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The Construction of Discrete Orthogonal Coordinates

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An orthogonalization procedure for the transformation of finite nonorthogonal coordinates to an equivalent finite set of orthogonal coordinates is described. The procedure involves the direct solution of a series of 'exact' matrix equations and is independent of the amount of shear or nonorthogonality of the original coordinates. The method may be applied to the solution of complex boundary value problems and generally at each timestep to the Lagrangian solution of multidimensional initial value problems.

1. INTRODUCTION

The use of generalized orthogonal coordinates in differential analysis has been of widespread importance. In simulations on the computer, however, their application has been very limited, mainly because the problem of mapping one orthogonal space to another is a difficult partially unsolved and nonlinear problem. This paper describes an "exact" method of constructing generalized discrete orthogonal coordinates, suitable for use in digital computation.

A common example of the need for such orthogonal coordinates occurs in the Lagrangian representation of fluid and magneto-fluid flows. In one space-dimension, a point Lagrangian method is frequently used with success [9, 12]. The extension of such a point Lagrangian method to two- or three-dimensional problems has on the whole been unsuccessful, since sheared flow rapidly induces a nonorthogonal, distorted and complex mesh, on which the physical equations of interest are difficult to represent accurately. Hirt and Amsden [8] have suggested an inexact prescription which tends to drive the mesh towards orthogonality.

These difficulties arise since the concept of a point Lagrangian method, appropriate in one space-dimension, does not extend to two or more space-dimensions. Rather than defining a set of Lagrangian points in two dimensions, it is appropriate to define a contour along which a state variable of interest, f, does not alter. Thus, advection, or Lagrangian motion along the contour of f, does not alter f and the contour need only be advected or moved in a Lagrangian manner perpendicular to the contour. The advantages of an orthogonal mesh may therefore be obtained, provided that, at each timestep, we may construct the lines orthogonal to the contours. In three dimensions we may define Lagrangian surfaces.

Elsewhere, orthogonal coordinates are important in many boundary-value problems and in simulations where the mesh needs to be related to complex boundaries [7].

We may define the mapping problem in two dimensions as follows. Let x and y be orthogonal coordinates in the domain R, so that the set of points $\mathbf{r} = (x, y)$ define what we shall call the "real" or laboratory space. Let μ and j be non-orthogonal coordinates defined in the domain Γ. We shall assume that there is a one-to-one correspondence between R and Γ, such that for each point $\rho = (\mu, j)$ in Γ, there exists a unique point $\mathbf{r} = \mathbf{r}(\mu, j)$ in R. Then, given $\mathbf{r} = \mathbf{r}(\mu, j)$, we are required to determine $\mathbf{r} = \mathbf{r}(i, j)$ where i and j are orthogonal coordinates. The set of points $\mathbf{l} = (i, j)$ in the domain L defines what we shall call the "logical" or natural space.

Given boundary conditions on the surface S of R, the problem is uniquely defined. In particular, we shall consider the "closed" problem in which the boundary S corresponds to the line $j = 1$. The boundary conditions then specify,

$$\mathbf{r}^S = \mathbf{r}(i, 1), \tag{1}$$

for all i. For this case, the two orthogonal spaces R and L are represented schematically in Figs. (1) and (2).

We shall here devise an orthogonalization procedure whereby, given any set of nonorthogonal coordinates, the corresponding orthogonal coordinates may always be constructed. In Section 2, the equations for orthogonal coordinates are discussed

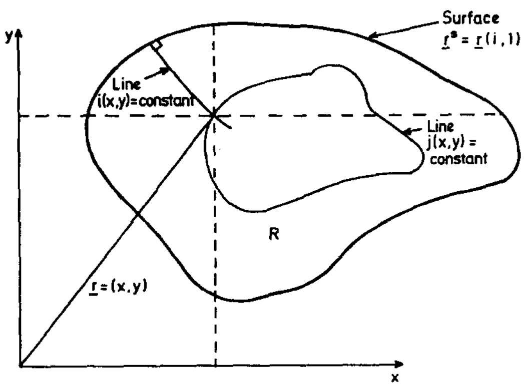


FIG. 1. The 'real' space R. The region of interest is bounded by $\mathbf{r}^S$. Constant values of the functions i and j map out orthogonal lines.

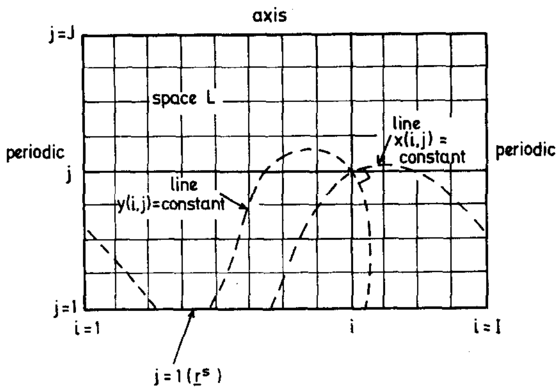


FIG. 2. The 'logical' space L. The line $j = 1$ corresponds to the boundary $\mathbf{r}^S$ on R. The boundaries at $i = 1$ and $i = I$ are periodic.

in the differential case and it is shown that the above specification uniquely defines a set of orthogonal coordinates, which are in principle readily soluble. Unlike the differential case, only a finite set of points in R are defined in the mesh problem and the meaning of orthogonality needs to be considered. In Section 4, matrix equations which relate the positions of i-points on each pair of j lines are obtained and the exact method of solution is outlined. The procedure is summarized in Section 5 and a number of illustrative solutions using the method are shown in Section 6.

2. ORTHOGONALITY IN THE CONTINUOUS DOMAIN

We shall consider the (i, j) lines in the domain R (Fig. 3):

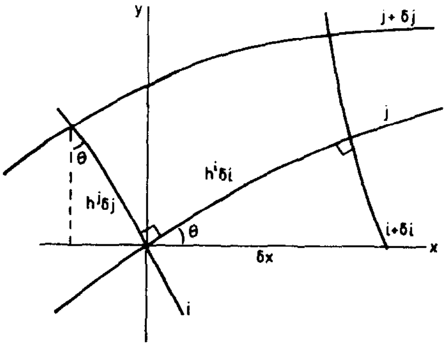
$$i = i(x, y); \qquad j = j(x, y). \tag{2}$$

If i and j are to be orthogonal, the functions i and j must satisfy (Fig. 3),

$$\begin{aligned} (\partial i/\partial x)_y &= \cos\theta/h^i, & (\partial j/\partial x)_y &= -\sin\theta/h^j, \\ (\partial i/\partial y)_x &= \sin\theta/h^i, & (\partial j/\partial y)_x &= \cos\theta/h^j \end{aligned} \tag{3}$$

where $\theta = \theta(x, y)$ is the angle between the unit vectors $\mathbf{e}_i$ and $\mathbf{e}_x$ in R. h^i and h^j are the usual scale factors defined by

$$d\mathbf{r}^2 = (h^i\, di)^2 + (h^j\, dj)^2$$



$$h^i \frac{\partial i}{\partial x} = \cos\theta \qquad h^j \frac{\partial j}{\partial x} = -\sin\theta$$

$$h^i \frac{\partial i}{\partial y} = \sin\theta \qquad h^j \frac{\partial j}{\partial y} = \cos\theta$$

FIG. 3. Lines of constant i and constant j orthogonal in R.

or, according to Eqs. (3),

$$\begin{aligned} 1/(h^i)^2 &= (\partial i/\partial x)^2 + (\partial i/\partial y)^2, \\ 1/(h^j)^2 &= (\partial j/\partial x)^2 + (\partial j/\partial y)^2. \end{aligned} \tag{4}$$

By eliminating h^i in Eqs. (3), a first-order equation in $i(x, y)$ is obtained:

$$(\partial i/\partial x) - \cot\theta(\partial i/\partial y) = 0. \tag{5}$$

In the differential problem defined in Section 1, $\theta = \theta(x, y)$ is defined by the nonorthogonal coordinates $\mathbf{r} = \mathbf{r}(\mu, j)$. Since $i(x, y)$ is known on the bounding surface $\mathbf{r}^S$, an integration of Eq. (5) for each point i on $\mathbf{r}^S$ will trace out a contour of i, solving the mapping problem.

3. Discrete Orthogonal Coordinates

On a finite mesh, the function $\theta(x, y)$ is not known at all between the given finite set of contours j, while on the contour j it may only be approximated. We may eliminate θ in the orthogonal equations (3) to obtain two elliptic equations for the functions $i = i(x, y)$ and $j = j(x, y)$:

$$\frac{\partial}{\partial x}\left(\frac{h^i}{h^j}\frac{\partial i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{h^i}{h^j}\frac{\partial i}{\partial y}\right) = 0, \tag{6}$$

$$\frac{\partial}{\partial x}\left(\frac{h^j}{h^i}\frac{\partial j}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{h^j}{h^i}\frac{\partial j}{\partial y}\right) = 0. \tag{7}$$

These are nonlinear equations since h^i and h^j are functions of i and j. Barfield [2] has considered this problem and approximated the solution by linearizing the equations, assuming the function h^i/h^j is constant everywhere. In general, this assumption is not reasonable, particularly when applied to the whole mesh. Godunov and Prokopov [6] have used a similar technique, assuming an optimized constant value h^i/h^j.

To determine i and thus obtain the orthogonal coordinates, we wish to solve Eq. (6) between each pair of j lines in sequence. In general without prescribing $\theta(x, y)$ or the functional form of h^i/h^j, Eqs. (6) and (4) admit of an infinite set of solutions. We shall therefore seek conditions on the function h^i/h^j which establish a unique and unambiguous correspondence between the i-points on each pair of j-lines. This may be achieved by demanding that no sources or sinks for i exist between each pair of j-lines.

The path of a constant i-line is found by following the *direction* of the vector ∇j. A vector of arbitrary magnitude in this direction is:

$$\mathbf{k} = \nabla q(j), \tag{8}$$

where $q(j)$ is any continuous function with continuous first and second derivatives. It follows that the sources σ of i-lines are defined by,

$$\nabla \cdot \mathbf{k} = \sigma.$$

Thus the condition for a unique correspondence between the i-points on each pair of j-lines is that the vector $\mathbf{k}$ be divergence free:

$$\nabla \cdot \{(dq/dj)\, \nabla j\} = 0,$$

or,

$$(dq/dj)\, \nabla^2 j + (d^2q/dj^2)(\nabla j)^2 = 0 \tag{9}$$

$\nabla^2 j$ and $|\nabla j|$ are defined by Eqs. (7) and (4):

$$\begin{aligned} \nabla^2 j &= (1/h^i h^j)(\partial/\partial j)(h^i/h^j), \\ |\nabla j| &= 1/h^j. \end{aligned} \tag{10}$$

Substituting these expressions into Eq. (9), we obtain:

$$\frac{dq}{dj} \frac{\partial}{\partial j} \left\{ \frac{h^i}{h^j} \right\} + \frac{d^2q}{dj^2} \frac{h^i}{h^j} = 0,$$

or,

$$\frac{\partial}{\partial j} \left\{ \frac{dq}{dj} \frac{h^i}{h^j} \right\} = 0, \tag{11}$$

which has the general solution:

$$(dq/dj)(h^i/h^j) = f(i).$$

Since q is a function only of j, h^i/h^j must have the functional form:

$$h^i/h^j = f(i)\,g(j). \tag{12}$$

This is the condition on h^i/h^j which we seek and which establishes a unique correspondence between the i-points on each pair of j-lines. An interpretation of the arbitrary function $g(j)$ is that it alters only the density or relative placement of the j-lines between j and $j+1$ without varying i.

It is therefore assumed that *between* each pair of j-lines (but not on the j-th line), h^i/h^j has the form of Eq. (12). It is to be noted that $f(i)$ and thus h^i/h^j changes discontinuously across each j line of the mesh. The form (Eq. (12)) for h^i/h^j is inserted in Eq. (6) for the function i:

$$\frac{\partial}{\partial x}\left\{f(i)\frac{\partial i}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{f(i)\frac{\partial i}{\partial y}\right\} = -\frac{f(i)}{g(j)}\cdot\frac{dg}{dj}\cdot\left\{\frac{\partial i}{\partial x}\frac{\partial j}{\partial x} + \frac{\partial i}{\partial y}\frac{\partial j}{\partial y}\right\}, \tag{13}$$

and using Eqs. (3) to eliminate the right-hand side:

$$\frac{\partial}{\partial x}\left\{f(i)\frac{\partial i}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{f(i)\frac{\partial i}{\partial y}\right\} = 0. \tag{14}$$

A similar equation in $j(x, y)$ and involving $g(j)$ is equally obtained. Thus, if the function $p = p(i)$ is defined:

$$f(i) = dp/di; \tag{15}$$

then, according to Eq. (14), p (and, equally, q) satisfies Laplace's equation:

$$\nabla^2 p = 0, \tag{16}$$

$$\nabla^2 q = 0. \tag{17}$$

Now h^i/h^j is a positive definite function (Eqs. 4). Along the line $j =$ constant, g is a constant, and from Eqs. (12) and (15),

$$dp/di = (h^i/h^j)/g. \tag{18}$$

If g is positive, it follows that along the line $j =$ const., p is a monotonically increasing function of i. If g is negative, p is a monotonically decreasing function of i. The form of the function p between each pair of j lines is drawn in Fig. (4). Thus for each value of i, there corresponds a unique value of p. It follows that if Laplace's equation (16) is solved for p between each pair of lines, for each point i

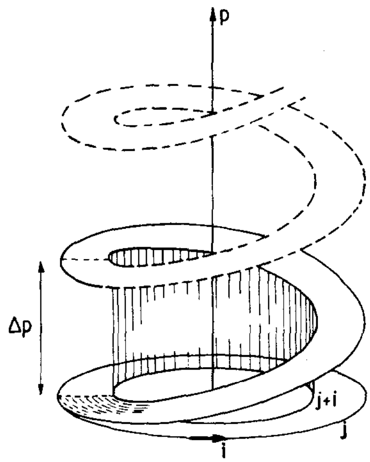


FIG. 4. Representation of the function $p(i)$ between the lines j and $j+1$. p is a monotonically increasing function of i, with period $\Delta p : p(i) = \Delta p\, \tilde{p}(i) + n\Delta p$, where n is an integer. For each value of i, there corresponds a *unique* value of $\tilde{p}$.

on j there corresponds a unique value p with which again the point i on the line $j+1$ may be associated. All the i points on the line $j+1$ may therefore be determined and the procedure continued to the next pair of j lines $j+1$ and $j+2$.

4. Orthogonalization by the Solution of a Sequence of Matrix Equations

According to the previous sections, we may orthogonalize the nonorthogonal mesh $\mathbf{r} = \mathbf{r}(\mu, j)$ by considering pairs of adjacent j lines (Fig. 5) in a sequence of $J-1$ operations. At the j-th step, the points i on j are known $\mathbf{r}(i, j)$ and the nonorthogonal points μ on $j+1$ are known $\mathbf{r}(\mu, j+1)$. We wish to determine $\mathbf{r}(i, j+1)$. Laplace's equation for $p = p(i)$ is to be satisfied in the space between j and $j+1$. The boundary conditions are of the Neumann type:

$$\partial p/\partial n = (1/h^j)\, \partial p/\partial j = 0, \tag{19}$$

where n is the direction normal to the boundaries on j and $j+1$. The region is not simply connected and a branch cut must be introduced.

Applying Green's theorem [4] for Laplace's equation (16) to a point on the contour C of a closed two-dimensional region, an integral equation for p is obtained:

$$p(\mathbf{r}) = -\frac{1}{\pi}\oint_C p \frac{\partial}{\partial n}\left\{\log \frac{1}{|\mathbf{r}-\mathbf{r}'|}\right\} dr' + \frac{1}{\pi}\oint_C \log\frac{1}{|\mathbf{r}-\mathbf{r}'|}\frac{\partial p}{\partial n}\, dr'. \tag{20}$$

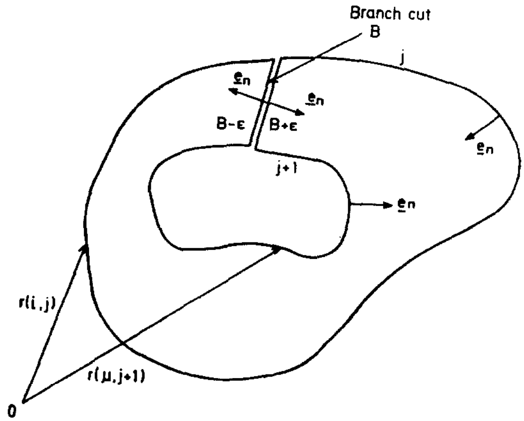
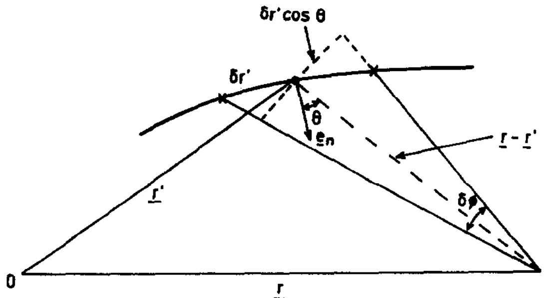


FIG. 5. Pairs of adjacent j lines are considered in sequence. The points specifying the line j lie on the orthogonal lines i. By solving Laplace's equation for $p(i)$ between j and $j + 1$, the i points on the line $j + 1$ can be identified. A branch cut B is introduced between j and $j + 1$ to obtain a simply connected region.

Using the boundary conditions (Eq. (19)), the second term on the right-hand side vanishes on the boundaries j and $j + 1$. Equally the contributions to the second term induced on each side of the branch cut B are exactly equal and opposite, no matter where the branch cut is taken:

$$\left.\frac{\partial p}{\partial n}\right|_{B+\epsilon} = -\left.\frac{\partial p}{\partial n}\right|_{B-\epsilon}, \tag{21}$$

when ϵ is vanishingly small. It is therefore only the first term on the right-hand side



$$\delta r' \; \underline{e}_n \cdot \underline{\nabla} \log \frac{1}{|\underline{r} - \underline{r}'|} = \frac{\delta r' \cos\theta}{|\underline{r} - \underline{r}'|}$$
$$= \delta\phi$$

FIG. 6. The angle subtended by the arc $\delta r'$ as observed by the point $\mathbf{r}$.

of Eq. (20) which remains. It is to be noted that the coefficient of p in this term may be written as a perfect differential:

$$\begin{aligned}(\partial/\partial n)\{\log(1/|\mathbf{r}-\mathbf{r}'|)\}\,\delta r' &= -\delta r' \cos\theta/|\mathbf{r}-\mathbf{r}'|,\\ &= -\delta\phi,\end{aligned} \tag{22}$$

where $\delta\phi$ is the angle, subtended by the arc $\delta r'$ from the point $\mathbf{r}$ (Fig. 6). Applying this notation to Eq. (20), we may determine p at the points i on the line j and p at the points μ (nonorthogonal) on the line $j+1$ according to the following equations (Fig. 7):

$$\begin{aligned}p(i,j) = {}& \frac{1}{\pi}\oint_j p(k,j)\,d\phi_{ki} + \frac{1}{\pi}\oint_{j+1} p(\nu, j+1)\,d\phi_{\nu i}\\ &+ \frac{1}{\pi}\int_{B+\epsilon} p(B)\,d\phi_{Bi} + \frac{1}{\pi}\int_{B-\epsilon} p(B)\,d\phi_{Bi}\,.\end{aligned} \tag{23}$$

$$\begin{aligned}p(\mu, j+1) = {}& \frac{1}{\pi}\oint_j p(k,j)\,d\phi_{k\mu} + \frac{1}{\pi}\oint_{j+1} p(\nu, j+1)\,d\phi_{\nu\mu}\\ &+ \frac{1}{\pi}\int_{B+\epsilon} p(B)\,d\phi_{B\mu} + \frac{1}{\pi}\int_{B-\epsilon} p(B)\,d\phi_{B\mu}\,.\end{aligned} \tag{24}$$

$d\phi_{ki}$ is the infinitesimal angle subtended by the boundary at the k-th point from the i-th point. On either side of the branch cut,

$$d\phi_{B+\epsilon,i} = -d\phi_{B-\epsilon,i}\,, \tag{25}$$

and

$$p(B+\epsilon) = p(B-\epsilon) + \Delta p, \tag{26}$$

where Δp is constant along any branch cut. It follows that the second two terms in Eq. (23), for example, reduce to:

$$\Delta p\,\frac{1}{\pi}\int_j^{j+1} d\phi_{Bi} = \Delta p\,\frac{\phi_{Bi}}{\pi}\,. \tag{27}$$

In finite form, the integral equations (23) and (24), applied to a finite set of points along the lines j and $j+1$, become matrix equations:

on line j:

$$p_i = \sum_{k=1}^{I} L_{ik} p_k + \sum_{\nu=1}^{I} M_{i\nu} p_\nu + \Delta p\, c_i\,, \tag{28}$$

on line $j+1$:

$$p_\mu = \sum_{k=1}^{I} M'_{\mu k} p_k + \sum_{\nu=1}^{I} L'_{\mu\nu} p_\nu + \Delta p\, c_\mu\,, \tag{29}$$

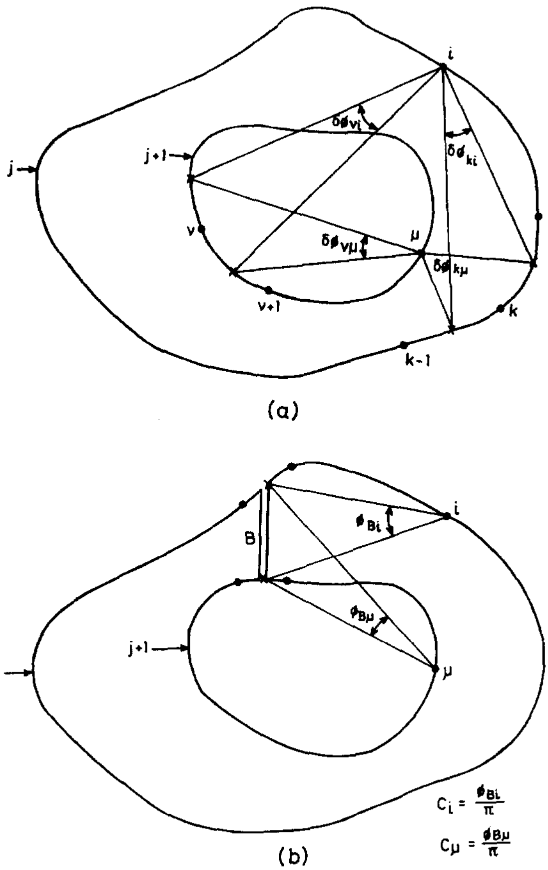


FIG. 7. The matrix equation for $\tilde{p}$ is defined in terms of angles. (a) The matrix elements must be defined so as to conserve angles, which may be achieved by defining intermediate points (crosses). (b) The angles subtended from each point by the branch cut, B, define the known vector in the matrix equation.

where we have used an indexing notation to denote each point i and μ. The matrix element L_{ik} for example is the angle relative to π subtended by the arc at the point k, by the point i on the line j (Fig. 7). The matrix element $M_{i\nu}$ is the angle relative to π subtended by the arc at the point ν on the line $j+1$ by the point i on the line j, and an equivalent meaning applies to the other matrix elements. The vector elements c_i and c_μ are the angles relative to π subtended by the branch cut at the points i and μ respectively (Fig. 7).

We may rewrite Eqs. (28) and (29) as a matrix equation:

$$(I - A)\,\tilde{\mathbf{p}} = \mathbf{c}, \tag{30}$$

where the vectors $\tilde{\mathbf{p}} = \{p_i/\Delta p, p_\mu/\Delta p\}$ and $\mathbf{c} = \{c_i, c_\mu\}$ are of length $2I$ and the matrix A, of dimension $2I \times 2I$, has the form:

$$A = \begin{pmatrix} L & \vdots & M \\ \cdots & \vdots & \cdots \\ M' & \vdots & L' \end{pmatrix} \tag{31}$$

In the finite mesh case, the matrix A must be defined to have the same properties as the angles in the integral equations (23), (24), namely,

for all i:

$$\oint_j d\phi_{ki} = \pi, \tag{32}$$

$$\oint_{j+1} d\phi_{\nu i} = 0. \tag{33}$$

for all μ:

$$\oint_j d\phi_{k\mu} = 2\pi, \tag{34}$$

$$\oint_{j+1} d\phi_{\nu\mu} = -\pi. \tag{35}$$

To reflect these properties, the matrix elements A must be defined to *conserve* angles (Fig. 7). This may be achieved by defining intermediate points (crosses) midway between the points i and $i+1$ and between μ and $\mu+1$. Thus, by conserving angles, it is clear that the partitioned matrices of A have the properties (Fig. 7):

all i:

$$\sum_{k=1}^{I} L_{ik} = 1, \tag{36}$$

$$\sum_{\nu=1}^{I} M_{i\nu} = 0, \tag{37}$$

all μ:

$$\sum_{k=1}^{I} M'_{\mu k} = 2, \tag{38}$$

$$\sum_{\nu=1}^{I} L'_{\mu\nu} = -1. \tag{39}$$

Equations (36) and (39) result from observing that a radius vector from a point on a closed curve to every other point on the curve sweeps out an angle $\pm\pi$, the sign depending on whether the acute or obtuse angle is taken. The curve $j+1$ is entirely enclosed within the curve j so that a radius vector from a point on j to every other point on $j+1$ sweets out a zero angle, while a radius vector from a point on $j+1$ to every point on j sweeps out an angle 2π.

From the relations (Eqs. (36), (37), (38), and (39)), it follows that the vector $\mathbf{e} = \{1\}$, constructed of all elements equal to one, is an eigenvector of the matrix A, with eigenvalue 1. Accordingly, the matrix $(I - A)$ is singular, so that Eqs. (30) may not be solved. This is the matrix consequence of the well-known fact that Laplace's equation (16) with Neumann boundary conditions only has a solution up to an arbitrary constant. The constant value in $\mathbf{p}$ is not relevant to our argument and we may readily specify:

$$\tilde{p}_{i=1,j} = 0. \tag{40}$$

Thus, for example, solutions may be obtained by eliminating the first row in the matrix equation (30) and defining,

$$\begin{aligned} A_{1i} &= 2\delta_{i1}, \\ c_1 &= 0. \end{aligned} \tag{41}$$

In practice, a "better-conditioned" matrix equation is obtained by adding the null vector $\tilde{p}_1\mathbf{e}$ to the left-hand side of the matrix equation (30). $I - A$ is no longer singular and solutions for $\tilde{\mathbf{p}}$ may readily be obtained by either exact or iterative methods. In the solutions illustrated (Sect. 6), the Gauss elimination method is used [5]. It is to be noted that, for the first I elements of the vector $\tilde{\mathbf{p}}$ (dimension $2I$), $\tilde{\mathbf{p}}$ is monotonically increasing and lies in the range 0 to 1.

The solution for $\tilde{\mathbf{p}}$ allows the line $\mathbf{r}(\mu, j+1)$ to be reconstructed by interpolation so as to be defined on the orthogonal space L, namely, $\mathbf{r}(i, j+1)$. For each point i on j, there exists a value $\tilde{p}_i$. By finding the corresponding value on the line $j+1$ between the pair of points μ and $\mu + 1$, say, the point $\mathbf{r}(i, j+1)$ may be constructed by interpolation.

Other properties of the mapping of R to L are immediately determined by the orthogonalization procedure. From Eqs. (12) and (15), the aspect ratio of the mesh is accurately found,

$$h^i/h^j = \Delta p\, g(j)(d\tilde{p}/di), \tag{42}$$

where the "constant" $\Delta p\, g(j)$ is readily determined around a constant j line. The area elements and length elements of each cell are defined in the usual way:

$$h^i h^j = \partial(x, y)/\partial(i, j), \tag{43}$$

$$h^{i2} = (\partial x/\partial i)^2 + (\partial y/\partial i)^2, \tag{44}$$

$$h^{j2} = (\partial x/\partial j)^2 + (\partial y/\partial j)^2. \tag{45}$$

5. Summary of the Orthogonalization Procedure

The prescription for generating the orthogonalized mesh is summarized:

(a) $\mathbf{r}(i, 1)$ is specified on the boundary (the line $j = 1$)—the boundary conditions.

(b) In matrix form, Laplace's equation for the function $\tilde{p}$ is solved between the lines $j = 1$ and $j = 2$.

(c) For each point i on the line $j = 1$ there exists a unique value of $\tilde{p}$. The points $\mathbf{r}(\mu, 2)$ on the line $j = 2$ are interpolated as a function of $\tilde{p}$ until each point has a value of $\tilde{p}$ which corresponds precisely to the values of $\tilde{p}$ for each i point on the line $j = 1$. The new points $\mathbf{r}(i, 2)$ now lie on contours of i.

(d) The i orthogonal contours have now been marched from the $j = 1$ line to cross the $j = 2$ line at the points specifying the $j = 2$ line. The whole procedure is now repeated for the pair of lines $j = 2$ and $j = 3$, and for subsequent pairs.

6. Application of the Method

Solutions from the application of the method are illustrated in Figs. (8) and (9) for meshes of dimension 8×32. In Fig. (8a), the lines $j =$ const are a set of concentric ellipses while the lines of constant μ (numbered 1 to w) are clearly nonorthogonal. The orthogonalized solution is illustrated in Fig. (8b). The method of solution in no way relies on an expansion and is therefore quite independent of the extent of the initial nonorthogonality. In Fig. (10), the sequence of steps which orthogonalize each pair of j lines in turn, from the lines $j = 7$ to the line $j = 1$, is illustrated. It is clear here that the method is quite independent of the extent of the shear in the original coordinates.

The amount of central processor time used depends predominantly on the solution of the set of $J - 1$ matrix equations (30) which are each of dimension $2I$. Since the exact Gauss elimination method has been used [5], the total number of arithmetic operations required in solving the problem is of the order $(2/3)(2I)^3(J - 1)$, or in principle, less than one second on, say, the CDC 6600. In practice, the solutions illustrated used 3 seconds of central processor time. Since the matrices (Eq. 30) concerned are diagonally dominant, an iterative method for the solution of the matrix equations (30) will provide an even faster solution. Using cylindrical coordinates for which the solutions are known (r, θ), an accuracy of one part in 10^8 on the CDC 6600 has been obtained.

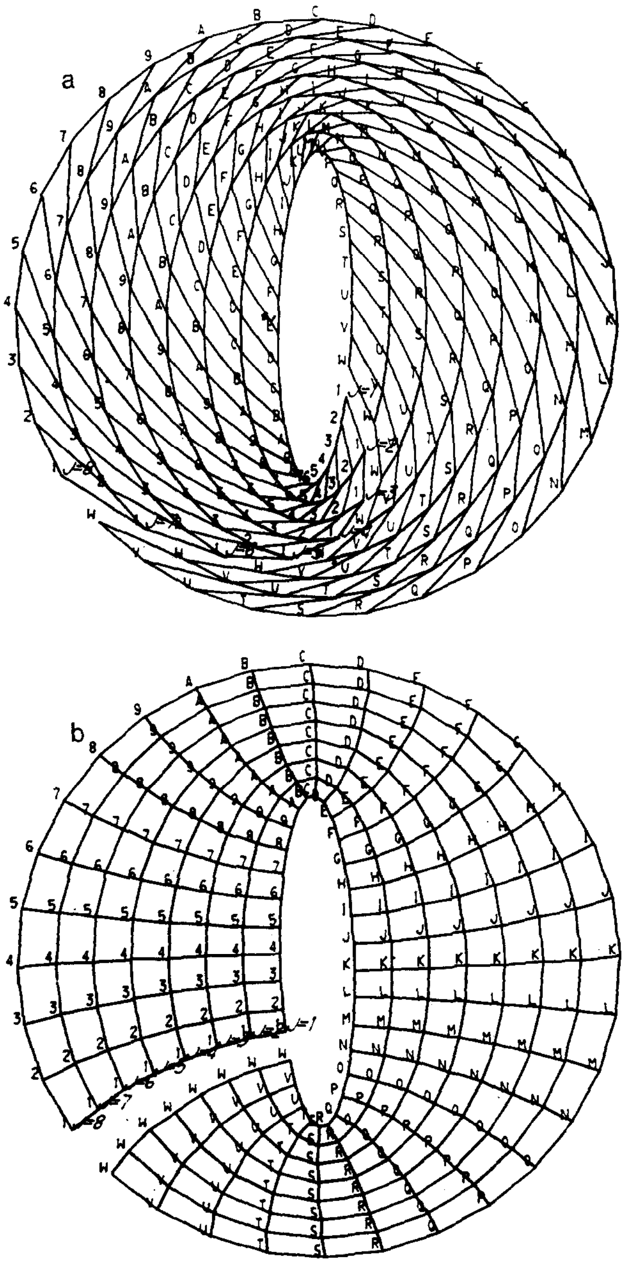


FIG. 8. (a) Nonorthogonal lines. The lines of constant j are a set of concentric ellipses. (b) The orthogonalized solutions. The j lines are now defined by points lying on orthogonal lines.

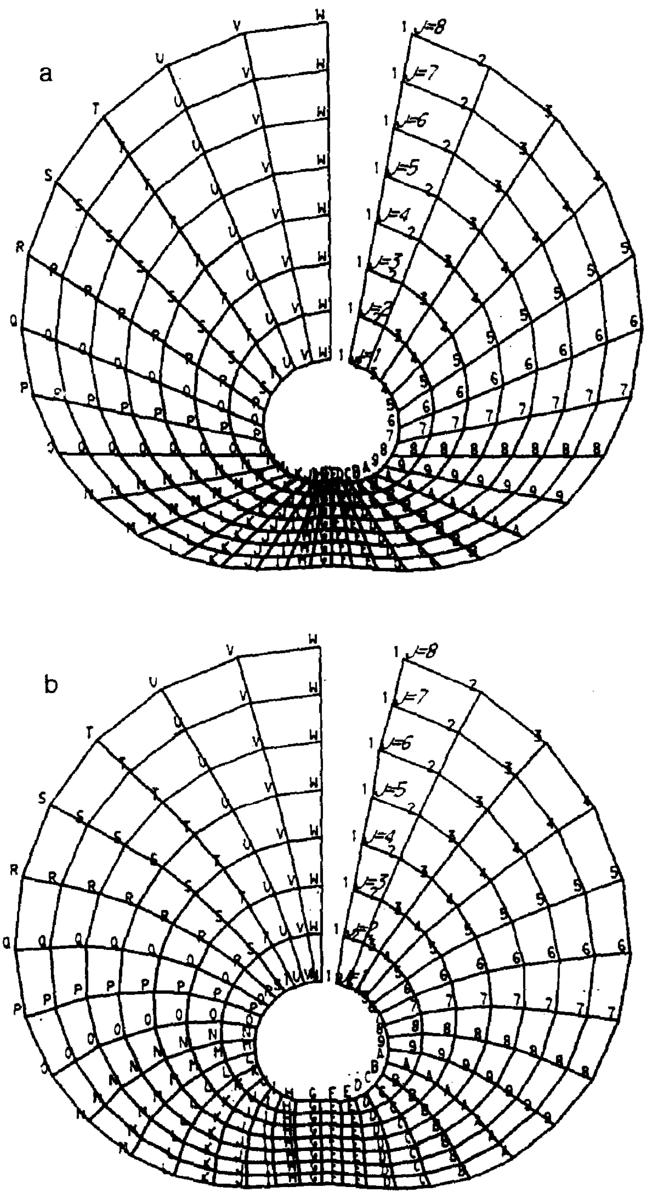
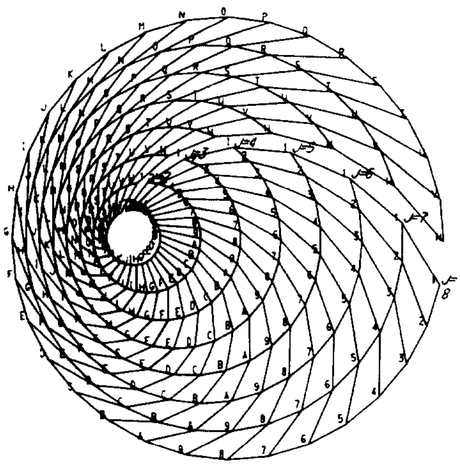
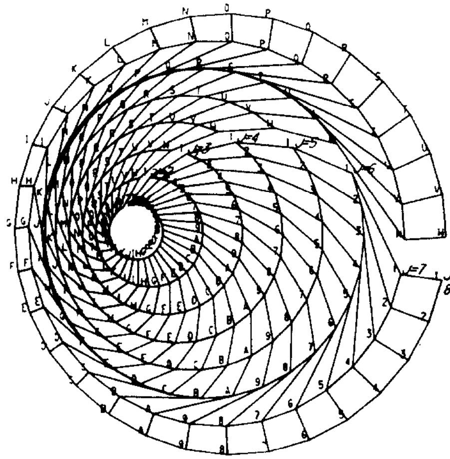
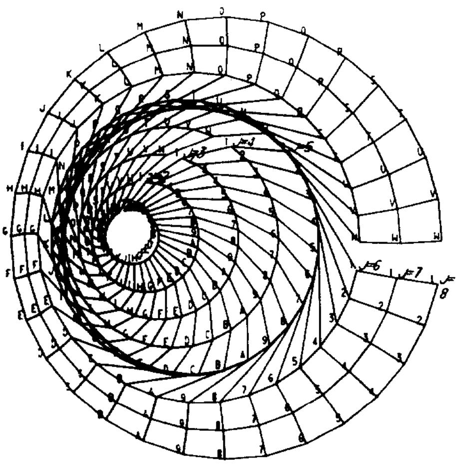
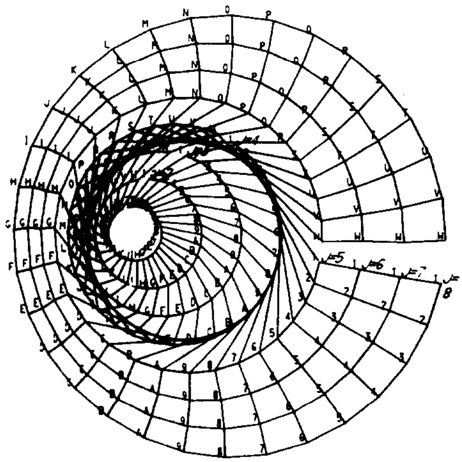
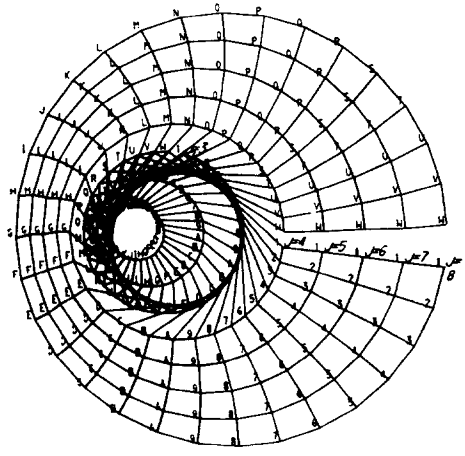
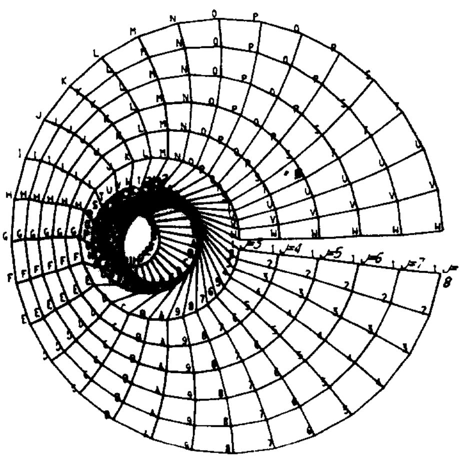


FIG. 9. Orthogonal solutions (b) produced from the nonorthogonal lines (a). The boundary here is taken as $J = 8$.

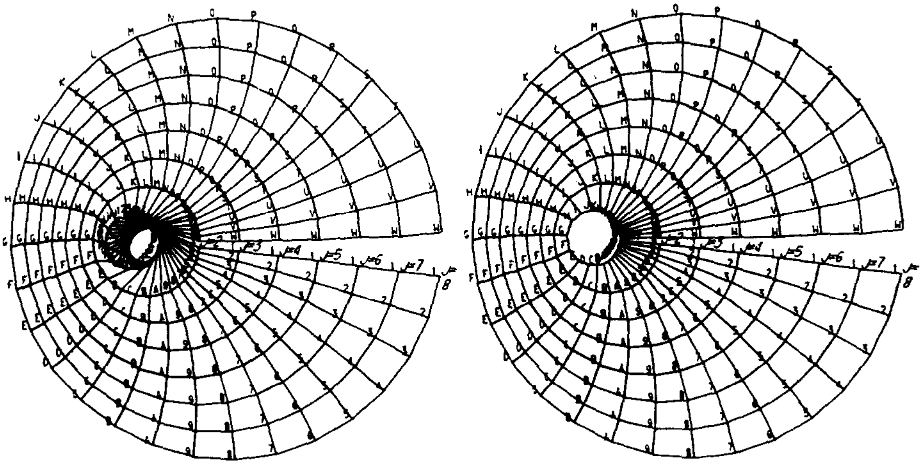


FIG. 10. The orthogonalization procedures involve a sequence of $J - 1$ operations. Starting at the boundary ($J = 8$), pairs of j lines are considered in sequence, each inner j line being redefined on points lying along constant i lines. The method is independent of the amount of shear in the given nonorthogonal coordinates.

7. Discussion

Generalized orthogonal coordinates for the simulation of problems on the computer have a very wide application. In the first instance, the method of constructing orthogonal coordinates described here may be applied to complex boundary value problems and to Eulerian coordinates in time-dependent problems [7].

The use of generalized orthogonal coordinates simplifies both the logic of indexing arrays and the difference formulation of boundary conditions. In a numerical simulation, the natural coordinates in the computer are the indices by which arrays are addressed. These indices define an "indexing mesh" of points. Fetching, storing, and the application of boundary conditions is most simple when the indexing mesh is rectangular. However, it is only in the simplest multidimensional problems that the spatial boundaries can be defined along the rectangular boundaries of a known coordinate system. Thus in an awkwardly shaped region, the logic in indexing an Eulerian mesh which does not match the boundaries can become excessively complex. In addition, boundary conditions are difficult to apply accurately in difference form, in such a region.

With any suitable *a priori* choice of one set of lines (the j-lines), the procedure described here will determine the orthogonal i-lines, and any awkwardly shaped domain will thereby be mapped onto a rectangular orthogonal mesh. Thus, if

Eulerian codes are written in terms of generalized orthogonal coordinates such that the real space R is a variable $\mathbf{r} = \mathbf{r}(i, j)$, to be determined according to the boundaries of the problem at hand, considerable generality in the application of such codes can be achieved.

Alternative methods for determining Eulerian orthogonal coordinates in this class of problem have been devised by Godunov and Prokopov [6, 7] and by Barfield [1, 2]. In the procedures developed by these authors, a variational technique is used to obtain elliptic difference equations, the solutions of which define an optimised quasiorthogonal mesh which is related to the boundaries of the problem at hand. In these methods, however, the aspect ratio of the mesh, h^i/h^j, is not defined self-consistently as a variable everywhere on the mesh.

The second major application of the procedure described here is in the use of orthogonalized Lagrangian coordinates, particularly in time-dependent fluid problems. Conventionally, in each time step of a multidimensional Lagrangian solution, advection creates a nonorthogonal mesh. As in the representation of collisionless fluids in phase-space [3], a class of "waterbag" methods may be envisaged whereby the system is represented by a set of contours of the functions of interest. An orthogonal mesh can therefore be defined, and calculated according to the direct method described here, without altering the positions of the contours, or one of the sets of lines (the j-lines). Thus, for example, by defining contours of vorticity, solutions have been obtained for incompressible hydrodynamic phenomena [10]. The authors have also applied such a technique to contours of the magnetic vector potential (the field lines) in two-dimensional magnetohydrodynamic problems [11].[1]

In summary, given a nonorthogonal, finite mesh, a procedure has been developed which defines and determines a unique orthogonal mesh. In two dimensions this is achieved by keeping one set of lines (the j-lines) fixed while varying the other set. The method is direct, in the sense of avoiding iteration, and is simple to apply.

The procedure for open-ended lines is entirely analagous. In lieu of the contribution from the branch-cut, however, sources at the two open ends of the lines give rise to the constant vector $\mathbf{c}$ (Eq. (30)).

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