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Transformation of Three-Dimensional Regions onto Rectangular Regions by Elliptic Systems*

C. Wayne Mastin and Joe F. Thompson

Institute for Computer Applications in Science and Engineering and Mississippi State University, Mississippi State, MS 39762, USA

Summary. A transformation method is developed which may be used to solve various types of boundary value problems on three-dimensional regions with an arbitrary boundary. The implementation of the method is illustrated in the solution of a potential flow problem. All computations are performed on a cubic mesh in a rectangular region.

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Introduction

In many engineering problems, a primary difficulty in implementing finite difference schemes is dealing with complicated computational regions having irregular boundaries. One method of circumventing this problem is to transform the original physical region onto a rectangular or other type of canonical region, and then solve the problem on the canonical region. This method has been used to solve various two-dimensional fluid flow problems by Chu [2] and Thompson et al. [9] and [10]. An alternate approach, employed by Winslow [11], Godunov and Prokopov [5], Amsden and Hirt [1], and Hirt et al. [6], is to use the transformation to construct a curvilinear mesh on the original region and then solve the problem on the curvilinear mesh.

The success of transformation methods for two-dimensional problems leads one to the consideration of such methods for three-dimensional problems. In this report a three-dimensional transformation method will be developed and tested by numerically solving a potential flow problem where analytic solutions are known. However, before any numerical considerations, the basic concept is analyzed for general applicability. If it is desired to solve a partial differential equation on a simply-connected region by transforming to a rectangular region, then the transformation should be a homeomorphism (one-to-one, continuous,

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and continuous inverse) which is differentiable and has a nonvanishing Jacobian. This requirement restricts the use of many simple algebraic transformations in regions with irregular boundaries.

As a final note some attention is given to the generalization of this method to higher dimensions. It appears that it would have limited application to physical problems, although it may be of some theoretical interest.

Transformation to Rectangular Region

Let D be a simply-connected region in xyz-space bounded by one surface. Let R be a rectangular region in uvw-space given by

$$R = \{(u, v, w) \mid a_1 < u < b_1, a_2 < v < b_2, a_3 < w < b_3\}.$$

Suppose that the boundary of D, denoted by ∂D, and the boundary of R, denoted by ∂R, are homeomorphic and such a homeomorphism is defined by the equations

$$\begin{aligned} u &= h_1(x, y, z) \\ v &= h_2(x, y, z) \\ w &= h_3(x, y, z) \end{aligned} \tag{1}$$

for (x, y, z) on ∂D. In order to avoid difficulties at the boundary in the proofs of the following theorems, additional assumptions will be imposed on the boundary correspondence. We assume that ∂D is analytic and the transformation from ∂D to ∂R is differentiable except possibly on subsets of ∂D which correspond to edges of ∂R. As will be evident later, no numerical difficulties were encountered when this smoothness condition was violated. The image of the points (x, y, z) in D are defined to be the points (u, v, w) where u, v, and w are solutions of the following system of elliptic partial differential equations

$$\begin{aligned} \nabla^2 u &= f_1(u, v, w) \\ \nabla^2 v &= f_2(u, v, w) \\ \nabla^2 w &= f_3(u, v, w) \end{aligned} \tag{2}$$

where ∇^2 denotes the Laplacian operator and f_1, f_2, f_3 are functions defined in uvw-space. As in the case of a single equation (see Courant and Hilbert [3, pp. 369–374]), the system (2) with Dirichlet boundary conditions (1) will have a solution under the appropriate smoothness and boundedness hypotheses.

Simple conditions can be imposed on the functions f_1, f_2, f_3 to guarantee that the image of every point in D is an element of $\bar{R} = R \cup \partial R$. Namely, $u < a_1$ implies $f_1(u, v, w) < 0$ and $u > b_1$ implies $f_1(u, v, w) > 0$ with the analogous relations holding for f_2 and f_3. Since a_1 and b_1 are the maximum and minimum values of u in $\bar{R}$, we are assuming a weak form of the maximum and minimum principles. Note that if $f_1 = f_2 = f_3 = 0$, then u, v, w are harmonic implying that D maps into R. The above condition does not limit the utility of the transformation method. In practice it is the values of f_1, f_2, f_3 on $\bar{R}$ which one perturbs to produce a transformation with high resolution, or some other essential property, in critical subregions of R (see Thompson et al. [10]).

From now on we will work under the assumption that sufficient conditions hold so that a transformation T, defined by (1) and (2), exists which maps $\bar{D}=D\cup\partial D$ into $\bar{R}$. In general, the Jacobian of T may vanish on a nonempty subset of D. This will not happen for harmonic transformations as the next theorem indicates.

Theorem 1. *If $f_1=f_2=f_3=0$, then the Jacobian of the transformation T does not vanish in D.*

Proof. Suppose that the Jacobian

$$\begin{vmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix}=0$$

at some point $P_0=(x_0, y_0, z_0)$ of D. Then there exists constants c_1, c_2, c_3 such that the gradient ∇s of the function $s=c_1u+c_2v+c_3w$ vanishes at P_0. The following results on spherical harmonics and level sets are stated without proof. The proofs may be found in Kellogg [7, pp. 273–275]. Let L be the level set (or equipotential set) in $\bar{D}$ defined by

$$L=\{P\,|\,s(P)=s(P_0)\}.$$

Since s is harmonic in D, it can be written in some neighborhood of P_0 as

$$s(P)=s(P_0)+\sum_{i=1}^{\infty}H_i(P-P_0)$$

where H_i is a spherical harmonic of order i. Now $\nabla s=0$ implies $H_1=0$ at P_0 and L cannot consist of a single analytic surface element or sheet. Let S_1 and S_2 be two sheets containing the point P_0. In some neighborhood N of any point where $\nabla s\neq 0$, $L\cap N$ is a single sheet. Since L is a compact subset of $\bar{D}$, the sheets S_1 and S_2 can be continued in L to ∂D. By the prescribed boundary correspondence, $L\cap\partial D$ is a simple closed coutour C which separates ∂D into two components. Since $D-(S_1\cup S_2)$ has more than two components, at least one of the components K must have ∂K contained in $S_1\cup S_2$. The harmonic function s is constant on ∂K and hence must be constant on K. However, since K is open, s must be constant on D. This violates the boundary conditions on u, v, and w.

The following result holds for more general transformations than considered in this report. In fact it is likely that the theorem follows as a corollary of some known theorem on transformations with nonvanishing Jacobians. However, a direct proof can be obtained from the ideas developed in the proof of Theorem 1 and is included for completeness.

Theorem 2. *If the Jacobian of the transformation T does not vanish in D, then T is a differentiable homeomorphism of D onto R.*

Proof. Since the transformation is a solution of the system of partial differential Equations (2), it will be differentiable on D. It is therefore sufficient to show that T is one-to-one and onto. Suppose T is not one-to-one. Then there exists two points P_1 and P_2 in D such that

$$T(P_1) = T(P_2) = (u_0, v_0, w_0).$$

Define the following level sets in $\bar{D}$.

$$L_1 = \{P \mid u(P) = u_0\},$$
$$L_2 = \{P \mid v(P) = v_0\},$$
$$L_3 = \{P \mid w(P) = w_0\}.$$

Let $K = L_2 \cap L_3$ and P be a point in $K \cap D$. Considerable use will be made of the Inverse Mapping Theorem (IMT) which may be found in any multivariable calculus text; e.g., [4, p. 185]. One consequence of the IMT is the fact that there is a neighborhood N of P such that $K \cap N$ is a smooth curve C. Now suppose the curve C is continued on K in both directions to ∂D. From the assigned boundary correspondence, K contains only two points of ∂D. Assume the two endpoints of C coincide. Then the function u, restricted to C, has an extremum at a point Q of D. Thus u is not one-to-one in any neighborhood of Q and since v and w are constant on C, the transformation T is not one-to-one in any neighborhood of Q. This contradicts the IMT. Therefore the smooth curve C has the two points of $K \cap \partial D$ as endpoints. Now consider the two points P_1 and P_2 of D where $T(P_1) = T(P_2)$. Since P_1 and P_2 belong to $L_1 \cap L_2 \cap L_3$, there exist smooth curves C_1 and C_2 in K which contain P_1 and P_2, respectively, and have endpoints $K \cap \partial D$. Since K is locally a smooth curve, the two curves C_1 and C_2 cannot intersect at a point of D unless they coincide. In the case $C_1 = C_2$, the curve C_1 contains an arc A in D with endpoints P_1 and P_2. The function u, restricted to A, will have a relative extrema on A which again leads to a contradiction as above. Now suppose C_1 and C_2 have only endpoints in common. Let S be the surface in L_2 bounded by the closed curve $C_1 \cup C_2$. The set $L_1 \cap S$ contains the point P_1 and hence, in some neighborhood of P_1, is a curve C_0 in S having P_1 as one endpoint. Suppose that C_0 is continued as a subset of L_1 on the surface S until C_0 intersects $C_1 \cup C_2$ at a point P_3. Now $\partial D \cap (L_1 \cap L_2 \cap L_3)$ is the empty set and hence P_3 is in D. Since $T(P_1) = T(P_3)$, a contradiction of the IMT follows as before. The same results used in the proof that T is one-to-one can be used to prove that the mapping is onto. Suppose (u_0, v_0, w_0) is an arbitrary point of R. Let L_2 and L_3 be the level sets as previously defined. It has been shown that $K = L_2 \cap L_3$ contains a smooth curve C whose endpoints are the two points of $K \cap \partial D$. The function u assumes its maximum and minimum values at the endpoints of C and since u is continuous on C, it will assume the value u_0 at some interior point P_0 of C. Since $P_0 \in L_1 \cap L_2$, $T(P_0) = Q_0$.

Throughout the remainder of this report, it will be assumed that the Jacobian of T does not vanish. Thus an inverse transformation will exist.

Inverse Transformation

In most of the two-dimensional problems which have been solved using a numerical transformation method, it is not the transformation from the physical region D to the rectangular region R that is constructed, but rather the transformation from the region R to the region D. Our work proceeds in the same direction. The first task is to invert the system of Equations (2). That is, to find an equivalent system with u, v, w as independent variables and x, y, z as dependent variables.

Define the matrix M by

$$M=\begin{bmatrix} x_u & x_v & x_w \\ y_u & y_v & y_w \\ z_u & z_v & z_w \end{bmatrix}.$$

Then the determinant of M, which is the Jacobian of T^{-1} and will be denoted by J, is a nonvanishing, real-valued function defined on R.

Theorem 3. *The functions u, v, w satisfy the system* (2) *if and only if the functions x, y, z satisfy the system of quasilinear elliptic equations*

$$\begin{aligned} &\alpha_{11} x_{uu}+2\alpha_{12} x_{uv}+2\alpha_{13} x_{uw}+\alpha_{22} x_{vv}+2\alpha_{23} x_{vw}+\alpha_{33} x_{ww} \\ &\qquad +J^2[f_1 x_u+f_2 x_v+f_3 x_w]=0 \\ &\alpha_{11} y_{uu}+2\alpha_{12} y_{uv}+2\alpha_{13} y_{uw}+\alpha_{22} y_{vv}+2\alpha_{23} y_{vw}+\alpha_{33} y_{ww} \\ &\qquad +J^2[f_1 y_u+f_2 y_v+f_3 y_w]=0 \\ &\alpha_{11} z_{uu}+2\alpha_{12} z_{uv}+2\alpha_{13} z_{uw}+\alpha_{22} z_{vv}+2\alpha_{23} z_{vw}+\alpha_{33} z_{ww} \\ &\qquad +J^2[f_1 z_u+f_2 z_v+f_3 z_w]=0 \end{aligned} \tag{3}$$

where

$$\alpha_{jk}=\sum_{m=1}^{3} \beta_{mj}\beta_{mk}$$

and β_{jk} is the cofactor of the (j, k) element in the matrix M.

Proof. Let u, v, w be solutions of (2). Suppose s is a function defined on D. By the chain rule,

$$\begin{aligned} s_x &= s_u u_x + s_v v_x + s_w w_x, \\ s_y &= s_u u_y + s_v v_y + s_w w_y, \\ s_z &= s_u u_z + s_v v_z + s_w w_z, \end{aligned}$$

and

$$\begin{aligned} \nabla^2 s = {} & (u_x^2+u_y^2+u_z^2)\, s_{uu} + 2(u_x v_x + u_y v_y + u_z v_z)\, s_{uv} \\ & + 2(u_x w_x + u_y w_y + u_z w_z)\, s_{uw} + (v_x^2+v_y^2+v_z^2)\, s_{vv} \\ & + 2(v_x w_x + v_y w_y + v_z w_z)\, s_{vw} + (w_x^2+w_y^2+w_z^2)\, s_{ww} \\ & + \nabla^2 u\, s_u + \nabla^2 v\, s_v + \nabla^2 w\, s_w. \end{aligned}$$

By substituting $s = x, y$, and z in each of the first three equations, expressions can be found for the partial derivatives of u, v, and w with respect to x, y, and z in terms of the partial derivatives of x, y, and z with respect to u, v, and w. If these values are substituted in the last equation, $\nabla^2 u$, $\nabla^2 v$, and $\nabla^2 w$ are replaced by f_1, f_2, and f_3, and then s is replaced by x, y, and z, the result is the system of Equations (3). It is well known that the type of a partial differential equation is preserved under a transformation with a nonvanishing Jacobian. Thus $\nabla^2 s = 0$ transforms into an elliptic equation and hence the system (3) is elliptic.

Conversely, suppose, x, y, z are solutions of (3). Then again computing $\nabla^2 s$ and setting $s = x, y$, and z, we obtain three equations which together with (3) yield the system

$$(\nabla^2 u - f_1)\, x_u + (\nabla^2 v - f_2)\, x_v + (\nabla^2 w - f_3)\, x_w = 0,$$
$$(\nabla^2 u - f_1)\, y_u + (\nabla^2 v - f_2)\, y_v + (\nabla^2 w - f_3)\, y_w = 0,$$
$$(\nabla^2 u - f_1)\, z_u + (\nabla^2 v - f_2)\, z_v + (\nabla^2 w - f_3)\, z_w = 0.$$

The matrix M is nonsingular and the trivial solution of the system of equations is equivalent to (2).

In the construction of the transformation of R onto D, the one-to-one boundary correspondence (1) furnishes boundary conditions for the elliptic Equations (3) of the form

$$\begin{aligned} x &= g_1(u, v, w) \\ y &= g_2(u, v, w) \\ z &= g_3(u, v, w) \end{aligned} \tag{4}$$

for (u, v, w) on ∂R. The construction of T^{-1} is equivalent to solving an elliptic boundary value problem with Dirichlet boundary conditions. It should also be noted that the coefficients α_{jk} in (3) depend only on the derivatives and not on the values of the functions u, v, w. This result may be used to prove that the solution of (3) with boundary values (4) is unique (see [3], pp. 323, 324).

Potential Flow with Symmetry

The problem of determining the potential function for the flow of an ideal fluid about a finite body in an infinite fluid region has been studied extensively. The only restriction we impose is that the fluid region have at least one plane of symmetry. Thus we include all axisymmetric problems where many exact solutions are available and the accuracy of our numerical method can be tested. The potential function will be computed using finite difference techniques and a free stream condition will be assumed on some sphere far from the body. Because of symmetry, only half of the truncated fluid region is used in the calculations.

The transformation is indicated in Figure 1. Under the inverse transformation, the horizontal faces of the rectangular region map to the body and the hemispherical outer boundary. The vertical faces map to the plane of symmetry.

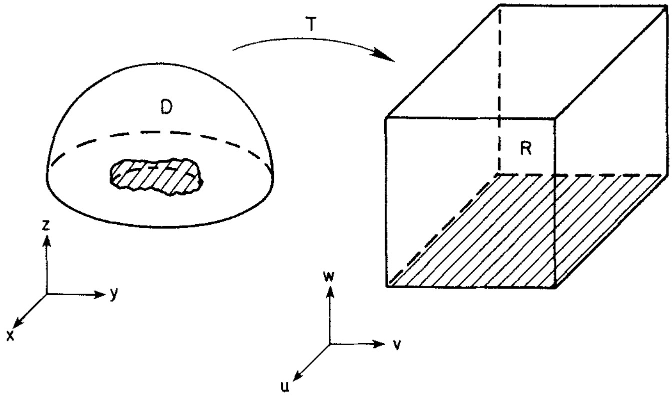

Fig. 1. Physical and computational regions

Let ϕ be the potential function defined on $\bar{D}$. Assume a unit free stream velocity in the direction of the positive y axis. Then $\nabla^2\phi=0$ in $D, \phi=y$ on the outer boundary and $\phi_n=0$ on the body and the plane of symmetry where n denotes the exterior normal on ∂D. In the region R, the equation and boundary conditions become

$$\begin{aligned}&\alpha_{11}\phi_{uu}+2\alpha_{12}\phi_{uv}+2\alpha_{13}\phi_{uw}+\alpha_{22}\phi_{vv}+2\alpha_{23}\phi_{vw}+\alpha_{33}\phi_{ww}\\&\qquad+J^2[f_1\phi_u+f_2\phi_v+f_3\phi_w]=0 \quad \text{on} \quad R,\end{aligned} \tag{5}$$

$$\begin{aligned}&\phi=y && \text{if } w=b_3\\&\alpha_{13}\phi_u+\alpha_{23}\phi_v+\alpha_{33}\phi_w=0 && \text{if } w=a_3\\&\alpha_{12}\phi_u+\alpha_{22}\phi_v+\alpha_{23}\phi_w=0 && \text{if } v=\alpha_2 \text{ or } b_2\\&\alpha_{11}\phi_u+\alpha_{12}\phi_v+\alpha_{13}\phi_w=0 && \text{if } u=a_1 \text{ or } b_1.\end{aligned} \tag{6}$$

The following procedure was used to construct an approximation to the potential function. For these examples, take $f_1=f_2=f_3=0$. A cubic mesh was placed on $\bar{R}$. The equations in (3) and (5) were converted to difference equations using second order central differences. The boundary conditions in (4) and (6) were used with second order central differencing for all derivatives in the equations except where a neighboring mesh point was outside of $\bar{R}$ in which case the derivative was replaced by a first order forward or backward difference. The derivative conditions in (6) degenerate at certain edges of ∂R and there an average value for the function was chosen. The system of equations was solved by non-linear SOR with an initial free stream potential function.

Three body configurations are included. The first is a sphere. The exact solution is well known and our computed value is compared with the exact value. The second body is an ellipsoid with axes ratio 1:2:4 and the third is the union of two circular cones joined at a common base lying in the xy-plane. In all cases the outer boundary was the sphere of radius e^2. Various surfaces and cross-sections are shown in Figures 2 and 3. The mesh in these figures is the

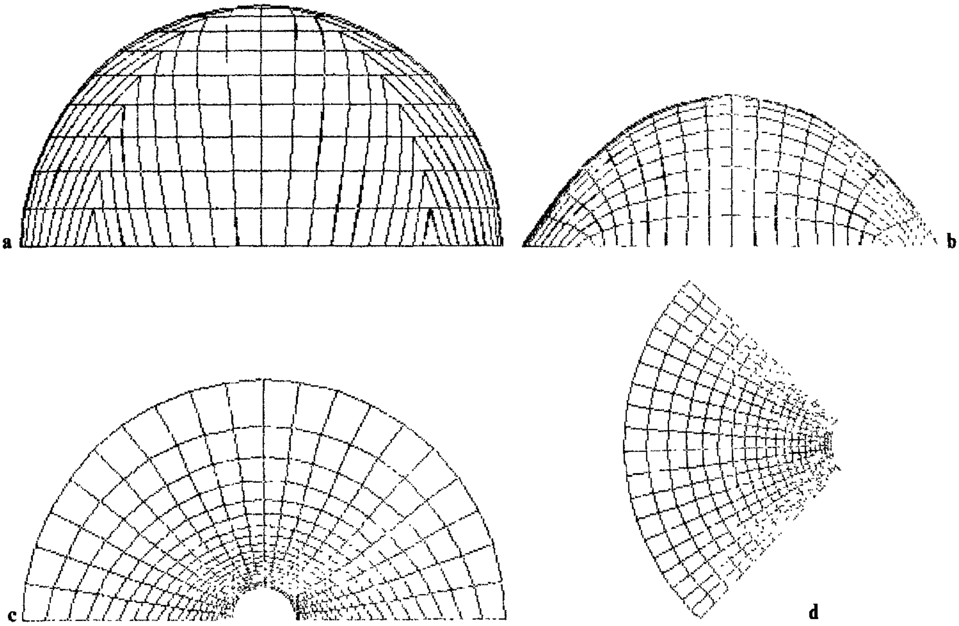

Fig. 2a–d. Spherical body $x^2+y^2+z^2=1$, $z \geqq 0$. **a** $w=b_3$. **b** $w=\frac{1}{2}(b_3+a_3)$. **c** $u=\frac{1}{2}(b_1-a_1)$. **d** $v=a_2$

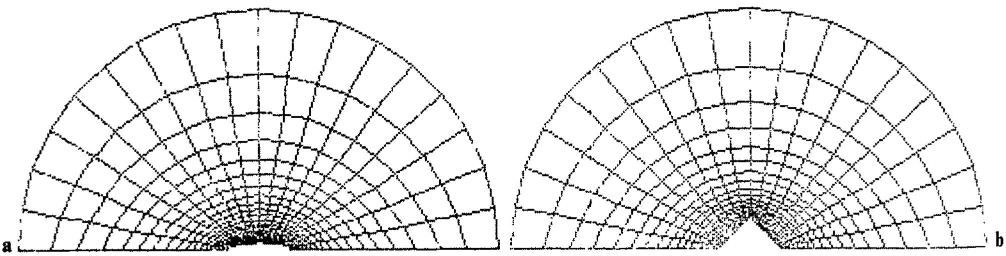

Fig. 3. **a** Ellipsoidal body $4x^2+y^2+16z^2=16$, $z \geqq 0$; $u=\frac{1}{2}(b_1-a_1)$. **b** Conical body $x^2+y^2=(z-1)^2$, $0 \leqq z \leqq 1$, $u=\frac{1}{2}(b_1-a_1)$

Table 1. Maximum difference in successive iterates after n iterations

n	Spherical body			Elliptical		Conical	
	mesh	potential	error	mesh	potential	mesh	potential
10	2.63014	1.17530	0.12645	1.70716	0.77372	1.34065	0.55443
20	2.19094	0.77492	0.05571	0.47050	0.20634	0.37055	0.18059
30	0.25112	0.08907	0.03191	0.11962	0.02564	0.06961	0.01985
40	0.03266	0.00840	0.01756	0.01681	0.00144	0.00580	0.00181
50	0.00377	0.00194	0.01565	0.00061	0.00049	0.00095	0.00159

image of the cubic mesh in $\bar{R}$. Although no computing was done on this mesh, it is advisable to examine its general appearance since extreme aspect ratios and nonorthogonality may slow iterative convergence and increase discretization error.

Selected output from the program written to solve the difference equations is presented in Table 1. A rectangular region with $19 \times 19 \times 20$ equally spaced mesh points was used. For each configuration, the first column contains the maximum difference of the x, y, and z values after the (n − 1)th and nth iteration. The second column contains the maximum difference of the ϕ values. For the spherical configuration, the third column contains the maximum difference between the computed value of ϕ and the exact value which is

$$y[1+\tfrac{1}{2}(x^2+y^2+z^2)^{-\frac{3}{2}}].$$

The maximum differences were taken over all interior points. For the spherical body, the maximum error on the surface of the body, excluding points on the symmetry plane, was about 0.02 or 2% of the free stream velocity after 50 iterations. The error at the outer boundary caused by the free stream assumption was nearly 0.01. A value for the potential function on the surface of the ellipsoid is given by Pien [8] to be 1.12659 y. Our computed values, after 50 iterations, differed by a maximum of 0.01 except on the symmetry plane. At the intersection of the body and the symmetry plane, errors increased to a maximum of 0.04 for the sphere and 0.03 for the ellipsoid. Increasing the number of iterations beyond $n=50$ increased accuracy very little if any.

The results of this simple example are encouraging. With less than 7500 points, we have attempted to solve a three-dimensional mixed boundary value problem. Still, when comparisons were made, the approximation was accurate to one decimal place. This is comparable to the accuracy of the integral equation methods reported by Pien [8].

Transformations in Higher Dimensions

Since there are problems involving more than three unknowns, one might ask if this method could be useful in higher dimensions. In this final section, that possibility will be examined.

Let D be a bounded region in the space of ordered *n-tuples* of real numbers $(x_1, \ldots, x_n)$. Suppose that ∂D is homeomorphic to the boundary of a rectangular region R given by

$$R=\{(u_1, \ldots, u_n) \mid a_i<u_i<b_i,\ i=1, \ldots, n\}.$$

Let T be a one-to-one transformation of $\bar{D}$ onto $\bar{R}$ which has a nonvanishing Jacobian on D. Then T is a solution of the system

$$\nabla^2 u_i=f_i(u_1, \ldots, u_n), \qquad i=1, \ldots, n$$

if and only if T^{-1} is a solution of the quasilinear elliptic system

$$\sum_{j,k=1}^{n} \alpha_{jk} \frac{\partial^2 x_i}{\partial u_j \partial u_k}+J^2 \sum_{k=1}^{n} f_k(u_1, \ldots, u_n) \frac{\partial x_i}{\partial u_k}=0, \qquad i=1, \ldots, n$$

where J is the Jacobian of T^{-1} and

$$\alpha_{jk} = \sum_{m=1}^{n} \beta_{mj} \beta_{mk}$$

with β_{jk} the cofactor of $\frac{\partial x_j}{\partial u_k}$ in the matrix $\left[\frac{\partial x_p}{\partial u_q}\right]$.

The method would appear to generalize to higher dimensions, but there are limitations to its implementation. First of all it is necessary to define some homeomorphism between ∂D and ∂R which are $(n-1)$-dimensional subsets. Secondly, the number of distinct terms in each equation defining the inverse transformation is $n(n+3)/2$. Also, the determination of the coefficient α_{jk} requires the calculation of determinants of order $n-1$. Consequently, any attempt to carry out the calculations in this report would be a formidable task for larger values of n.

Conclusions

A transformation method which has proven useful in two-dimensional fluid flow problems has been generalized to three-dimensions. The method may even prove more valuable in the construction of three-dimensional transformations since three-dimensional conformal mappings can only be used in trivial cases. Even the determination of simple algebraic transformations is more difficult since the three gradient vectors must be linearly independent at each point of the region.

No attempt has been made to give a complete list of all variants of the method which may be used in solving other physical problems. In the study of time dependent problems, the physical domain may change with time so that the mesh functions may depend on the temporal variable as well as the spatial variables. For example, free surface problems could be studied in the manner of Godunov and Prokopov [5] and Thompson et al. [10]. Transformations of certain multiply-connected regions can also be constructed provided appropriate branch cuts are made as in Thompson et al. [9].

The example is intended to be a test of the method and not an improved method for solving the stated potential flow problems. It illustrates how the method handles both Dirichlet and Neumann boundary conditions. In the transformations there are boundary points where the Jacobian vanishes and points where the body is not smooth.

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