos(m\pi y), \quad \psi = \frac{-(m-n)}{(m^2+n^2)\pi} \sin(n\pi x) \sin(m\pi y), \quad m \neq n.$$

In all of the numerical experiments we took the finest grid to be such that $N = 32$ and considered a total of five grids in the multigrid context. The initial approximation was taken to be zero everywhere except where the solution was specified by the boundary conditions. The iterations were terminated when the ℓ_2-norm of the residual had been reduced by a factor of 10^{-4} from its initial value. After solving Eq. (27) for ϕ and/or ψ, we obtain the corresponding values of u and v by approximating the left-hand-side of Eq. (20) by central differences. We note that increased accuracy could have been obtained if we had used some global interpolation scheme.

The first problem corresponds to one of the examples considered by Phillips [3]. Results very similar to those for u and v discussed in [3] are obtained using the modified least squares approach outlined in this paper. Close agreement was achieved in measurements of different norms of the errors in the discrete solution and in the convergence histories of the two techniques. Similar conclusions were reached for the second problem.

With the normal component of the velocity specified around the boundary, the boundary conditions in terms of ϕ and ψ take the form:

$$\begin{aligned} \phi_x + \psi_y &= u_0 \quad \text{along} \quad x = 0,\ x = 1, \\ \phi_y - \psi_x &= v_0 \quad \text{along} \quad y = 0,\ y = 1. \end{aligned} \tag{28}$$

We have chosen to decouple these boundary conditions in terms of ϕ and ψ by putting $\psi = 0$ on the boundary and obtaining conditions for ϕ from Eq. (28).

The details of the algorithm applied to the third problem are given in Tables I, II, and III. In Table I we give the details of the ϕ calculation. We give the number of work units required to attain the convergence criterion, and the asymptotic convergence factor $\bar{\lambda}$ for various values of m and n. Similar information is furnished in Table II for the ψ calculation. In Table III we give norms of the errors in the velocities u and v for various values of m and n. We have used the notation a.b − c for $a.b \times 10^{-c}$.

It can be seen that the method exhibits the usual multigrid behaviour by examining the asymptotic convergence factors obtained. The accuracy of the discrete approximation to the third problem decreases as m and n increase as one might expect since the number of mesh points per wavelength of the solution decreases.

Table I. Details of the ϕ Calculation

m	n	WU	$\bar{\lambda}$
1	2	21.41	0.56
2	1	21.41	0.56
3	1	17.88	0.52
1	5	17.25	0.49

Table II. Details of the ψ Calculation

m	n	WU	$\bar{\lambda}$
1	2	18.13	0.55
2	1	18.13	0.55
3	1	17.81	0.52
1	5	17.50	0.49

Table III. Error Norms of the Solution

m	n	$\Vert u\Vert_\infty$	$\Vert u\Vert_1$	$\Vert u\Vert_2$	$\Vert v\Vert_\infty$	$\Vert v\Vert_1$	$\Vert v\Vert_2$
1	2	0.46-2	0.18-2	0.23-2	0.81-3	0.31-3	0.39-3
2	1	0.46-2	0.18-2	0.22-2	0.81-3	0.31-3	0.39-3
3	1	0.10-1	0.40-2	0.50-2	0.27-2	0.11-2	0.13-2
1	5	0.12-1	0.46-2	0.58-2	0.27-1	0.10-1	0.13-1

5. CONCLUDING REMARKS

An application of the least squares method to a system of first-order equations has led to a formulation in terms of second-order equations. The process has also determined the additional boundary conditions necessary for the higher order equations. The duality of problems in which either the normal or the tangential components of velocity are specified on the boundary has been indicated. Also, a modified least squares approach has been outlined. This approach avoids the need to differentiate the source or vorticity functions. Numerical examples demonstrate the effectiveness of the method.

Future work will concentrate on treatment of the nonlinear problem, i.e., when $\rho = \rho(u)$. Possible extensions of this technique to three dimensions using either two or three stream functions are under examination.

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