Orthogonal Mapping

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Received November 13, 1981; revised August 17, 1982

A technique of orthogonal mapping is proposed for constructing boundary-fitted orthogonal curvilinear coordinate systems in 2-D. The mapping is defined by the covariant Laplace equation, and constraints on the components of the metric tensor of the curvilinear coordinates are used to achieve orthogonality and to control the spacing of coordinate lines. Two different methods of implementing the mapping are presented. The first, termed the strong constraint method, is intended primarily for problems in which the boundary shape is not known in advance, but is to be determined as a part of the solution (e.g., free boundary problems in fluid mechanics). The second, termed the weak constraint method, is designed for the construction of an orthogonal mapping with a prescribed boundary correspondence, i.e., the production of boundary-fitted orthogonal coordinates for a domain of given shape with a prescribed distribution of coordinate nodes along the boundary. The method is illustrated by numerical examples, and it is shown that the problem of mapping infinite domains can be treated by mapping the infinite domain onto a finite one using a simple conformal transformation and then applying the orthogonal mapping technique developed here to the finite domain. The possibility of obtaining analytical solutions for the mapping functions is discussed. The Appendices contain connection (Christoffel) coefficients which provide a convenient means for deriving equations of a physical problem for the constructed coordinates in terms of physical components, using a slight extension of Cartesian tensor notation.

1. Introduction

The construction of a curvilinear coordinate system in which a boundary of arbitrary shape is represented by a coordinate line or surface is an important problem of applied mathematics. The best-known approach to this problem is typified by the method of Thompson et al. [1, 2], who also review previous research. In the Thompson et al. method [2], the transform relations $\xi(x, y)$ and $\eta(x, y)$ between Cartesian coordinates x, y and "boundary-fitted" curvilinear coordinates ξ , η are assumed to satisfy elliptic equations of the form

$$\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} = P(\xi, \eta), \qquad \frac{\partial^2 \eta}{\partial x^2} + \frac{\partial^2 \eta}{\partial y^2} = Q(\xi, \eta), \tag{1}$$

where the functions $P(\xi, \eta)$ and $Q(\xi, \eta)$ are chosen (essentially by trial and error) to

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control the spacing and configuration of coordinate lines in the domain of interest. It is suggested that "sums of decaying exponentials" provide a convenient form for P and Q, but the choice is otherwise ad hoc. To actually carry out the transformation, a set of coupled, nonlinear partial differential equations is derived for $x(\xi, \eta)$ and $y(\xi, \eta)$ from (1) by direct interchange of dependent and independent variables, and these equations are then solved numerically. Though undoubtedly useful, the Thompson et al. approach has the severe drawback, when applied to the numerical solution of differential equations from mathematical physics, of yielding a nonorthogonal coordinate system. In addition, the only control over spacing and configuration of coordinate lines is exercised by the ad hoc choice of $P(\xi, \eta)$ and $Q(\xi, \eta)$.

We consider the development of a method to generate orthogonal (boundary-fitted) coordinates. With this objective, the first and classical candidate in 2-D is, of course, conformal mapping. Indeed, efficient methods for numerical construction of conformal mappings have been developed (see [3, 4] and references therein); however, as Fornberg [3] points out, conformal mappings are ill-conditioned in the sense that very small changes in the shape of the domain can dramatically alter the position of mapped boundary points. Also, the density of boundary points (placed uniformly in the ξ , η plane) may vary by several orders of magnitude along the boundaries of the original x, y domain. Examples given by Fornberg [3, Figs. 1 and 7] show clearly that conformal mapping can yield coordinate grids which are completely unsuitable for numerical solution of partial differential equations.

The problem with conformal mapping is that the dual requirements of orthogonality and equality of the scale factors (so that a small square in the ξ , η plane is mapped onto a square in the physical x, y plane) are too restrictive. Hung and Brown [5] and Pope [6] have attempted to alleviate this problem by constructing orthogonal mappings in which the ratio of scale factors is not unity but rather some (adjustable) constant throughout the domain. However, the use of a constant ratio of scale factors is still too restrictive for a generally applicable transformation technique, and Mobley and Stewart [7] have thus suggested construction of an orthogonal mapping by nonuniform stretching of the conformal coordinates. The coordinates of Mobley and Stewart are thus a pair of variables, each of which is a monotonic function of a respective conformal variable. By eliminating the "intermediate" conformal variables, Mobley and Stewart obtained generating equations for their transformation functions. As will be seen in Sections 2 and 4, this procedure can lead to basically the same types of grids as the "strong constraint" subclass of the present method and the generating equation of Mobley and Stewart is just a covariant Laplace equation, though this important fact could not be recognized in the framework of their approach. Most recently, Haussling and Coleman [8] have attempted to produce orthogonal coordinate grids in two dimensions with prescribed nodal correspondence on all boundaries, using a pair of differential constraints on the mapping functions $x(\xi, \eta)$, $y(\xi, \eta)$ which are equivalent to our orthogonality constraint $g_{12} = 0$ (see Section 2). The single constraint of orthogonality is, however, insufficient to completely specify a mapping in two-dimensions, and the resulting procedure exhibits a number of problems including nonorthogonal mesh. One example, which is treated successfully by the method outlined in this paper (see Figs. 7 and 8), led to a completely unacceptable mesh in Haussling and Coleman [8].

Other recent attempts to construct orthogonal coordinates have been based on solving first order partial differential equations of the Cauchy-Riemann type as an initial value problem. Starius [9] used this idea to construct an orthogonal coordinate mesh in a strip near a given boundary, but was forced to use a different grid in the interior of his domain with interpolation between the two grids then required in the region of overlap. Following an earlier approach by Potter and Tuttle [10], Davies [11] used the same idea to construct a second set of coordinate lines orthogonal to a first set which was to be specified on an a priori basis, e.g., a set coincident with pathlines of the fluid in a semi-Lagrangian code. However, the application of this initial value approach is not generally suitable for the construction of a coordinate system for the complete domain, since it is usually necessary to specify conditions on all boundaries, and the generating equation should thus be elliptic.

We suggest a "covariant" approach for the generation of orthogonal mappings. Simple considerations from vector and tensor analysis are used in Section 2 to establish the covariant Laplace equation as the generating elliptic equation for the transformation functions $x(\xi, \eta)$ and $y(\xi, \eta)$. The properties of the resulting coordinate system are then determined by constraints on the components of its metric tensor. We consider three types of application. In the first, the boundary shape is to be determined as part of the solution of the problem, and we develop the so-called "strong constraint method" to determine the mapping. This case is discussed in Section 4. In the second type of application, the shape of the domain is known, and in the third, the spacing of boundary nodes is also specified, i.e., the complete boundary correspondence is prescribed. For these cases, we have developed the "weak constraint method," which is discussed in Section 5. Finally, a brief comparison with the classical method of conformal mapping is given in Section 6. A preliminary presentation of our technique of orthogonal mapping was given in [12], and an application of the "strong constraint method" to calculate the shapes of gas bubbles rising through a viscous fluid is summarized in [13].

2. Equations Defining the Mapping

A most important first step in the development of a mapping between a Cartesian and a "boundary-fitted" curvilinear coordinate system is to determine the equations to be satisfied by the transform functions $x(\xi, \eta)$ and $y(\xi, \eta)$. Fortunately, this is extremely simple even if the resulting "boundary-fitted" coordinates are required to have predetermined properties such as orthogonality, provided the well-known covariant point of view is adopted, according to which any physical or geometrical law must be expressible in a form that does not depend on the choice of a particular coordinate system (see, e.g., [14, Sect. 12.5]).

In particular, a covariant, coordinate-free form of the equations for x and y follows directly from the trivial observation that x, as a Cartesian coordinate in the physical

space, is obviously a linear scalar function of position and the same is true of y. Thus, grad(x) and grad(y) are constant valued vector fields, and it follows that

$$\operatorname{div} \operatorname{grad}(x) = 0, \qquad \operatorname{div} \operatorname{grad}(y) = 0 \tag{2}$$

everywhere, with div grad being the covariant Laplace operator ∇^2 . As is well known, this operator can be written in explicit form for any particular coordinate system ξ^1 , ξ^2 , including the one we want to construct, provided only that we know the components of the metric tensor $g_{\alpha\beta}$ which define the length of a line element according to the relation

$$ds^2 = g_{\alpha\beta} d\xi^{\alpha} d\xi^{\beta}.$$

Here, the Greek indices equal one or two in 2-D and summation on the repeated indices is implied.

The obvious question, then, is how the metric tensor is to be determined before the coordinate system is constructed. The answer is that the development of an appropriate coordinate transformation must begin by specifying the metric tensor—and it is this specification which determines the properties of the resulting coordinate system. For example, if the nondiagonal components of $g_{\alpha\beta}$ are zero, the coordinate system ξ^1 , ξ^2 is orthogonal. If, in addition, the diagonal components are all equal to one, the system is Cartesian, etc. Now, whatever physical problem is being considered, there are always *m* degrees of freedom (where m=2 in 2-D and m=3 in 3-D) in choosing the mapping functions (e.g., the functions $x(\xi, \eta)$, $y(\xi, \eta)$ in 2-D). The essential idea pursued in the remainder of this paper is to "use" these available degrees of freedom to impose m constraints on the components of the metric tensor in order to build the desired properties into the constructed coordinate system.

Although the metric tensor (being symmetric) generally has three independent components in 2-D (and six in 3-D), the m constraints referred to above are the maximum number that can be imposed if the space described by the resulting coordinate system is to be Euclidean ("flat"). Mathematically, the condition that the space is Euclidean is equivalent to requiring the Riemann curvature tensor of the coordinate system to be zero (see [14]). The Riemann tensor, which is a function of the metric tensor and its first and second derivatives, has only one independent component in 2-D (which is proportional to the Gaussian curvature), and the restriction to a Euclidean space thus imposes a single constraint on $g_{\alpha\beta}$, reducing the number of freely specifiable constraints to two. In 3-D, the Riemann tensor has six independent components, but they are linked by the differential Bianchi identities (see [14]), leaving only three "flatness" constraints on the metric tensor. Consequently, the number of freely specifiable constraints on $g_{\alpha\beta}$ in 3-D is three. Note that an explicit consideration of the "flatness" constraints is not necessary. If a solution of Eqs. (2) exists (thus defining a transformation from ξ , η to the Cartesian coordinates x, y), the space described by ξ , η is guaranteed to be Euclidean because Cartesian coordinates may be introduced only in a Euclidean space. In other words, the condition that the Riemann tensor be zero is just a condition of integrability for Eqs.

(2) (see [15, Sect. 39]) and so will be satisfied automatically when a solution of (2) is obtained.

It is, of course, not clear that the degrees of freedom in choosing the mapping functions $x(\xi, \eta)$, $y(\xi, \eta)$ can always be utilized as constraints on the metric tensor. In particular, it is not evident that mapping functions can always be found connecting some particular domains in the x, y and ξ, η planes which satisfy prescribed constraints on the metric tensor. To prove that this is indeed possible for arbitrary constraints would amount to a major result in theoretical mathematics, and is beyond the scope of the present work. However, for the particular pair of constraints in 2-D,

$$g_{12} = 0$$
 and $g_{22}/g_{11} = 1$

which define conformal mapping, the proof is, in fact, well known: it is the celebrated Riemann mapping theorem. This fact provides some theoretical support for the present approach, though we do not restrict ourselves to conformal maps.

The most obvious (and useful) constraint in the general case is to set all of the nondiagonal components of $g_{\alpha\beta}$ equal to zero, thereby ensuring that the resulting coordinate system is orthogonal. Since the number of independent nondiagonal components is one in 2-D and three in 3-D, it is evident that this is always possible in two- or three-dimensional systems. In fact, in the important 2-D case, one additional degree of freedom is still left. For m > 3, on the other hand, the orthogonality constraint cannot be satisfied—an arbitrary space of more than three dimensions does not generally admit an orthogonal coordinate system (see Eisenhart [16]). We restrict our attention to orthogonal systems in two dimensions in the remainder of this paper.¹

The metric tensor for 2-D orthogonal coordinates ξ , η can be written as

$$g_{\alpha\beta} = \begin{pmatrix} h_1^2 & 0 \\ 0 & h_2^2 \end{pmatrix},$$

where index 1 corresponds to ξ , and index 2 to η . Recall now that there is one degree of freedom left in 2-D after setting $g_{12}=0$, and we propose using this to impose an additional constraint on the scale factors h_1 and h_2 . A simple and useful constraint is to specify the ratio of the scale factors as a function of ξ and η , i.e., $f(\xi, \eta) \equiv h_2/h_1$. The ratio h_2/h_1 has a clear geometrical significance—it specifies the ratio of the sides of a small rectangle in the x, y plane which is an image of a small square in the ξ , η plane. It is therefore natural to call $f(\xi, \eta)$ the distortion function. By judicious choice of the distortion function, one can control the spacing of a computational grid in the x, y plane, which is the image of a uniform grid in the ξ , η plane (say, on a unit

Note that this case can also serve as a basis for three-dimensional orthogonal coordinates in the presence of either translational symmetry in the direction normal to the x, y plane (i.e., no dependence on z) or axial symmetry. For these special cases, the three-dimensional orthogonal coordinates are obtained, respectively, by either translating the ξ , η system in the z direction or rotating it about the axis of symmetry provided that the latter is also a coordinate line in ξ , η .

square). This should be particularly useful in problems involving disparate length scales in different directions (e.g., a boundary layer-like structure). Although the distortion function could, in principle, be adjusted automatically during the course of numerical solution to reflect the evolving gradients of the solution, such an algorithm would be expensive and has not been implemented in the current study.

The condition $f(\xi, \eta) = 1$, which corresponds to conformal mapping, is obviously a major restriction on the class of possible mappings; an adjustable function of two variables $f(\xi, \eta)$ evidently provides much greater flexibility while orthogonality is still maintained. Indeed, the "stiffness" of the conformal mapping, which makes it ill-suited for the present purposes (see Section 1), is due to this unnecessary restriction $f(\xi, \eta) = 1$. To a lesser degree, the same is true for other methods in which $f(\xi, \eta) = \text{const}(\text{Hung and Brown [5], Pope [6]})$. We note in passing that in 3-D no freedom is left after specification of the three orthogonality constraints $g_{12} = g_{13} = g_{23} = 0$, and so orthogonal mapping in 3-D is likely to be as "stiff" as conformal mapping in 2-D.

Equations (2) can now be written explicitly in the ξ , η coordinates using the conditions

$$g_{12} = 0$$

$$\frac{h_{\eta}}{h_{\xi}} = \frac{h_2}{h_1} = \frac{(g_{22})^{1/2}}{(g_{11})^{1/2}} = f(\xi, \eta)$$

and the well-known formula for the two-dimensional covariant Laplace operator in orthogonal coordinates, which is

$$\nabla^2 = \frac{1}{h_{\xi}h_{\eta}} \left[\frac{\partial}{\partial \xi} \left(\frac{h_{\eta}}{h_{\xi}} \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\frac{h_{\xi}}{h_{\eta}} \frac{\partial}{\partial \eta} \right) \right].$$

The generating equations are thus²

$$\frac{\partial}{\partial \xi} \left(f \frac{\partial x}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\frac{1}{f} \frac{\partial x}{\partial \eta} \right) = 0, \qquad \frac{\partial}{\partial \xi} \left(f \frac{\partial y}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\frac{1}{f} \frac{\partial y}{\partial \eta} \right) = 0. \tag{3}$$

² One of the referees has pointed out that Eqs. (3) can be obtained from the Thompson *et al.* Eqs. (1) with an appropriate choice for P and Q, thus suggesting that the present mapping techniques (and all related techniques intended to generate orthogonal mappings) should be considered as special cases of the Thompson *et al.* technique. While the first part of this statement is, of course, true, the specific choice

$$P = \frac{1}{h_{\ell}h_{\eta}} \frac{\partial f}{\partial \xi}, \qquad Q = \frac{1}{h_{\ell}h_{\eta}} \frac{\partial}{\partial \eta} \left(\frac{1}{f}\right)$$

which is necessary to obtain (3), was not, apparently, evident to Thompson and co-workers, who suggested that P and Q be chosen as sums of decaying exponentials and stated "An orthogonal system cannot be achieved with arbitrary spacing of the coordinate lines around the boundary," nor to subsequent workers (cf. Haussling and Coleman [8]) who actually attempted to generate the P and Q so as to ensure an orthogonal mesh. At any rate, this choice is not directly realizable since h_l and h_n cannot be specified in advance.

The solution of these equations with appropriate boundary conditions (to be discussed later) will provide the transformation from Cartesian coordinates x, y to an orthogonal curvilinear coordinate system ξ , η provided the mapping actually exists for the particular boundary shape³. The scale factors h_{ℓ} and h_{η} that are required in the governing equations of the physical problem, can be computed easily from the standard formulae of tensor analysis

$$h_{\alpha}^{2} \equiv g_{\alpha\alpha} = \delta_{\beta\gamma} \frac{\partial x^{\beta}}{\partial \xi^{\alpha}} \frac{\partial x^{\gamma}}{\partial \xi^{\alpha}} = \left(\frac{\partial x}{\partial \xi^{\alpha}}\right)^{2} + \left(\frac{\partial y}{\partial \xi^{\alpha}}\right)^{2}. \tag{4}$$

Of course, only one of the scale factors needs to be computed from (4) as the second one can be obtained from $h_n/h_i = f(\xi, \eta)$.

Three types of application should be distinguished.

- (1) The shape of the domain is not known in advance, but is to be determined as a part of the solution of a physical problem (e.g., free boundary problems in fluid mechanics).
- (2) The shape of the domain is known, but the distribution of the coordinate nodes along the boundary is not specified and may be determined by the mapping.
- (3) The shape of the domain is known and the distribution of coordinate nodes is specified along all boundaries, i.e., the complete boundary correspondence is prescribed.

The two methods, considered in the rest of the paper (the "strong constraint" method (Section 4) and "weak constraint" method (Section 5)) are not equally suitable for these problems. The strong constraint method (which includes conformal mapping as a special case) works well for problems of type (1), and might, in principle, also be applied to problems of type (2). The strong constraint method cannot be used to solve problems of type (3). The weak constraint method, on the other hand, is particularly well suited to problems of type (3), and thus also can be used conveniently for (2) by simply prescribing some reasonable boundary correspondence.

Since problems of types (2) and (3) are more common than those of type (1), the weak constraint method is likely to be the more important of the two methods of mapping.

It may be noted that the present orthogonal mapping corresponds to a special case of a so-called quasiconformal mapping [17, 18] when f and f^{-1} are bounded [the "complex dilatation" μ of the quasiconformal mapping being real and equal to (1-f)/(1+f) in this case]. An extensive mathematical theory of quasiconformal mapping has been developed, including the mapping theorem [17, 18] which establishes the existence of a quasiconformal mapping for a given μ (and thus of an orthogonal mapping for a given f if f and f^{-1} are bounded). It would obviously be of considerable interest to establish theoretically the existence of an orthogonal mapping for any given f, since some of the most useful orthogonal mappings do not satisfy the above boundedness conditions (e.g., the mapping which gives polar coordinates has $f = \pi \xi$, so that f = 0 at $\xi = 0$, see Section 4a). In this paper we take the existence of an orthogonal mapping for granted and proceed to the practical task of generating the mapping numerically.

3. APPLICATION TO AN INFINITE DOMAIN

In order to actually apply Eqs. (3) to the calculation of a boundary-fitted coordinate system, it is necessary to specify the distortion function f and determine boundary conditions for the functions $x(\xi, \eta)$ and $y(\xi, \eta)$. As a preliminary, however, we consider here the application to an infinite domain. Since the present investigation was originally motivated by the fluid mechanics problem of flow past a deformable bubble (or drop), we shall use this problem for illustration purposes in this and subsequent sections. In the case of a bubble, the interior flow can be ignored and it is therefore only necessary to develop boundary-fitted coordinates for the region exterior to the bubble. The objective, for a given bubble shape, is an orthogonal mapping $X(\xi, \eta)$, $Y(\xi, \eta)$ which maps the unit square $0 \le \xi \le 1$ and $0 \le \eta \le 1$ onto the exterior of the bubble. A "reasonable" correspondence of the boundaries for this case is sketched in Fig. 1a, with $\xi = 1$ being the bubble surface, $\xi = 0$ corresponding to "infinity" and η varying from 0 to 1 as the bubble surface is traversed from the finition to leading axis of summetry. Note that the ξ n coordinate system as

dinates X, Y, φ (where $Y \geqslant 0$) are right handed, but this presents no real problems and will actually be very useful in the case of a viscous drop where the matching of an exterior and interior coordinate system is most convenient when one is right handed and the other left handed. One should only remember that in a left-handed coordinate system all the expressions which involve the Levi-Civita alternating symbol ε_{ijk} (e.g., cross product and curl) change sign.

The first problem, and one whose resolution is of some general interest, is the mapping of an infinite domain by numerical solution of Eqs. (3) subject to some suitable boundary conditions. Since numerical solution cannot produce functions $X(\xi,\eta)$ and $Y(\xi,\eta)$ which reach infinite values, it is necessary to introduce some modification into the problem. One obvious possibility would be to simply truncate the X,Y domain at a large, but finite distance. However, a more satisfactory resolution is to combine a numerically generated orthogonal mapping from ξ,η to a ("fictitious") auxiliary domain in which $x(\xi,\eta)$ and $y(\xi,\eta)$ are finite, followed by a conformal mapping from this finite auxiliary domain to the infinite, "physical" domain in the X,Y space.

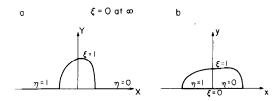


Fig. 1. Sketch of the coordinate system for the exterior of an axisymmetric bubble. (a) The final coordinate system in the infinite domain, and (b) the auxiliary mapping for the finite domain.

From the properties of conformal mapping it follows immediately that the ξ , η coordinates in the physical X, Y space will be orthogonal; moreover, the scale factors H_{ξ} , H_{η} for these coordinates will be related to the scale factors h_{ξ} , h_{η} of the auxiliary mapping via simple formulae

$$H_{\ell} = |F'| h_{\ell}, \qquad H_n = |F'| h_n$$

where F is the analytic function which defines the conformal mapping, i.e., X + iY = F(x + iy).

One especially simple and convenient conformal mapping (of the so-called second kind since it reverses orientation) which transforms from a finite to infinite domain is the inversion

$$F(w) = \frac{1}{\overline{w}}, \qquad X + iY = \frac{1}{x - iy} \tag{5}$$

which leads to

$$X = \frac{x}{r^2}, \qquad Y = \frac{y}{r^2}, \qquad H_{\xi} = \frac{h_{\xi}}{r^2}, \qquad H_{\eta} = \frac{h_{\eta}}{r^2},$$
 (6)

where

$$r^2 = x^2 + y^2.$$

A qualitative sketch of the auxiliary mapping $x(\xi,\eta)$, $y(\xi,\eta)$, which, when combined with (5) and (6), will yield an orthogonal, boundary-fitted coordinate system outside a bubble (or any particle), is seen in Fig. 1b. The point x=y=0 corresponds to infinity in the X, Y plane and is an image of the line $\xi=0$, i.e., the mapping is singular here. The distortion function $f(\xi,\eta)$ should thus be equal to 0 at $\xi=0$ (a concentration point of the coordinate system). Other factors concerning the choice of $f(\xi,\eta)$ will be discussed later.

4. Mapping by the Strong Constraint Method

a. Choice of the Distortion Function and Boundary Conditions

Let us now turn to the application of orthogonal mapping, beginning with the simplest case from a conceptual point of view, in which the distortion function $f(\xi, \eta)$ is specified completely throughout the ξ, η domain. In anticipation of the alternative approach outlined in Section 5, the method of mapping associated with this condition will be called the "strong constraint method." It is especially convenient when the shape of the domain must be determined as a part of the solution of the problem (e.g., the shape of a bubble in flow at finite Reynolds number), but cannot be used when the boundary correspondence is completely specified, where the "weak constraint" method of Section 5 must be adopted.

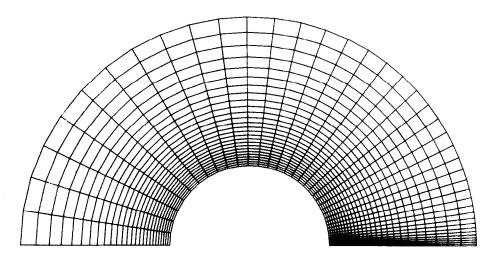


Fig. 2. Control over the density of coordinate lines by distortion function. Here, $f(\xi, \eta) = \pi \xi (1 - 0.9 \cos \pi \eta)$, $h_{\ell}(1, \eta) = 1$.

The most appropriate form for the distortion function depends on the domain of interest and any special features of the physical problem which must be resolved. Consider, for example, a bubble in a uniform fluid flow. The auxiliary domain has already been sketched in Fig. 1b, and we have noted that $f(0, \eta)$ should be 0. If one does not need the distortion to vary along the boundary $\xi = 1$, one can simply choose $f(\xi, \eta)$ to be the same as for polar coordinates, i.e., $f = \pi \xi$. Such a choice would, of course, produce polar coordinates if the shape of the boundary $\xi = 1$ were a semicircle with its center at x = y = 0, though very different coordinates will be produced when the shape of the boundary is noncircular. One potential advantage of equating $f(\xi, \eta)$ with the distortion function for some classical, "separable" coordinate system (such as polar coordinates) is that it may be possible to construct analytical expressions for the mapping functions, $x(\xi, \eta)$ and $y(\xi, \eta)$ (see Section 4c). On the other hand, if one wants the computational grid to be denser in the region downstream of the bubble (say, to resolve the wake), this can be accomplished easily by introducing the desired n dependence into the distortion function (see Fig. 2). Similarly, a higher resolution can be achieved in the boundary region by introducing a more complicated dependence on ξ into $f(\xi, \eta)$. Note that the finite-difference equations of the problem of interest will always be solved on a uniform grid in the unit square, $0 \le \xi$, $\eta \le 1$; it is well known that the uniform grid is preferable for the production of finite-difference schemes of high accuracy.

Let us now consider the boundary conditions for numerical generation of the mapping $x(\xi, \eta)$, $y(\xi, \eta)$. Referring to Fig. 1b, it is easy to see that

$$\left. \frac{\partial x}{\partial \eta} \right|_{\eta=0, \eta=1} = 0, \qquad y|_{\eta=0, \eta=1} = 0. \tag{7}$$

At $\xi=0$, which is a concentration point for the coordinate system and a singular point for differential equations (3), the only necessary condition is that x and y be finite (see Morse and Feshbach [19, pp. 713-716]), which reflects the fact that no real physical boundary is present. This condition will, of course, be satisfied by any numerical solution of (3), and it is permissible to choose arbitrary values (within some reasonable range of O(1)) for x and y at $\xi=0$, with the particular choice influencing the solutions for $x(\xi, \eta)$ and $y(\xi, \eta)$ by no more than the order of accuracy of the numerical scheme. Here, we simply choose

$$x|_{\xi=0}=0, y|_{\xi=0}=0.$$
 (8)

Finally we turn to conditions at the boundary $\xi = 1$, which corresponds to the bubble surface in the example considered here. In general, both $x(1, \eta)$ and $y(1, \eta)$ cannot be specified simultaneously if the resulting coordinate system is to be orthogonal. To demonstrate this fact, we need only examine the orthogonality constraint $g_{12} = 0$. With the definition of scale factors (4), and the distortion function, this yields

$$f\frac{\partial x}{\partial \xi} = \frac{\partial y}{\partial \eta}, \qquad \frac{\partial x}{\partial \eta} = -f\frac{\partial y}{\partial \xi}.$$
 (9)

These are obviously the analogue of the Cauchy-Riemann conditions in conformal mapping.⁴ Clearly, if $x|_{\xi=1}$ is given as a function of η , conditions (9) determine $\partial y/\partial \xi|_{\xi=1}$, and vice versa. Thus if both $x(1,\eta)$ and $y(1,\eta)$ are given, conditions (9) provide also $\partial x/\partial \xi|_{\xi=1}$ and $\partial y/\partial \xi|_{\xi=1}$, and the problem is overdetermined. Note, however, that a combination of a constant Dirichlet condition for one function and a zero Neumann condition for the other will satisfy (9) automatically (conditions (7) are of this type). If it is essential that both $x(1,\eta)$ and $y(1,\eta)$ be specified (i.e., the exact boundary correspondence of the mapping be prescribed), it is evident that the method of coordinate transformation must be substantially changed. This question is considered in Section 5.

We have noted earlier that the strong constraint method is particularly useful for problems in which the boundary shape must be determined as part of the solution. For the example of a deformed bubble, considered here, the shape of the boundary, $x(1, \eta)$, $y(1, \eta)$ must be attained as part of the problem solution. One approach is to use an iterative procedure starting from an initial shape (e.g., spherical). At each iteration, the position of the curve $\xi = 1$ which represents the bubble boundary (in either x, y or X, Y) must be changed incrementally in the normal direction, with the magnitude and sign of the increment (i.e., whether the boundary moves locally "in" or "out") to be determined by the magnitude and sign of the local normal-stress imbalance across the interface.

What is needed for application of the strong constraint method to problems involving an unknown boundary shape is a method for changing the mapping $x(\xi, \eta)$,

⁴ Note that the signs in (9) are for a mapping which preserves orientation, otherwise the signs are reversed.

 $y(\xi,\eta)$ so that the position of the curve $\xi=1$ is changed in the desired direction by a small increment normal to itself. This must be done without directly specifying both $x(1,\eta)$ and $y(1,\eta)$ as would seem to be necessary if one were to attempt somehow to specify the new position of a boundary point (say, $x^n(1,\eta)$, $y^n(1,\eta)$) directly from its position in the previous iteration $[x^{n-1}(1,\eta),y^{n-1}(1,\eta)]$. The approach proposed here is to alter the mapping, in a prescribed fashion, by changing its metric tensor (i.e., the scale factors). In particular, it is evident from the geometrical significance of $h_{\xi}(\xi,\eta)$ that a point of the boundary, say $\xi=1$, $\eta=\eta_0$, can be moved outward or inward along a ξ -coordinate line ($\eta=\eta_0$) which is locally normal to the boundary (due to the orthogonality of the coordinate lines) by simply increasing or decreasing $h_{\xi}(\xi,\eta_0)$. There is, of course, no way to modify h_{ξ} all along the line $\eta=\eta_0$ in an a priori fashion and still obtain a mapping which satisfies Eqs. (3). If a point on the

equivalent to changing h_{ℓ} locally in the limit as $\xi \to 1$. In order that this change in $h_{\ell}(1, \eta_0)$ actually cause the boundary $\xi = 1$ to move inward or outward in the x, y plane, it is necessary that it propagate inside the domain to produce changes of the same sign for $h_{\ell}(\xi, \eta_0)$ for $\xi < 1$. We can offer no rigorous proof at this time that this will always be true. For now, we simply accept it as a hypothesis. It should be noted, however, that this hypothesis is supported in the special case f = 1 of conformal mapping by the so-called Lindelöf principle [20] and has also turned out to be true for all test cases that we have considered to date.

The iterative procedure which we have adopted in the case of determining the unknown boundary shape for a bubble may be represented as follows. The value of $h_{\ell}(1, \eta_0)$ at the *n*th iteration is calculated as its value at the previous iteration plus a small change $\delta^{n-1}(\eta_0)$, dependent on (in the simplest case, proportional to) the normal stress imbalance at η_0 for the (n-1)th iteration, i.e.,

$$h_{\ell}^{n}(1,\eta_{0}) = h_{\ell}^{n-1}(1,\eta_{0}) + \delta^{n-1}(\eta_{0})$$
(10)

for $0 \le \eta_0 \le 1$. The new value of $h_{\ell}(1, \eta_0)$ is then transformed into boundary values for $\partial x/\partial \xi|_{\ell=1}$ and $\partial y/\partial \xi|_{\ell=1}$ by means of the definition

$$(h_{\ell}^{n})^{2} = \left(\frac{\partial x^{n}}{\partial \xi}\right)^{2} + \left(\frac{\partial y^{n}}{\partial \xi}\right)^{2} \tag{11}$$

and the constraint of orthogonality $g_{12} = 0$. The latter is implemented by noting that $g_{12} = 0$ can be expressed in the form

$$\frac{(\partial y/\partial \xi)}{(\partial x/\partial \xi)}\bigg|_{\xi=1} = -\frac{(\partial x/\partial \eta)}{(\partial y/\partial \eta)}\bigg|_{\xi=1}.$$
 (12)

The term on the left-hand side is the slope of a ξ -coordinate line at the boundary, while that on the right is the negative inverse of the slope of the boundary ($\xi = 1$)

itself. Thus, in order that the iterative procedure converge to a mapping in which the ξ -coordinate line at the boundary ($\xi = 1$) is orthogonal to the boundary, we interpret (and use) Eq. (12) as defining the slope of the ξ -coordinate line at the *n*th iteration via the slope of the boundary $\xi = 1$ at the previous iteration, i.e.,

$$\frac{(\partial y^n/\partial \xi)}{(\partial x^n/\partial \xi)}\bigg|_{\xi=1} = -\frac{(\partial x^{n-1}/\partial \eta)}{(\partial y^{n-1}/\partial \eta)}\bigg|_{\xi=1}.$$
 (13)

Equations (10), (11), and (13) provide sufficient information to determine boundary conditions for

$$\frac{\partial x^n}{\partial \xi}\Big|_{\xi=1}$$
 and $\frac{\partial y^n}{\partial \xi}\Big|_{\xi=1}$

at each new iteration. Equation (13) can be applied either in the given form or inverted, the choice being made in such a manner as to avoid division by very small numbers. The signs of $\partial x^n/\partial \xi|_{\xi=1}$ and $\partial y^n/\partial \xi|_{\xi=1}$ (which are found by a square root operation from (11)) are determined from the signs of $\partial y^{n-1}/\partial \eta|_{\xi=1}$ and $\partial x^{n-1}/\partial \eta|_{\xi=1}$ via (9).

The procedure outlined above can be implemented easily on a computer and leads to a stable and fast iterative process. It may be noted, however, that the boundary conditions for $x(\xi, \eta)$ are all of the Neumann type, with the exception of the "weak" condition at $\xi = 0$ and the solution is therefore determined only up to an arbitrary constant. Numerically, this "indeterminacy" manifests itself in the fact that the coordinate boundary (and, in fact, the whole coordinate system) may "creep" along the x axis during the iterative process (the point $\xi = 0$ stays at x = 0 but, being a singular point, it cannot "hold" the rest of the solution, see the discussion above). A simple way to eliminate this unwanted movement is to add a constant to $x(\xi, \eta)$ after each iteration, with the value chosen in such a way that the points closest to $\xi = 0$ on the x axis (i.e., x(h, 0) and x(h, 1), where h is the grid size) are required to fit symmetrically about the point x = 0.

b. Numerical Examples of the Strong Constraint Method

The proposed strong constraint method for generation of boundary-fitted, orthogonal coordinates has now been reduced to the solution of Eqs. (3), subject to the boundary conditions described above. A variety of finite-difference schemes can be used for this purpose. In our own computations we have adopted the ADI technique of Peaceman and Rachford (see, e.g., Richtmyer and Morton [21]) and used a 41×41 grid, i.e., h = 0.025.

First, we test the adequacy of Eqs. (11) and (13) for the generation of boundary conditions for $(\partial x/\partial \xi)_{\ell=1}$ and $(\partial y/\partial \xi)_{\ell=1}$ with $h_{\ell}(1,\eta)$ known. We consider two cases. In the first, we set

$$h_{\xi}(1,\eta)=1$$

and

$$f(\xi, \eta) = \pi \xi (1 - 0.9 \cos \pi \eta)$$

while the second has

$$h_l(1, \eta) = \sin^2 \pi \eta$$
 for $0 \le \eta \le 0.5$,
= 1 for $0.5 \le \eta \le 1$,

and

$$f(\xi, \eta) = \pi \xi.$$

In both cases, an iterative process is necessary even with $h_t(1, \eta)$ specified. For the calculations reported here, we start with an initial guess for x, y, use this to calculate $(\partial x/\partial \eta)$ and $(\partial y/\partial \eta)$ at the boundary $(\xi=1)$, use the specified form for h_{ℓ} and Eqs. (11) and (13) to obtain boundary values for $\partial x/\partial \xi|_{\xi=1}$ and $\partial y/\partial \xi|_{\xi=1}$, and finally calculate a new estimate for the mapping by numerically solving Eqs. (3) with $\partial x/\partial \xi|_{\xi=1}$ and $\partial y/\partial \xi|_{\xi=1}$ as boundary conditions. With this new estimate for $x(\xi,\eta)$ and $y(\xi, \eta)$ the process can be repeated. Presumably, if Eqs. (11) and (13) did not provide a sufficient means of obtaining boundary conditions for $x(\xi, \eta)$ and $y(\xi, \eta)$ (and this is by no means obvious), we might expect this iterative procedure to diverge. However, in both of the cases listed above, a convergent solution was obtained. In the first example, a very good initial guess can be generated analytically and the test of conditions (11) and (13) is rather weak. However, the resulting coordinate mapping, which is shown in Fig. 2, is of some qualitative interest in itself since it demonstrates how the density of a computational grid can be controlled by $f(\xi, \eta)$; this particular grid might potentially be useful for computation of the flow past a body with a developed wake. The "teardrop" shape shown in Fig. 3 was obtained for the second case and constitutes a much stronger test of convergence with

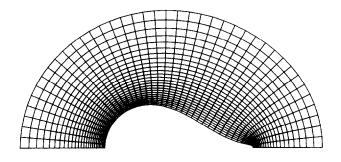


Fig. 3. "Teardrop" shape obtained with $f(\xi, \eta) = \pi \xi$ and $h_l(1, \eta) = \sin^2 \pi \eta$, if $\eta \le 0.5$, or 1, if $\eta > 0.5$.

boundary conditions generated from Eqs. (11) and (13). In this case, approximately 60 iterations (with a constant time step O(h)) were necessary to compute the mapping, starting with polar coordinates (and a circular boundary) as an initial guess (sixty iterations correspond to approximately 30 sec of CPU time on the VAX-11/780 computer which we used for our work). It should be noted that $h_{\ell}(1, \eta) = 1$ for all η in this initial guess and the change from this to the specified form for $h_{\ell}(1, \eta)$ is a very strong "jump," much greater than one might expect at each step in an overall solution scheme for a problem with unknown boundary shape where h_{ℓ} is incremented according to Eq. (10). The maximum nonorthogonality error in the final solution is approximately 0.5%, i.e., max $|g_{12}| \simeq 0.005$.

Let us now turn to an example of a problem in which an unknown boundary shape is to be calculated as part of the solution. This will constitute a final numerical test of the strong constraint method. Figure 4 gives a final converged solution for the axisymmetric steady shape of a bubble at finite Reynolds number, for a uniform streaming flow which moves from left to right. Of course, the shape is initially unknown and can be determined only in the course of solving the full fluid dynamical problem, described by the Navier-Stokes equations and appropriate boundary conditions. This is precisely the type of problem that the strong constraint method was designed to handle, but it is very important to establish the convergence of the overall solution scheme outlined in Section 4a, including iterative incremental changes in $h_l(1, \eta)$ as indicated in Eq. (10). In the present example, only an approximate solution of the fluid dynamics problem was obtained on the grid provided by the mapping at each overall iteration. This decreases the necessary computing time to the final steady state, but renders meaningless the transient results for bubble shape and velocity field at intermediate iterations in the solution scheme. The mapping and bubble shape illustrated in Fig. 4 were obtained starting from a sphere as the initial guess for bubble shape. After obtaining the solution of the fluid dynamics problem for a given boundary shape at each iteration in the overall solution scheme, the scale

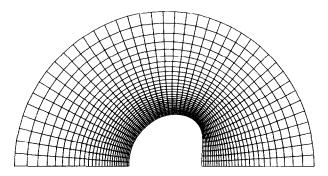


Fig. 4. Deformed bubble; obtained as a part of solution of the fluid mechanical problem described by the Navier-Stokes equations; $f(\xi, \eta) = \pi \xi$.

factor $h_i(1, \eta)$ was changed according to the sign and magnitude of the normal stress imbalance at the surface of the bubble, as discussed in Section 4a. The new scale factor was then used to redefine the mapping and the corresponding boundary shape for the bubble, and the whole process was repeated for this new shape, until overall convergence was achieved. A detailed account of this fluid mechanical problem will appear in a forthcoming publication. A brief description of the solution procedure and results was presented in [13].

c. On the Possibility of Analytical Solution by Separation of Variables

The present approach to the construction of an orthogonal mapping via the strong constraint method is primarily a numerical one. Nevertheless, it is of interest to note that the possibility exists for analytical solution in cases where the distortion function $f(\xi, \eta)$ of the mapping happens to coincide with the distortion function of some classical separable coordinate system. For example, in the previous section, the

solution could have been attempted. The reason for this is that the covariant Laplace Equation (3), which defines the orthogonal mapping, has exactly the same form for the general orthogonal coordinates ξ , η as it does in the classical polar coordinate system with the same $f(\xi, \eta)$ —simply because the form of the equation depends only on $f(\xi, \eta)$. The domain in the ξ , η plane is a unit square and one can solve Eqs. (3), in principle, as a series expansion in the appropriate eigenfunctions of the Laplace equation.

As an example, let us consider the distortion function $f(\xi, \eta) = \pi \xi$ for which the general solution of the Laplace equation, that is finite at $\xi = 0$, is (Morse and Feshbach [19, pp. 713-714]),

$$\sum_{l=0}^{\infty} \left[A_l \cos(l\pi\eta) + B_l \sin(l\pi\eta) \right] \xi^l.$$

one thus obtains

$$x = \sum_{l=1}^{\infty} A_l \cos(l\pi\eta) \, \xi^l, \qquad y = \sum_{m=1}^{\infty} B_m \sin(m\pi\eta) \, \xi^m$$

and the conditions for orthogonality (9) require

$$A_l = B_m$$
 for $l = m$.

The mapping is thus

$$x = \sum_{l=1}^{\infty} A_l \cos(l\pi\eta) \, \xi^l, \qquad y = \sum_{l=1}^{\infty} A_l \sin(l\pi\eta) \, \xi^l$$

and the coefficients are to be determined from the boundary conditions at $\xi = 1$, where

$$\sum_{l=1}^{\infty} A_l \cos(l\pi\eta) = x|_{\ell=1}, \qquad \sum_{l=1}^{\infty} A_l \sin(l\pi\eta) = y|_{\ell=1}.$$
 (14)

One can distinguish several possible cases insofar as determination of A_l is concerned. First, in the unlikely circumstance that *one* of the Cartesian coordinates, i.e., x or y, is known at the boundary $\xi = 1$ as a function of the transform variable η , the coefficients can be obtained directly from (14) using the orthogonality of $\cos(l\pi\eta)$ and/or $\sin(l\pi\eta)$. Second, in a more realistic situation, the shape of the boundary $\xi = 1$ is given parametrically, e.g.,

$$x|_{\xi=1} = u(s), y|_{\xi=1} = v(s), 0 \le s \le s_{\max},$$

where s is an arclength, i.e.,

$$\left(\frac{du}{ds}\right)^2 + \left(\frac{dv}{ds}\right)^2 = 1.$$

Since the correspondence between s and η is not ordinarily known, the coefficients A_l in this case cannot be found directly in closed form, but some version of a method of successive approximations can be used.

Finally, there may be cases like that discussed in Section 4a in which the boundary shape is not known in advance but must be determined as part of the solution. In this case, an iterative procedure like that adopted in Section 4a is appropriate.

Whatever method (numerical or analytical) is used to construct the mapping, the equations of the problem of interest, which are to be solved on the mapped domain, may still be solvable by separation of variables, provided $f(\xi, \eta)$ is of some classical form. This curious possibility of using classical analytical methods of solution, devised for some very special coordinate systems, in the case of a much more general orthogonal mapping is due to the fact that the form of the governing equations depends mainly (for the Laplace equation entirely) on the distortion function.

These analytical approaches are worth exploring in more detail than is done here. On the other hand, as Section 5 will show, in many cases it may be advantageous to use a distortion function which is not limited by the requirement of being of some classical form.

5. ORTHOGONAL MAPPING WITH A PRESCRIBED BOUNDARY CORRESPONDENCE (the Weak Constraint Method)

The strong constraint method, considered so far, could also be used, at least in principle, for problems of type (2) when the shape of the domain (but not the complete boundary correspondence) is prescribed from the beginning. In this case,

one might start from some initial approximation to the desired boundary shape and proceed iteratively by using the distance between the desired boundary and the numerical approximation to that boundary (measured along the direction normal to the current boundary) as a driving "normal force" for moving the boundary in or out. In practice, however, a much more powerful technique can be devised for dealing both with this problem, and the apparently more difficult one in which the complete boundary correspondence (i.e., the boundary shape and the spacing of coordinate nodes along the boundary) is specified. This is the topic of the present section.

Let us then consider the generation of an orthogonal mapping with a prescribed boundary correspondence. It has often been suggested that such a mapping is impossible (see, for example, Thompson et al. [1, p. 300]). Indeed, in the case of conformal mapping it is not possible to achieve a prescribed boundary correspondence, and this is crucial in limiting the application of conformal mapping to problems of practical importance.

It would be very beneficial in a number of applications to be able to construct an orthogonal mapping with a prescribed distribution of grid points along a boundary of given shape. Indeed, in the case of a boundary separating two domains of solution (e.g., the surface of a liquid drop), this ability is imperative in order that the normal coordinate lines on the two sides emanate from the same boundary points (otherwise, application of matching conditions is greatly complicated).

It may seem, at first, that the present approach could not be any more successful than conformal mapping as far as the determination of a mapping with prescribed boundary correspondence is concerned. Indeed, a complete prescription of boundary shape and mesh spacing along a boundary requires the imposition of Dirichlet boundary conditions for both functions $x(\xi, \eta)$ and $y(\xi, \eta)$ on the boundaries of the ξ, η domain—and this is clearly impossible with $f(\xi, \eta)$ specified (as discussed in Section 4a). However, we will see that the present approach does allow orthogonal mappings with prescribed boundary correspondence, provided one imposes what we shall call a "weak constraint" on $f(\xi, \eta)$, rather than specifying $f(\xi, \eta)$ completely throughout the whole ξ, η domain.

We have noted in Section 2 that two degrees of freedom exist in defining a mapping in two dimensions. In the method of the preceding section, these were used to impose the orthogonality condition $g_{12} = 0$, and to specify the distortion function, $f(\xi, \eta) \equiv h_{\eta}/h_{\xi}$, throughout the domain of ξ and η . It will be convenient to refer to contraints specified throughout ξ and η as utilizing a "domain degree of freedom," and call these "strong constraints." Evidently, in this terminology, a mapping in two dimensions allows imposition of two (and only two) strong constraints, and the imposition of an added "boundary constraint," in the form of a prescribed boundary correspondence, will cause the mapping to be over-determined unless one of the domain constraints, for g_{12} or f, is relaxed. The basic idea proposed here is to maintain orthogonality, i.e., $g_{12} = 0$, while giving up a part of the freedom to specify $f(\xi, \eta)$ everywhere in return for the ability to specify both $x(\xi, \eta)$ and $y(\xi, \eta)$ on the boundary of the ξ , η domain. In other words, we propose to relinquish a "part" of the "domain degree of freedom," available to specify f, in order to gain a "boundary

degree of freedom" for $x(\xi,\eta)$ (or $y(\xi,\eta)$) while still retaining the orthogonality condition $g_{12}=0$. Instead of prescribing the function $f(\xi,\eta)$ explicitly throughout the domain, we give a rule which determines f in the interior of the ξ , η domain as soon as it is known on the boundary. The boundary values of f are found using the definition of $f(\equiv h_{\eta}/h_{\ell})$, and formulas (4) to obtain h_{ℓ} and h_{η} from the mapping functions $x(\xi,\eta)$ and $y(\xi,\eta)$. The latter are obtained, in principle, by solving Eqs. (3) subject (for prescribed boundary correspondence) to Dirichlet conditions on the boundaries of the ξ , η domain. It is evident, since the governing Equations (3) for x and y involve f, that the boundary values for f (which are used to determine f in the interior) and the mapping functions $x(\xi,\eta)$ and $y(\xi,\eta)$ must be determined sequentially in a successive approximation scheme, starting from some initial guess for f. The exact manner in which this scheme is implemented will be discussed shortly. As a preliminary, however, it is useful to consider some additional factors that are intended to clarify the fundamental ideas behind the approach proposed here to obtain orthogonal mappings with a prescribed boundary correspondence.

First, the rule to determine f from its boundary values is essentially arbitrary, subject to the condition that f > 0. It may thus take the form of an algebraic ("interpolation") formula, or, for example, an elliptic differential equation which can be solved to determine f from its values on the boundary. For convenience, we denote this type of condition on f as a weak constraint to distinguish it from the strong constraint in which f is given explicitly throughout the domain. It is obvious that a weak constraint together with the values of f on the boundary is exactly equivalent to some strong constraint, and we have seen that a strong constraint on f is enough, together with the condition $g_{12} = 0$, to determine an orthogonal mapping in two dimensions. The available domain degree of freedom may thus be used either to impose a strong constraint on f (as in the previous section), or to impose a weak constraint together with values of f along the boundary. Heuristically, the second approach divides a domain degree of freedom into two "parts": the "interior degree of freedom" (used by a weak constraint) and the "boundary degree of freedom."

The key idea of the present development is to use a weak distortion constraint instead of a strong one, and to leave the values of f along the boundary unspecified, i.e., to let these values be determined by the mapping itself. The hope is that in this case one will be able to prescribe the boundary correspondence, since the boundary degree of freedom, available for the distortion constraint, is not used.

Let us now discuss how the method is to be applied. As we have noted, the problem of determining $x(\xi, \eta)$ and $y(\xi, \eta)$ is rather unusual in the sense that the coefficients of the governing partial differential Eqs. (3) depend via $f(\xi, \eta)$ on the coupling between the solutions $x(\xi, \eta)$ and $y(\xi, \eta)$. The problem is thus nonlinear and must be solved by some iterative procedure. Although this might seem a disadvantage in comparison with the strong constraint method of the previous section, this is not necessarily true since the latter also requires iteration (on boundary conditions) and it is not obvious which iteration will converge most rapidly. At any rate, this nonlinearity is a small price to pay for the ability to construct an orthogonal mapping with a prescribed boundary correspondence.

The iterative procedure mentioned above may be realized as follows:

- (1) Choose an initial guess for $x(\xi, \eta)$, $y(\xi, \eta)$, thus obtaining an initial guess for $f(\xi, \eta)$ via its definition and expressions for scale factors (4). It is preferable, but probably not absolutely necessary, that the initial $f(\xi, \eta)$ satisfy the chosen weak constraint, i.e., the chosen rule for determining f from its boundary values.
- (2) Using this $f(\xi, \eta)$ and the Dirichlet boundary conditions for $x(\xi, \eta)$, $y(\xi, \eta)$ known from the prescribed boundary correspondence, calculate new $x(\xi, \eta)$, $y(\xi, \eta)$ from the basic Eqs. (3); if some iterative scheme is used to solve (3), it will be sufficient to advance the solution by only a few (or even one) iterations.
 - (3) Calculate new scale factors on the boundary from $x(\xi, \eta)$, $y(\xi, \eta)$ using (4).
- (4) Use the weak contraint and the new boundary values for $f(\xi, \eta)$, calculated from the scale factors of step (3), to find new $f(\xi, \eta)$ in the interior of the domain.
 - (5) Go to step (2) and repeat.

This algorithm appears to work fairly well. It has been tried with two types of weak distortion constraints (rules)—algebraic "interpolation" and an elliptic partial differential equation (EPDE). The weak constraint may apparently be chosen quite arbitrarily, but it should give $f(\xi, \eta)$ which is nonnegative and, preferably, smooth. Since the freedom to prescribe the boundary correspondence already gives a considerable degree of control over the spacing of coordinate lines near the boundaries (which is usually the most important area), the weak constraint can often be chosen as a rule which determines the values of $f(\xi, \eta)$ in the interior of a domain as some kind of simple interpolation between its boundary values.

To obtain interpolation by EPDE, $f(\xi, \eta)$ is defined as a solution of some EPDE with Dirichlet boundary conditions. The EPDE may, for example, be the ordinary Laplace equation $(\partial^2 f/\partial \xi^2) + (\partial^2 f/\partial \eta^2) = 0$, and the motivation for this approach is the fact that a linear interpolation in 1-D can be thought of as defined by the differential equation $d^2 f/d\xi^2 = 0$. It is, of course, known that the solution of the ordinary Laplace equation provides a means of (local) averaging throughout the domain.

Although this EPDE approach appears quite sophisticated, experience obtained in the course of the present study indicates that the simpler, algebraic, approach is often to be preferred, and this will now be described in more detail.

To obtain a convenient formula for an algebraic interpolation, consider first the case when the given boundary values of $f(\xi, \eta)$ are zero in all four corners of the $0 \le \xi$, $\eta \le 1$ domain. Then the formula

$$f^{0}(\xi,\eta) = (1-\xi)f(0,\eta) + \xi f(1,\eta) + (1-\eta)f(\xi,0) + \eta f(\xi,1)$$

gives a suitable, smooth interpolation. If the corner values are not zero, however, this formula is not suitable, since each corner value appears in it twice, giving a spurious

contribution. To obtain a useful interpolation formula in this case, we need to subtract a bilinear "corner function"

$$f^{c}(\xi, \eta) = (1 - \xi)(1 - \eta) f(0, 0) + (1 - \xi) \eta f(0, 1) + \xi(1 - \eta) f(1, 0) + \xi \eta f(1, 1).$$

The final formula for an algebraic interpolation thus reads⁵

$$f^{a}(\xi, \eta) = f^{0}(\xi, \eta) - f^{c}(\xi, \eta).$$
 (15)

This algebraic interpolation is very easy to apply both as a weak constraint for a distortion function $f(\xi, \eta)$ and as an intial guess for $x(\xi, \eta)$ and $y(\xi, \eta)$ (if a better guess is not available). We note in passing that if orthogonality of the boundary-fitted coordinates is not required (as in the method of Thompson *et al.* (see Section 1)), a direct algebraic interpolation for $x(\xi, \eta)$, $y(\xi, \eta)$ provides the simplest possible way to construct a complete coordinate system with prescribed boundary correspondence.

It should be borne in mind that one has almost complete freedom in choosing the weak constraint rule, and the above suggestions are simply examples. In particular, some control over the spacing of the coordinate lines can obviously be achieved by the form chosen for the weak constraint, in addition to the strong control obtained by prescribing the boundary correspondence. The only limitation is that $f(\xi, \eta)$ must be greater than zero inside the domain. In some cases, this will follow automatically from the fact that $f(\xi, \eta) > 0$ at the boundaries (where it is calculated as a ratio of two positive quantities: the scale factors). In other cases, the condition $f(\xi, \eta) > 0$ inside the domain may be quite simply satisfied by adding some function of ξ and η to (15), which vanishes at the boundaries; the same function can also be efficiently used for control of the coordinate mesh. Other possibilities are conceived easily, but the details of choosing the weak constraint rule are much better discussed in the context of a particular application and we will not deal with them further here.

Let us finally consider numerical examples of the weak constraint method. These examples were obtained using an ADI technique to solve Eqs. (3) and algebraic interpolation (15) as an initial guess for $x(\xi, \eta)$, $y(\xi, \eta)$. The number of iterations needed was of the same order (50–100) as required by the strong constraint method of Section 4. The "peanut" shape, shown in Fig. 5, was obtained by simply specifying arbitrarily chosen values of x and y (i.e., prescribing the boundary correspondence) at $\xi = 1$, $\eta = 0$, and $\eta = 1$; plus the boundary conditions $y(0, \eta) = 0$ and $\frac{\partial x}{\partial \xi}|_{\xi=0} = 0$ at the boundary $\xi = 0$ (which in this case corresponds to a segment of the x axis). This last pair satisfies orthogonality conditions (9) for any $f(0, \eta)$ which means that

⁵ We are indebted to one of the referees for pointing out the existence of an elaborate mathematical framework [22] for constructing expressions of this type. In mathematical terminology, Eq. (15) is a "bivariate interpolation by a Boolean sum of projection operators" $P_l \oplus P_n \equiv P_l + P_n - P_l P_n$, where the projection operator P_l has been defined in our case as $P_l f(\xi, \eta) \equiv (1 - \xi) f(0, \eta) + \xi f(1, \eta)$, i.e., P_l and P_n realize linear interpolations in 1-D. Obviously, much more sophisticated interpolation formulae can be obtained by using more complicated forms for P_l and P_n .

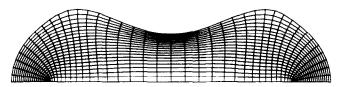


Fig. 5. "Peanut" shape obtained by the weak constraint method (only every second of the η -coordinate lines are drawn).

at this part of the boundary (only) the value of $f(\xi, \eta)$ needs to be given; it was chosen as $f(0, \eta) = 4 \sin^2 \pi \eta$. The algebraic interpolation (15) served then as a weak constraint on the distortion function $f(\xi, \eta)$. Note that in order to make the picture legible, only every second of the η -coordinate lines were drawn.

The mapping shown in Fig. 6 gives a coordinate system in the interior of the axisymmetric bubble, deformed by the flow. The distribution of the coordinate nodes at the surface of the bubble (i.e., the boundary correspondence $x(1, \eta)$, $y(1, \eta)$ at the boundary $\xi = 1$) was taken from the mapping of the exterior of the bubble (see Fig. 4) which was obtained previously as a part of the solution of the fluid mechanical problem using the strong constraint method. The boundary conditions for $x(\xi, \eta)$ and $y(\xi, \eta)$ at $\xi = 0$, $\eta = 0$, and $\eta = 1$ were assumed to be the same as in Section 4a (see (7) and (8)) and hence, they too satisfy (9) for any distortion $f(\xi, \eta)$. Thus, $f(\xi, \eta)$ must be specified independently at $\xi = 0$, $\eta = 0$, and $\eta = 1$. If $\xi = 0$ is to be a concentration point of the coordinate system, then $f(0, \eta)$ should be equal to zero, and if $f(\xi, 0)$ and $f(\xi, 1)$ are taken to be linear functions of ξ , one obtains the simplest possible variety of the algebraic weak constraint

$$f(\xi, \eta) = \xi f(1, \eta),$$

which was, in fact, used to construct the mapping in Fig. 6.

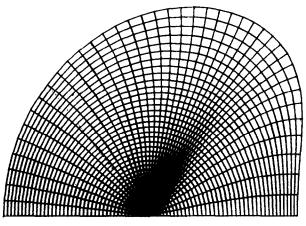


FIG. 6. Interior of the deformed bubble obtained by the weak constraint method with the distribution of the points at the surface taken from the exterior mapping (Fig. 4).

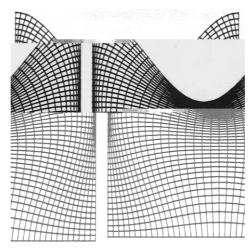


FIG. 7. Orthogonal mapping by the weak constraint method with prescribed boundary correspondence on all four boundaries and algebraic interpolation (15) used as the weak constraint.

In the last two examples, shown in Figs. 7 and 8, we consider mapping in a concave region whose shape is similar to a domain in which the recent method of Haussling and Coleman [8] failed to produce an orthogonal grid even for shapes with smaller boundary curvature. It is important to note that the boundary correspondence in Figs. 7 and 8 was prescribed on all four boundaries. The mapping in Fig. 7 was computed with the weak constraint given by (15). The mapping in Fig. 8 was obtained using (15) multiplied by $(1-0.8 \sin \pi \xi \sin \pi \eta)$ as the weak constraint. Comparing Figs. 7 and 8, it can be seen that the form chosen for the weak constraint does provide a degree of control over the spacing of the coordinate grid inside the domain; however, the main features of the mapping are determined by the prescribed boundary correspondence. Though the numerical examples that we have considered show that an orthogonal mapping can be computed with a prescribed boundary correspondence for reasonably complicated geometries, they do not, of course, prove either the existence or uniqueness of such mappings for arbitrary geometries and/or boundary correspondence. This is a very important and interesting question, but one that is far beyond the scope of the present study and probably requires the attention of theoretical mathematicians.

A final important point about the weak constraint method concerns the prescription of the boundary correspondence. Apart from the difficult question of the existence of a mapping, some care must also be exercised to minimize the possibility of the resulting coordinates being ill-suited for numerical solutions. Consider, for example, the problem of generating orthogonal coordinates inside an acute angle with coordinate nodes distributed in equal increments along the sides. Evidently, orthogonal coordinates can be generated quite easily if these nodes are connected by one family of coordinate lines, with the other family emanating from the vertex (thus giving, essentially, polar coordinates inside the angle). However, if it were assumed

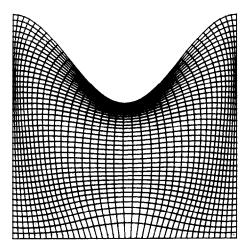


Fig. 8. Same as Fig. 7 but the weak constraint is now (15) multiplied by $(1-0.8 \sin \pi \xi \sin \pi \eta)$.

that the side boundary nodes belonged to different families of coordinate lines (as might initially seem to be the obvious choice if one were to think of the acute angle as being obtained starting from a right angle with Cartesian coordinates inside it and simply decreasing the included angle), the configuration of the corresponding coordinates is less obvious and the numerically generated coordinates would likely have a larger nonorthogonality error due to discretization.

6. Conclusions

The mapping techniques proposed in this paper provide a method for the construction of an orthogonal, boundary-fitted coordinate system in two dimensions. The strong constraint method of orthogonal mapping is obtained by specifying $f(\xi, \eta)$ throughout the ξ, η domain in advance and is especially suitable for cases when the shape of the boundary in the x, y plane is not known but is to be found as a part of the solution of some physical problem ("free boundary problems"). The weak constraint method of orthogonal mapping is obtained by specifying a rule which determines the values of $f(\xi, \eta)$ in the interior of the ξ, η domain as soon as its boundary values are known. This method is capable of solving the most important and difficult problem, namely, the contruction of an orthogonal mapping with a prescribed boundary correspondence, or, in other words, the construction of an orthogonal coordinate system fitted to a boundary of given shape, with a prescribed distribution of coordinate nodes along this boundary.

The governing equations of any physical problem of interest can be written out easily in the resulting orthogonal coordinate system in terms of *physical* components of vectors and tensors, using the standard expressions for invariant differential operations in orthogonal coordinates. Alternatively, the technique of tensor analysis can be employed directly for this purpose if the connection coefficients in the

orthonormal basis and a "physical tensor" notation (given in the Appendices) are used.

The most serious rival of the present method is, of course, conformal mapping. The main advantage of conformal mapping is that a harmonic function of the x, y coordinates remains a harmonic function of the ξ , η coordinates. This reduces the solution of the Laplace equation on some domain in the x, y plane to a problem of finding the conformal mapping for this domain. However, this reduction is not of much help unless a conformal mapping function has already been tabulated; moreover, the solution of the Laplace equation, though significant, is certainly not the only important problem to be solved.

The important drawbacks of conformal mapping include the difficulty of construction by the direct approach, closely connected with the inability to prescribe the boundary correspondence, and the potentially poor quality of the resulting grid for numerical solutions. The method proposed here for orthogonal mapping is free of these problems. In addition, it has the potential of extension to a three-dimensional space.

APPENDIX A: Connection Coefficients in Orthonormal Basis

In order to use the orthogonal mapping techniques which are presented in the main body of this paper, it is necessary to express the governing differential equations and boundary conditions of a physical problem, which are normally given in terms of the invariant differential operators for vectors and/or tensors, in terms of a general orthogonal coordinate system. In most instances this can be done by simply using the standard expressions for the various invariant differential operations in orthogonal curvilinear coordinates which are given in numerous texts and require only a knowledge of the scale factors h_i . However, expressions for some differential operations are not readily accessible, and it is necessary, in general, to have a method available for their derivation from the invariant (tensorial) form. The most commonly advocated approach is to use the expression for the ∇ operator, together with the expressions for the spatial derivatives of the unit basis vectors. This is a rather cumbersome and outdated procedure in comparison with the powerful technique of tensor analysis; the trouble is, however, that the connection coefficients, which are necessary for covariant differentiation, are usually given only for a coordinate basis (whose vectors $\mathbf{e}_i \equiv \partial \mathbf{r}/\partial \xi^i$ are not generally of unit length). In this case (only) they are called "Christoffel symbols." Correspondingly, covariant differentiation can usually be performed only for covariant and contravariant components of vectors and tensors.

In the case of an orthogonal coordinate system, it is highly preferable to use an orthonormal basis (whose basis vectors $\mathbf{e}_i \equiv \mathbf{e}_i/h_i$ are of unit length) and physical components of the vectors and/or tensors. In this case, we need only the normal rules for covariant differentiation and the connection coefficients for an orthonormal basis. These connection coefficients are derived easily, following the methods of [14] (see,

in particular, Chap. 8), but we do not intend to spell out the details here. Instead, we simply state the results, first using the standard notation of tensor analysis. In Appendix B, a much simplified notation is introduced for "physical tensors," which is a natural and obvious extension of the Cartesian tensor formalism.

We use the gradient of a second rank tensor, say

$$G \equiv \nabla T$$

as a suitable invariant object (a third rank tensor) for illustration purposes. This entity can be expressed for any particular coordinate system in terms of its components calculated in any basis according to the rules of covariant (absolute) differentiation (denoted by the semicolon ";")

$$G_{ik}^i \equiv T_{j,k}^l = T_{j,k}^i + \Gamma_{lk}^i T_j^l - \Gamma_{jk}^l T_l^i,$$

where indices run through 1, 2, 3 and summation over repeated indices is implied. The connection coefficients are denoted Γ_{np}^m , and the comma "," indicates differentiation of the tensor component as if it were a scalar (for example, $f_{,k}$ indicates the kth component of the gradient of a scalar field f). It should be noted that this "scalar differentiation" coincides with partial differentiation $\partial/\partial \xi^k$ only in a coordinate basis; in the orthonormal basis it is given by

$$f_{,\hat{i}} \equiv \mathbf{e}_{\hat{i}} \cdot \nabla f = \frac{1}{h_i} \frac{\partial f}{\partial \xi^i}.$$
 (A1)

Scale factors h_i , being a shorthand notation for $(g_{ii})^{1/2}$, are exempt from the summation convention. Carets are employed to indicate the use of an orthonormal basis.

Now, in a general three-dimensional space, there are 27 connection coefficients. However, in an orthonormal basis, only 12 are nonzero, and these can be expressed in the compact form

$$\Gamma_{\hat{n}\hat{m}}^{\hat{m}} = -\Gamma_{\hat{n}\hat{m}}^{\hat{n}} = h_{m,\hat{n}}/h_m \qquad (m \neq n, \text{ no summation}).$$
 (A2)

The general rule for covariant differentiation, together with formulas (A1) and (A2) are all that is needed to write any differential expression in terms of physical components in a general orthogonal coordinate system.

APPENDIX B: A SIMPLIFIED "PHYSICAL TENSOR" NOTATION FOR COVARIANT DIFFERENTIATION IN ORTHOGONAL COORDINATES

An orthonormal basis (with a positive definite metric) is identical with its dual (reciprocal), so that covariant and contravariant components coincide (and are called "physical") and the usual distincton between these quantities, by the use of upper and lower indices, becomes unnecessary. In other words, the metric tensor of an

orthonormal basis is always a unit tensor, i.e., $g_{ij} = \delta_{ij}$. (This tensor should be distinguished, however, from the metric tensor of the coordinate basis g_{ij} , which is used in the main body of this paper and is often called "the metric tensor of the coordinate system" because it defines the line element.) Although an attempt has previously been made to formulate the rules of tensor calculus specifically for

notation is introduced which is a natural generalization of Cartesian tensor formalism. Since the physical components are by definition (see McConnell [24]) the components in the local Cartesian coordinate system, whose basis vectors coincide with the orthonormal basis vectors at a given point, the similarity between physical and Cartesian tensor analysis is not surprising.

The transition to a simplified notation for physical tensors from the general covariant formalism is accomplished by writing all indices of tensor or vector components as subscripts and switching to the convention of summation over repeated subscripts which is typical of Cartesian tensors. The carets, which indicated an orthonormal basis before, will be dropped since we deal with orthonormal bases only. All tensor algebra for physical tensors is formally identical to Cartesian tensor calculus, but the rules of differentiation are different. Specifically, the gradient of a tensor field $\mathbf{G} \equiv \nabla \mathbf{T}$ is calculated according to the following rule of covariant (meaning here "invariant") differentiation for physical tensors

$$G_{ii...nk} \equiv T_{ii...nk} = T_{ii...nk} + \Gamma_{iik}T_{ii...n} + \Gamma_{iik}T_{ii...n} + \cdots + \Gamma_{nlk}T_{ii...l},$$
 (B1)

where the comma "," denotes scalar differentiation defined by

$$f_{,k} = \frac{1}{h_{k}} \frac{\partial f}{\partial \xi_{k}} \tag{B2}$$

(as always, scale factors h_i are exempt from the summation convention). For a Cartesian coordinate system where

all
$$h_i = 1$$
, all $\Gamma = 0$

rule (B1) reduces to the familiar partial differentiation of Cartesian tensor calculus. Otherwise, one has to correct for the change of scale (thus (B2)) and for the variation of basis vectors in space (the " ΓT " terms in (B1), one for each index of T). To remember the pattern of these latter terms, the following mnemonic rule is useful: (1) The last index of Γ is always the differentiation index; (2) The index being corrected shifts to the first subscript on Γ and is replaced on T by a dummy summation index, identical to the middle index on Γ . The 12 nonzero connection coefficients can be taken directly from (A2),

$$\Gamma_{iji} = -\Gamma_{jii} = h_{i,j}/h_i \equiv \frac{1}{h_i h_i} \frac{\partial h_i}{\partial \xi_i}$$
 ($i \neq j$, no summation). (B3)

The basic rule of tensor analysis is that a tensorially correct equation (formula), which is true in a particular coordinate system (say, Cartesian), is true in any other coordinate system. It is thus evident that a physical law expressed in terms of the physical components for some arbitrary orthogonal system is formally identical to its component form for Cartesian tensors, provided only that ordinary partial derivatives with respect to coordinates are replaced by covariant derivatives, i.e., one simply has to substitute a semicolon for the symbol used to indicate partial differentiation in the Cartesian expression and then use (B1). This makes relatively complicated differential expressions very easy to calculate assuming a familiarity with the corresponding Cartesian tensor quantities. By way of illustration, we may consider the derivation of formulae for the physical components of the rate-of-strain tensor in a general orthogonal coordinate system. A diagonal component, such as e_{11} , is simply

$$e_{11} \equiv u_{1;1} = u_{1,1} + \Gamma_{1l1} u_l = \frac{1}{h_1} \frac{\partial u_1}{\partial \xi_1} + \frac{u_2}{h_1 h_2} \frac{\partial h_1}{\partial \xi_2} + \frac{u_3}{h_1 h_3} \frac{\partial h_1}{\partial \xi_3}$$

while the off-diagonal (2, 3) component is

$$\begin{split} e_{23} &\equiv \frac{1}{2}(u_{2;3} + u_{3;2}) = \frac{1}{2}(u_{2,3} + \Gamma_{2l3}u_l + u_{3,2} + \Gamma_{3l2}u_l) \\ &= \frac{1}{2} \left(\frac{1}{h_3} \frac{\partial u_2}{\partial \xi_3} - \frac{u_3}{h_2 h_3} \frac{\partial h_3}{\partial \xi_2} + \frac{1}{h_2} \frac{\partial u_3}{\partial \xi_2} - \frac{u_2}{h_2 h_3} \frac{\partial h_2}{\partial \xi_3} \right). \end{split}$$

Although these formulas are identical to those derived by direct differentiation of the basis vectors (see, e.g., [25, p. 600]), they are obviously much easier to obtain using the physical tensor notation.

So far we have been dealing with general orthogonal coordinates in 3-D. However, the orthogonal coordinate system used in practice is most likely to be axisymmetric or two dimensional, in which cases even fewer connection coefficients remain nonzero. Consider first the axisymmetric case, with $\xi_3 \equiv \varphi$ being the azimuthal angle. In this case, $h_3 = \sigma$, where σ is the distance between the point of interest and the symmetry axis, and only eight connection coefficients remain nonzero

$$\begin{split} &\Gamma_{121} = -\Gamma_{211} = h_{1,2}/h_1 \equiv \frac{1}{h_1 h_2} \frac{\partial h_1}{\partial \xi_2}, \qquad \Gamma_{212} = -\Gamma_{122} = h_{2,1}/h_2 \equiv \frac{1}{h_2 h_1} \frac{\partial h_2}{\partial \xi_1}, \\ &\Gamma_{313} = -\Gamma_{133} = \sigma_{,1}/\sigma \quad \equiv \frac{1}{\sigma h_1} \frac{\partial \sigma}{\partial \xi_1}, \qquad \Gamma_{323} = -\Gamma_{233} = \sigma_{,2}/\sigma \quad \equiv \frac{1}{\sigma h_2} \frac{\partial \sigma}{\partial \xi_2}. \end{split} \tag{B4}$$

In the two-dimensional case with $\xi_3 = z$ and $h_3 = 1$, only Γ_{121} , Γ_{211} , Γ_{212} , and Γ_{122} remain nonzero.

The formalism presented above provides an easy method for writing any differential expression in terms of physical components for the boundary-fitted orthogonal coordinates (ξ, η, φ) whose construction we have discussed in the main body of the paper. A final quantity of interest, relevant to the boundary conditions in

some problems, is the boundary curvature. The geometric definition of the connection coefficients for the orthonormal basis (see [14, Chap. 8]) is

 $\Gamma_{ijk} \equiv (i \text{ component of the rate of change in } \mathbf{e}_i \text{ along } \mathbf{e}_k).$

Thus, it is evident that

$$\Gamma_{ijj} = \kappa_{(g)}^{(ij)}, \qquad \Gamma_{kij} = \kappa_{(g)}^{(ij)},$$

where $\kappa_{(n)}^{(ij)}$ is the normal curvature in the direction \mathbf{e}_j of the coordinate surface with normal \mathbf{e}_i and $\kappa_{(g)}^{(ij)}$ is the geodesic curvature of the ξ_j coordinate line on the same surface (note, there is a slight difference here from the classical definition of geodesic curvature which usually takes it to be always positive; see [15, 24]).

If one considers the ξ_j coordinate line as a curve on the coordinate surface $\xi_k = \text{const}$, the geometrical meaning of Γ_{ijj} and Γ_{kjj} is reversed, i.e.,

$$\Gamma_{ijj} = -\kappa_{(g)}^{(kj)}, \qquad \Gamma_{kjj} = \kappa_{(n)}^{(kj)}.$$

The half-sum of the normal curvatures in two perpendicular directions [say, $\kappa_{(n)}^{(ij)}$ and $\kappa_{(n)}^{(ik)}$] gives the mean curvature of the surface; and since the coordinate lines of an orthogonal coordinate system are also the lines of curvature of a coordinate surface ([15, p. 195]), these normal curvatures are also the principal curvatures and hence their product gives the Gaussian (intrinsic) curvature of the surface.

ACKNOWLEDGMENTS

This work was supported by a grant from the National Science Foundation. The authors wish to thank J. R. A. Pearson and P. R. Eiseman for valuable comments on an earlier draft of this paper.

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