GRID GENERATION USING DIFFERENTIAL SYSTEMS TECHNIQUES*

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I. INTRODUCTION

In recent years a multitude of techniques has been developed for generating computational grids required in the finite difference or finite element solutions of partial differential equations on arbitrary regions. The importance of the choice of the grid is well known. A poorly chosen grid may cause results to be erroneous or may fail to reveal critical aspects of the true solution. Some considerations that are involved in grid selection can be noted from the papers of Blottner and Roache [1], Crowder and Dalton [2], and Kalnay de Rivas [3]. While these papers discuss error for one-dimensional problems, few results exist for higher dimensions. This report will examine the errors in approximating the derivatives of a function by traditional central differences at grid points of a curvilinear coordinate system. The implications concerning the accuracy of the numerical solution of a partial differential equation will be explained by considering several numerical examples. Although this study only considers the two-dimensional case, the techniques and implications are equally valid for three-dimensional grids.

An interesting feature of the error analysis in this report is its simplicity. Most of the results follow by merely working with the truncation terms of some power series expansion. It is noted that these series expansions also give rise to higher-order difference approximations which can significantly reduce error when the grid spacing changes rapidly, as might be the case in problems with shock waves or thin boundary layers.

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When transforming a partial differential equation from rectangular to curvilinear coordinates, the derivatives of the functions defining the transformation must be evaluated. If the relation between rectangular and curvilinear variables is given by a simple analytic expression, the transformation derivatives may be computed either analytically or numerically. Truncation errors in both cases are considered for comparison.

One objective of this work is to provide tools to examine a grid, together with a computed solution, and predict possible inaccuracies due to the grid. The grid may thus be redefined to give a better solution. Directions for future work could be an extension to higher dimensions of the one-dimensional grid optimization technique of Pierson and Kutler [4].

This report also discusses the control of coordinate line spacing through functions incorporated in the elliptic generating system for the curvilinear coordinates. Attraction of coordinate lines to other coordinate lines and also attraction to fixed lines in physical space are covered. Appropriate forms of the control functions required to produce desired spacing distributions are derived. Finally a procedure for distribution of points around a boundary curve according to local boundary curvature is given. In addition a few examples of recent generation of coordinate systems are given.

II. TRUNCATION ERROR ANALYSIS

Suppose a curvilinear coordinate system is generated by transforming an arbitrary physical region of the xy-plane onto a rectangular computational region of the $\xi\eta$-plane. The relationship between partial derivatives of a function f with respect to physical and computational variables is well-known. It will be included here for later comparison with approximations derived from series expansions. Only first and second order derivatives will be considered:

$$\frac{\partial f}{\partial \xi} = \frac{\partial x}{\partial \xi}\frac{\partial f}{\partial x} + \frac{\partial y}{\partial \xi}\frac{\partial f}{\partial y}$$

$$\frac{\partial^2 f}{\partial \xi^2} = \frac{\partial^2 x}{\partial \xi^2}\frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi^2}\frac{\partial f}{\partial y} + \left(\frac{\partial x}{\partial \xi}\right)^2\frac{\partial^2 f}{\partial x^2} + 2\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \xi}\frac{\partial^2 f}{\partial x \partial y}$$

$$+ \left(\frac{\partial y}{\partial \xi}\right)^2\frac{\partial^2 f}{\partial y^2} \tag{1}$$

$$\frac{\partial^2 f}{\partial \xi \partial \eta} = \frac{\partial^2 x}{\partial \xi \partial \eta}\frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi \partial \eta}\frac{\partial f}{\partial y} + \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \eta}\frac{\partial^2 f}{\partial x^2}$$

$$+ \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right)\frac{\partial^2 f}{\partial x \partial y} + \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta}\frac{\partial^2 f}{\partial y^2}$$

The derivatives with respect to η can be obtained by replacing ξ with η in the first two equations of (1).

Although this change of variables formulation can be easily used in deriving difference approximations for derivatives with respect to x and y, nothing can be said about truncation error. An error analysis can, however, be based on Taylor series expansion of function values at neighboring points about a single point in the physical region. In order to distinguish between derivatives and differences in the following, the <u>differential notation is used for derivatives</u> while <u>subscripts denote the usual second order central difference expressions</u>. The following approximations for the central differences are valid when all series are truncated after

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second derivative terms. A unit mesh width in the $\xi\eta$-plane is assumed without loss of generality.

$$f_\xi \simeq x_\xi \frac{\partial f}{\partial x} + y_\xi \frac{\partial f}{\partial y} + \frac{1}{2}x_\xi x_{\xi\xi} \frac{\partial^2 f}{\partial x^2} + \frac{1}{2}(x_\xi y_{\xi\xi} + y_\xi x_{\xi\xi})\frac{\partial^2 f}{\partial x \partial y}$$

$$+ \frac{1}{2} y_\xi y_{\xi\xi} \frac{\partial^2 f}{\partial y^2}$$

$$f_{\xi\xi} \simeq x_{\xi\xi} \frac{\partial f}{\partial x} + y_{\xi\xi} \frac{\partial f}{\partial y} + (x_\xi{}^2 + \frac{1}{4}x_{\xi\xi}{}^2)\frac{\partial^2 f}{\partial x^2} + 2(x_\xi y_\xi + \frac{1}{4}x_{\xi\xi} y_{\xi\xi})$$

$$+ \frac{\partial^2 f}{\partial x \partial y} + (y_\xi{}^2 + \frac{1}{4}y_{\xi\xi}{}^2)\frac{\partial^2 f}{\partial y^2} \qquad (2)$$

$$f_{\xi\eta} \simeq x_{\xi\eta} \frac{\partial f}{\partial x} + y_{\xi\eta} \frac{\partial f}{\partial y} + \frac{1}{2}((x^2)_{\xi\eta} - 2xx_{\xi\eta})\frac{\partial^2 f}{\partial x^2}$$

$$+ ((xy)_{\xi\eta} - xy_{\xi\eta} - yx_{\xi\eta})\frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2}((y^2)_{\xi\eta} - 2yy_{\xi\eta})\frac{\partial^2 f}{\partial y^2}$$

Together with the corresponding two equations for f_η and $f_{\eta\eta}$, this constitutes a system of five simultaneous equations which can be solved to produce difference expressions of two first and three second derivatives of f with respect to x and y. Assuming the third order derivatives of f are bounded, the truncation error in the above expressions is $O(h^3)$, where h is some measure of the local mesh spacing. Consequently, when (2) is solved for the difference approximations of the physical derivatives of f, the truncation error is $O(h^2)$ for first derivatives and O(h) for second order derivatives. In contrast, solving the system (1) with the f, x, and y derivatives replaced by differences (and including the corresponding equations for f_η and $f_{\eta\eta}$) simultaneously to produce expressions for the five physical derivatives of f gives rise to O(h) and O(1) truncation errors for the first and second order derivatives.

In both cases it has been assumed that the coefficient matrices on the right hand sides of (1) and (2), i.e., the coordinate derivatives, including the omitted η differences, are well conditioned. Ill conditioned matrices which may result from extremely skewed coordinate lines could cause further deterioration in accuracy. Higher order accuracy can be obtained using (1) if second order coordinate differences are assumed to be $O(h^2)$. This effectively limits the rate of change in coordinate line spacing and the curvature of coordinate lines, however. No simple relation between the coefficients of the second order derivatives in the last equation of (1) and (2) was found except for the fact that they would be equal if the differences in (2) were replaced by derivatives.

The variation in numerical solutions using (1) and (2) is illustrated in the solution of Laplace's equation. The function

$$u(x, y) = x(1 + 1/(x^2 + y^2))$$

satisfies Laplace's equation for $x^2 + y^2 > 1$ and has a vanishing normal derivative on the boundary. This boundary value problem was solved numerically on $1 \leq x^2 + y^2 \leq 100$. A grid was selected with 39 radial coordinate lines and 49 circular coordinate lines. The first 23 circular coordinate lines were uniformly spaced after which the spacing was increased by a factor of 5. The difference between the exact and numerical solution is indicated in Figure 1 for difference equations derived from (1) and (2). The effect of the sudden change in coordinate line spacing was clearly less severe when using difference expressions from the higher order series expansion.

A similar error analysis can be carried out where the derivatives of x and y with respect to ξ and η are computed analytically rather than approximated by differences. In this case a series expansion in the $\xi\eta$-plane is required, followed by substitution of expressions for the higher-order ξ and η derivatives in terms of the x and y derivatives (see Ref. 5 for complete detail). Retaining physical derivatives of f through second order, as in (2), the following approximations are generated. The second derivative approximations, $f_{\xi\xi}$ and $f_{\xi\eta}$, are very lengthy and only the first and second order derivatives of x and y are included here, the complete expressions being given in Ref. 5. The first derivative approximation includes third order derivatives:

$$
\begin{aligned}
f_{\xi} &\simeq \left(\frac{\partial x}{\partial \xi} + \frac{1}{6}\frac{\partial^3 x}{\partial \xi^3}\right)\frac{\partial f}{\partial x} + \left(\frac{\partial y}{\partial \xi} + \frac{1}{6}\frac{\partial^3 y}{\partial \xi^3}\right)\frac{\partial f}{\partial y} + \frac{1}{2}\frac{\partial x}{\partial \xi}\frac{\partial^2 x}{\partial \xi^2}\frac{\partial^2 f}{\partial x^2} \\
&\quad + \frac{1}{2}\left(\frac{\partial x}{\partial \xi}\frac{\partial^2 y}{\partial \xi^2} + \frac{\partial y}{\partial \xi}\frac{\partial^2 x}{\partial \xi^2}\right)\frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2}\frac{\partial y}{\partial \xi}\frac{\partial^2 y}{\partial \xi^2}\frac{\partial^2 f}{\partial y^2} \\
f_{\xi\xi} &\simeq \frac{\partial^2 x}{\partial \xi^2}\frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi^2}\frac{\partial f}{\partial y} + \left(\left(\frac{\partial x}{\partial \xi}\right)^2 + \frac{1}{4}\left(\frac{\partial^2 x}{\partial \xi^2}\right)^2\right)\frac{\partial^2 f}{\partial x^2} \\
&\quad + 2\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \xi} + \frac{1}{4}\frac{\partial^2 x}{\partial \xi^2}\frac{\partial^2 y}{\partial \xi^2}\right)\frac{\partial^2 f}{\partial x \partial y} + \left(\left(\frac{\partial y}{\partial \xi}\right)^2 + \frac{1}{4}\left(\frac{\partial^2 y}{\partial \xi^2}\right)^2\right)\frac{\partial^2 f}{\partial y^2} \qquad (3) \\
f_{\xi\eta} &\simeq \frac{\partial^2 x}{\partial \xi \partial \eta}\frac{\partial f}{\partial x} + \frac{\partial^2 y}{\partial \xi \partial \eta}\frac{\partial f}{\partial y} + \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{1}{2}\frac{\partial^2 x}{\partial \xi \partial \eta}\left(\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial^2 x}{\partial \eta^2}\right)\right)\frac{\partial^2 f}{\partial x^2} \\
&\quad + \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi} - \frac{1}{2}\frac{\partial^2 x}{\partial \xi \partial \eta}\left(\frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 y}{\partial \eta^2}\right) - \frac{1}{2}\frac{\partial^2 y}{\partial \xi \partial \eta}\right. \\
&\quad \left.\left(\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial^2 x}{\partial \eta^2}\right)\right)\frac{\partial^2 f}{\partial x \partial y} + \left(\frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{1}{2}\frac{\partial^2 y}{\partial \xi \partial \eta}\left(\frac{\partial^2 y}{\partial \xi^2} + \frac{\partial^2 y}{\partial \eta^2}\right)\right)\frac{\partial^2 f}{\partial y^2}
\end{aligned}
$$

Considerable similarity exists between the approximations in (2) and (3) and corresponding statements can be made about the effects of the coordinate system on truncation error. For example, it can be noted that for the first derivative approximations to be second order accurate, the second and third order derivatives of x and y must be $O(h^2)$ and $O(h^3)$, respectively. Due to the additional restriction on the third order derivatives, it is not difficult to find examples where solutions of (1) with numerically computed derivatives of x and y are much more accurate than solutions using the analytical expressions for these derivatives.

With reasonable care in the selection of the grid any of the above difference formulations will give equally good results. For example, consider the grid for the region about a Joukowski airfoil depicted in Figure 2. This grid was constructed by the conformal mapping of an annular region with uniformly spaced circular coordinates. As in the above example, Laplace's equation is solved with vanishing normal derivative imposed on the airfoil. The solution is the velocity potential for flow about the airfoil at zero angle of attack. Table 1 indicates the

the difference between the computed solution and the exact solution on the surface of the airfoil where the error was greatest.

Table 1. Comparison of Difference Formulations

Differencing Method	Max Error	RMS Error
Taylor Series (2)	.03123	.00864
Analytic (1)	.02216	.01256
Numerical (1)	.02411	.00795

For this example there is clearly no advantage in using the difference expression from the series expansion in (2) over using (1) with the derivatives of x and y computed either analytically or numerically. There is another aspect to the question of the use of analytically calculated coordinate derivatives, as opposed to numerical difference representatives, when fully conservative difference formulations are used. In that case the formulation will not be fully conservative with the analytical expression in the sense that a uniform solution on the field will not be strictly preserved. This can lead to instability if the differences of the coordinate derivatives are large.

Thus far only problems of error which deal directly with the coordinate system have been considered. This source of error can be controlled by limiting the higher order differences of derivatives of x and y. A more serious problem in numerical computations is the error in the approximate solution which results from large higher order derivatives of f. In transforming from physical to computational variables, the derivatives of f with respect to ξ and η are replaced by differences regardless of whether derivatives or differences are used for x and y. The truncation error in approximating the computational derivatives of f can be minimized to some degree by a properly chosen grid. However, there are limitations in the grid choice since, as we have previously observed, a highly distorted grid also contributes to large truncation errors in the approximation of the physical derivatives of f. To analyze the total truncation error due to solution and grid, it is convenient to introduce matrix notation.

Suppose the derivatives in the physical and computational planes are related by (1). This relation can be written

$$\Delta = AD \qquad (4)$$

where

$$\Delta = \begin{bmatrix} \frac{\partial f}{\partial \xi} \\ \frac{\partial f}{\partial \eta} \\ \frac{\partial^2 f}{\partial \xi^2} \\ \frac{\partial^2 f}{\partial \xi \partial \eta} \\ \frac{\partial^2 f}{\partial \eta^2} \end{bmatrix}, \quad D = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial^2 f}{\partial x^2} \\ \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y^2} \end{bmatrix}, \quad A = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & 0 & 0 & 0 \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & 0 & 0 & 0 \\ \frac{\partial^2 x}{\partial \xi^2} & \frac{\partial^2 y}{\partial \xi^2} & (\frac{\partial x}{\partial \xi})^2 & 2 \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \xi} & (\frac{\partial y}{\partial \xi})^2 \\ \frac{\partial^2 x}{\partial \xi \partial \eta} & \frac{\partial^2 y}{\partial \xi \partial \eta} & \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} \\ \frac{\partial^2 x}{\partial \eta^2} & \frac{\partial^2 y}{\partial \eta^2} & (\frac{\partial x}{\partial \eta})^2 & 2 \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \eta} & (\frac{\partial y}{\partial \eta})^2 \end{bmatrix}$$

Difference expressions for D are generated by replacing the elements of Δ (and possibly A) by the appropriate difference approximations. If the truncation term is retained, the equation (4) becomes

$$\delta + \varepsilon = AD \tag{5}$$

where δ is the vector containing the difference approximations and

$$\varepsilon = \begin{bmatrix} -\frac{1}{6} \frac{\partial^3 f}{\partial \xi^3} \\ -\frac{1}{6} \frac{\partial^3 f}{\partial \eta^3} \\ -\frac{1}{12} \frac{\partial^4 f}{\partial \xi^4} \\ \frac{1}{6}(\frac{\partial^4 f}{\partial \xi^3 \partial \eta} + \frac{\partial^4 f}{\partial \xi \partial \eta^3}) \\ -\frac{1}{12} \frac{\partial^4 f}{\partial \eta^4} \end{bmatrix}$$

Solving for D in (5) we have

$$D = A^{-1}\delta + A^{-1}\varepsilon \tag{6}$$

Now ε is unknown but can be estimated using differences of f. Although such numerical differentiation does not tend to be very accurate when applied to an approximate solution of a partial differential equation, the value of $A^{-1}\varepsilon$ has been used successfully to distinguish regions of high error from regions of low error. This can be illustrated by returning to the numerical solution of potential flow about the Joukowski airfoil in Figure 2. The comparison of truncation error with error in the solution is indicated in Figure 3 for grid points beginning near the trailing edge and ending near the leading edge of the airfoil. The grid points were chosen to lie on the second coordinate line from the airfoil surface so that no extrapolation was needed to estimate the elements of ε.

Each factor in the truncation error estimate can be analyzed independently. The factor A^{-1} deals only with the grid coordinates, while ε involves only the solution of the partial differential equation. In the above example consideration of ε alone would seriously underestimate the order of accuracy near the leading and trailing edge since the distortion in the coordinate system would not be taken into account. The influence of the factor A^{-1} can be analyzed by examining the condition of the matrix A. An ill-conditioned matrix not only magnifies the effect of the truncation terms in ε but also the effect of deleting the additional terms which appeared in the series expansions (2) and (3).

We will now consider a case where an extremely ill-conditioned matrix is encountered. The Navier-Stokes equations in stream function-vorticity formulation were solved numerically for viscous flow about a circular cylinder. The data in Table 2 illustrates the growth in the condition number of A as the circular coordinate lines are concentrated near the cylinder to resolve the boundary layer. Only the Laplacian of vorticity was included in the truncation error computation since this truncation term clearly dominated the remaining truncation terms in the equations. As n increases, the dominating factors in the truncation term shifts from the elements of ε to the elements of A^{-1}. An examination of vorticity values revealed a clear deterioration of the numerical solution for $n = 4$.

Table 2. Maximum truncation error for $\nabla^2\omega$ and condition number of A. Circular coordinate lines $r = 1 + 9(1 - \exp(n\eta/48)) / (1 - \exp(n))$, $\eta = 0, 1, ---, 48$. Reynolds no. = 5.

n	Max Truncation	Max Cond_1 (A)
1	.1079	45
2	.0482	78
3	.0891	259
4	3.0918	1017

For later reference, we have from (2) for the one-dimensional case that the simple two-point central difference expression for the first derivative, f_ξ/x_ξ, has a truncation error term given by

$$\frac{1}{2}x_{\xi\xi}\,\frac{\partial^2 f}{\partial x^2}$$

which acts as a numerical diffusion. This effect was pointed out earlier in Ref. 1.

III. COORDINATE SYSTEM CONTROL

A. Original Generating System

In the formulation of boundary-fitted coordinate systems generated from elliptic systems as given in Ref. 6 the curvilinear coordinates (ξ, η) were determined as the solution of the system

$$\nabla^2 \xi = P(\xi,\eta) \tag{7a}$$

$$\nabla^2 \eta = Q(\xi,\eta) \tag{7b}$$

which in the transformed plane becomes (from here on, subscripts indicate derivatives)

$$\alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} = -J^2(Px_\xi + Qx_\eta) \tag{8a}$$

$$\alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} = -J^2(Py_\xi + Qy_\eta) \tag{8b}$$

with

$$\alpha \equiv x_\eta^{\ 2} + y_\eta^{\ 2} \tag{9a}$$

$$\beta \equiv x_\xi x_\eta + y_\xi y_\eta \tag{9b}$$

$$\gamma \equiv x_\xi^{\;2} + y_\xi^{\;2} \tag{9c}$$

$$J \equiv x_\xi y_\eta - x_\eta y_\xi \tag{9d}$$

B. Attraction to Coordinate Lines

Here the functions P and Q are to be chosen to control the coordinate line spacing. In Ref. 6 those control functions were taken as sums of decaying exponentials of the form

$$P = -\sum_{i=1}^{n} a_i \operatorname{sgn}(\xi - \xi_i)\exp(-c_i|\xi - \xi_i|) \tag{10a}$$

$$- \sum_{i=1}^{m} b_i \operatorname{sgn}(\xi - \xi_i)\exp(-d_i((\xi - \xi_i)^2 + (\eta - \eta_i)^2)^{1/2})$$

$$Q = -\sum_{i=1}^{n} a_i \operatorname{sgn}(\eta - \eta_i)\exp(-c_i|\eta - \eta_i|) \tag{10b}$$

$$- \sum_{i=1}^{m} b_i \operatorname{sgn}(\eta - \eta_i)\exp(-d_i((\xi - \xi_i)^2 + (\eta - \eta_i)^2)^{1/2})$$

Here the a_i, b_i, c_i, and d_i of the Q functions are not necessarily the same as those in the P function.

In the P function the effect of the amplitude a_i is to attract ξ-

coordinate lines toward the ξ_i-line, while the effect of the amplitude b_i is to attract ξ-lines toward the single point (ξ_i, η_i). Note that this attraction to a point is actually attraction of ξ-lines to a point on another ξ-line, and as such acts normal to the ξ-line through the point. There is no attraction of η-lines to this point via the P function. In each case the range of the attraction effect is determined by the decay factors, c_i and d_i. With the inclusion of the sign changing function, the attraction occurs on both sides of the ξ-line, or the (ξ_i, η_i) point, as the case may be. Without this function, attraction occurs only on the side toward increasing ξ, with repulsion occuring on the other side.

A negative amplitude simply reverses all of the above-described effects, i.e., attraction becomes repulsion and vice versa. The effect of the Q function on η-lines follows analagously. A number of examples of this type of coordinate line control have been given in Ref. 6.

In the case of a boundary that is an η-line, positive amplitudes in the Q function will cause η-lines off the boundary to move closer to the boundary, assuming that η increases off the boundary. The effect of the P function will be to alter the angle at which the ξ-lines intersect the boundary, since the points on the boundary are fixed, with the ξ-lines tending to lean in the direction of decreasing ξ. If the boundary is such that η decreases off the boundary then the amplitudes in the Q function must be negative to achieve attraction to the boundary. In any case, the amplitudes a_i cause the effects to occur all along the boundary, while the effects of the amplitudes b_i occur only near selected points on the boundary.

If the attraction line and/or the attraction points are in the field, rather than on a boundary, then the attraction is not to a fixed line or point in space, since the attraction line or points are themselves solutions of the system of equations, the functions P and Q being functions of the variables ξ and η. It is, of course, also possible to take these control functions as functions of x and y, instead of ξ and η, and achieve attraction to fixed lines and/or points in the physical field. This case becomes somewhat more complicated, since it must be ensured that coordinate lines are not attracted parallel to themselves, and its discussion follows in a later section.

C. Control Functions for Certain Spacings

For certain simple geometries it is possible to integrate (8) analytically for appropriately selected forms of the control functions, and thus to determine the control functions required to produce a certain line spacing. In this regard consider the case of two concentric circular boundaries of radii r_1 and r_2, with $r_2 > r_1$.

With $\eta = 1$ on the inner boundary, $\eta = J$ on the outer boundary, and ξ varying monotonically from 1 to I around these boundaries, a solution of (8) can be given in the form

$$x = r(\eta) \cos \left[2\pi \left(\frac{\xi-1}{I-1}\right)\right] \tag{11a}$$

$$y = r(\eta) \sin \left[2\pi \left(\frac{\xi-1}{I-1}\right)\right] \tag{11b}$$

Substitution of these expressions into the equations of (8) with $P(\xi,\eta) = 0$ yields

$$\frac{r''}{r'} - \frac{r'}{r} + r'^2 Q = 0 \tag{12}$$

This can be made a perfect differential by taking the control function Q to be of the form (following the direction of Ref. 7)

$$Q \equiv - \frac{f''(\eta)}{f'(\eta)} \frac{1}{r'^2}$$

where the minus sign has been introduced merely for convenience. Since $\frac{1}{r'^2}$ is equal to $\frac{\gamma}{J^2}$ for the solution given by (11), this form of Q suggests taking Q to be of the form

$$Q = - \frac{\gamma}{J^2} \frac{f''(\eta)}{f'(\eta)} \tag{13}$$

Substitution of (13) into (12) yields

$$\frac{r''}{r'} - \frac{r''}{r} - \frac{f''}{f'} = 0 \tag{14}$$

which can be integrated twice to yield

$$r(\eta) = c_2 e^{c_1 f(\eta)}$$

The constants of integration may be evaluated from the boundary conditions, $r(1) = r_1$, $r(J) = r_2$, so that

$$r(\eta) = r_1 \{(r_2/r_1)^{\left[\frac{f(\eta) - f(1)}{f(J) - f(1)}\right]}\} \tag{15}$$

This equation may then be solved for $f(\eta)$ to yield

$$\frac{f(\eta) - f(1)}{f(J) - f(1)} = \frac{\ln[\frac{r(\eta)}{r_1}]}{\ln[\frac{r_2}{r_1}]} \tag{16}$$

If the distance from the body to the Nth η-line is specified to be r_N, the following equation must be satisfied:

$$\frac{f(N) - f(1)}{f(J) - f(1)} = \frac{\ln[\frac{r_N}{r_1}]}{\ln[\frac{r_2}{r_1}]} \tag{17}$$

It should be noted that the form of $f(\eta)$ is still arbitrary, subject to (17).

Alternatively, to set r' at the inner boundary, $\eta = 1$, we have, upon differentiation of (15) with respect to η and subsequent evaluation at $\eta = 1$, that $f(\eta)$ must satisfy

$$\frac{f'(1)}{f(J) - f(1)} = \frac{\dfrac{r'(1)}{r_1}}{\ln(\dfrac{r_2}{r_1})} \tag{18}$$

The two derivatives appearing in the truncation error of first derivatives, as given in last equation in section II, are, from repeated differentiation of (15),

$$r' = \frac{\ln(\dfrac{r_2}{r_1})}{f(J) - f(1)} [rf'(\eta)] \tag{19a}$$

$$r'' = \frac{\ln(\dfrac{r_2}{r_1})}{f(J) - f(1)} [r'f'(\eta) + rf''(\eta)) \tag{19b}$$

Thus if a function $f(\eta)$ with a free parameter is selected, (17) may be used to determine the parameter in the function such that the Nth η-line lies at a specified distance, $r_N - r_1$, from the inner boundary. Alternatively, the free parameter may be determined by (18) such that the spacing at the boundary is set by specification of r' there. The derivatives in the truncation error terms may then be calculated from (19). With the function $f(\eta)$ determined, the control function Q is then given by (13).

For example, with the function (Ref. 7)

$$f(\eta) \equiv \eta K^{\eta-1}$$

where K is a free parameter, we have, by (17), that K must be the solution of the nonlinear equation

$$\frac{NK^{N-1} - 1}{JK^{J-1} - 1} = \frac{\ln(\dfrac{r_N}{r_1})}{\ln(\dfrac{r_2}{r_1})} \tag{20}$$

to set the Nth η-line at r_N. Alternatively, the value of K required to set r' to a specified value at the inner boundary is determined by (18) as the solution of the nonlinear equation

$$\frac{1 + \ln K}{JK^{J-1} - 1} = \frac{\dfrac{r'(1)}{r_1}}{\ln\left(\dfrac{r_2}{r_1}\right)} \tag{21}$$

For this function, the derivatives appearing in the truncation error term, (19), are given by

$$f'(\eta) = (1 + \eta\ln K)K^{\eta-1} \tag{22a}$$

$$f''(\eta) = (2 + \eta\ln K)(\ln K)K^{\eta-1} \tag{22b}$$

The control function Q is given by (13) as

$$Q = -\frac{\gamma}{J^2}\left(\frac{2 + \eta\ln K}{1 + \eta\ln K}\right)\ln K \tag{23}$$

It can be shown by consideration of the ratios of successive derivatives that the higher derivatives of this function are progressively decreasing if K is in the range

$$0 < \ln K < \frac{1}{2}(\sqrt{5} - 1) \tag{24}$$

Since the left side of (21) is a decreasing function of K for positive K, the smallest value of the spacing at the boundary, r'(1), that can be achieved while maintaining progressively decreasing higher derivatives of $f(\eta)$ occurs with K at the upper limit of the inequality (24), viz

$$r'(1)_{min} = r_1\ln\left(\frac{r_2}{r_1}\right)\frac{\frac{1}{2}(1 + \sqrt{5})}{J\exp[\frac{1}{2}(\sqrt{5} - 1)(J - 1)] - 1} \tag{25}$$

It is not reasonable to use smaller values of $r'(1)$ since the progressively increasing higher derivatives of $f(\eta)$ will result in significant truncation error introduced by the coordinate system.

Another choice of $f(\eta)$ might be

$$f(\eta) = \sinh\,[K(\eta - 1)] \tag{26}$$

for which, from (17), the Nth line occurs at r_N for K given by the solution of the equation

$$\frac{\sinh\,[K(N-1)]}{\sinh\,[K(J-1)]} = \frac{\ln(\frac{r_N}{r_1})}{\ln(\frac{r_2}{r_1})}$$

or the spacing at the inner boundary is $r'(1)$ for K given by (18):

$$\frac{K}{\sinh\,[K(J-1)]} = \frac{\frac{r'(1)}{r_1}}{\ln(\frac{r_2}{r_1})} \tag{27}$$

The first two derivatives and the control function are given by

$$f'(\eta) = K\cosh[K(\eta - 1)] \tag{28a}$$

$$f''(\eta) = K^2 \sinh\,[K(\eta - 1)] \tag{28b}$$

$$Q = -\frac{\gamma}{J^2} K\tanh\,[K(\eta - 1)] \tag{29}$$

In this case progressively decreasing higher derivatives occur for K in the range $0 < K < 1$, so that the smallest practical spacing at the inner boundary is

$$r'(1)_{min} = \frac{r_1 \ln(\frac{r_2}{r_1})}{\sinh (J - 1)}$$

The control function for the spacing distribution of Roberts, Ref. 8, can be determined in the same manner as follows. With the notation of Ref. 8 adjusted so that the boundaries occur as used above, we have

$$r(\eta) = r_2 + \frac{G(\eta) - 1}{G(\eta) + 1}(1 - \frac{r_1}{r_2})b \tag{30}$$

with

$$G(\eta) = (\frac{b + r_2}{b - r_2})^{(\frac{\eta - J}{J - 1})}$$

with b a free parameter.

Although the form of $f(\eta)$ could be extracted by substitution of (30) into (16), it is simpler to determine the parameter b from either $r(N) = r_N$, or for a specified value of $r'(1)$. The derivatives are

$$r'(\eta) = \frac{2}{J - 1} \ln(\frac{b + r_2}{b - r_2}) \frac{G}{(G + 1)^2} (1 - \frac{r_1}{r_2})b \tag{31a}$$

$$r''(\eta) = 2(\frac{1}{J - 1})^2 \ln^2 (\frac{b + r_2}{b - r_2}) \frac{G(1 - G)}{(G + 1)^3} (1 - \frac{r_1}{r_2})b \tag{31b}$$

The control function Q is then given by (13) and (14) as

$$Q = - \frac{\gamma}{J^2}(\frac{r''}{r'} - \frac{r'}{r}) \tag{32}$$

with r, r', and r'' to be substituted from (30) and (31).

Finally, another type of function is a patched function using different functions near and away from the inner boundary to achieve a group of closely spaced lines near the inner boundary with fairly rapid expansion outside this inner group. This is done as follows: Let the spacing of the inner group be such that the same change in velocity would occur between each two lines for a velocity distribution given by u(r). To do this, invert the velocity function such that r = r(u), and then take

$$u(\eta) = \frac{\eta - 1}{N - 1} u_N \qquad 1 \leq \eta \leq N$$

when u_N is the velocity at the edge of the inner group of lines. Then

$$r(\eta) = r\left(u = \frac{\eta - 1}{N - 1} u_N\right) \qquad 1 \leq \eta \leq N$$

From this function all the derivatives and the control function may be calculated, the latter being determined by (13) and (14).

Now outside the inner group of lines, i.e., for $N \leq \eta \leq J$, let $r(\eta)$ be a quartic polynomial:

$$r(\eta) = r'_N(\eta - N) + \frac{1}{2}r''_N(\eta - N)^2 + \frac{1}{6}r'''_N(\eta - N)^3$$
$$+ a(\eta - N)^4 + r_N \qquad N \leq \eta \leq J$$

where the three derivatives at $\eta = N$ are determined from the derivatives of the inner function, all being evaluated at $\eta = N$. The final parameter, a, is determined such that $r(J) = r_2$. Thus

$$a = \frac{(r_J - r_N) - r'_N(J - N) - \frac{1}{2}r''_N(J - N)^2 - \frac{1}{6}r'''(J - N)^3}{(J - N)^4}$$

The outer control function is then determined from (13) and (14). This composite control function has only one continuous derivative, and thus could possibly lead to truncation error introduced by the coordinate system.

It is, of course, also possible to integrate the coordinate equation (8) for the one-dimensional case. In that case the control function Q is given by

$$Q = -\frac{\gamma}{J^2}\frac{r''}{r'} = -\frac{\gamma}{J^2}\frac{f''(\eta)}{f'(\eta)} \tag{33}$$

and

$$r(\eta) = r_2 + (r_2 - r_1)\left[\frac{f(\eta) - f(1)}{f(J) - f(1)}\right] \tag{34}$$

All the other steps follow in analogy with the two-dimensional case.

Now, although the two-dimensional case given above applies only to concentric circular boundaries, the effect of using the same control functions for the general case will be qualitatively the same, with even closer spacing near inner boundary with stronger curvature. Thus the control functions derived in the above manner can be expected to produce the type of spacing desired in general applications. A version of the TOMCAT code incorporating several of these functions has been written and has been used to produce coordinate systems for airfoils with the spacing at the airfoil set at $\frac{0.01}{\sqrt{R}}$ automatically through (18). An example is shown in Fig. 4, using the function above (20). Other examples are given in Ref. 9.

D. Revised Generating System

The form of the control function Q taken in (13) naturally leads to the idea of replacing the original elliptic system, (7), with the system

$$\nabla^2\xi = ({\xi_x}^2 + {\xi_y}^2)\ P\ (\xi,\eta) \tag{35a}$$

$$\nabla^2\eta = ({\eta_x}^2 + {\eta_y}^2)\ Q\ (\xi,\eta) \tag{35b}$$

since the terms multiplying P and Q here are, respectively, equal to $\frac{\alpha}{J^2}$ and $\frac{\gamma}{J^2}$. With this system the transformed equations are

$$\alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} = -(\alpha P x_\xi + \gamma Q x_\eta) \tag{36a}$$

$$\alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} = -(\alpha P y_\xi + \gamma Q y_\eta) \tag{36b}$$

This form has also been given by Shanks and Thompson, Ref. 10, and by Thomas and Middlecoff, Ref. 11. This form has now been adopted in the latest version of the TOMCAT code.

The exponential forms of the functions P and Q, and the discussion given therewith above, are still applicable with this system. Appropriate values of the attraction amplitudes are several orders of magnitude smaller with this new system because of the relatively large values attained by the terms multiplying P and Q for small Jacobians.

Finally, it is useful to solve (36) simultaneously to display P and Q explicitly as

$$P = -\frac{1}{\alpha J}(y_\eta Dx - x_\eta Dy) \tag{37a}$$

$$Q = \frac{1}{\gamma J}(y_\xi Dx - x_\xi Dy) \tag{37b}$$

with

$$Dx \equiv \alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} \tag{38a}$$

$$Dy \equiv \alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} \tag{38b}$$

With (37) the control functions required to produce any specified solution $x(\xi,\eta)$, $y(\xi,\eta)$ could be calculated. Although such a procedure is normally of only academic interest, since the solution $x(\xi,\eta)$, $y(\xi,\eta)$ is yet to be determined, it might be useful in some cases to determine

P and Q from (37) for some approximate solution generated, say, by simple interpolation from the boundaries, and then to use smoothed values of these functions as the control functions for the actual solution. Although the approximate solution might have lacked continuity of derivatives, the actual solution determined by solving the elliptic system with the smoothed control functions will have continuous derivatives, while following generally the form of the approximate solution.

E. Control Functions for Near Orthogonality at Boundary

Another example of the usefulness of (37) is as follows. The solution for the concentric circle case can be generalized slightly to include variable spacing of points along the boundaries by taking, instead of (11),

$$x = r(\eta) \cos \left[2\pi \frac{g(\xi) - g(1)}{g(I) - g(1)}\right] \tag{39a}$$

$$y = r(\eta) \sin \left[2\pi \frac{g(\xi) - g(1)}{g(I) - g(1)}\right] \tag{39b}$$

Substitution of these functions in (37) then results in

$$P = -\frac{g''}{g'} \tag{40a}$$

$$Q = \frac{r'}{r} - \frac{r''}{r'} \tag{40b}$$

The second of these is the same as (13), using (14) and considering the above re-definition of Q, and was used above to generate the control function Q.

With $g(\eta)$ determined by the boundary point spacing, the control function P given here will maintain the ξ-lines as radial lines, i.e., normal to the circular boundaries. Note that arc length along the circular boundary is given by

$$s(\xi) = 2\pi \frac{g(\xi) - g(1)}{g(I) - g(1)} r \tag{41}$$

so that the function $g(\xi)$ may be related to arc length by

$$g(\xi) = g(1) + \frac{g(I) - g(1)}{2\pi r} s(\xi) \tag{42}$$

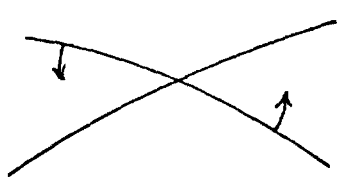
Thus (40a) can be rewritten in terms of arc length as

$$P = -\frac{s''}{s'} \tag{43}$$

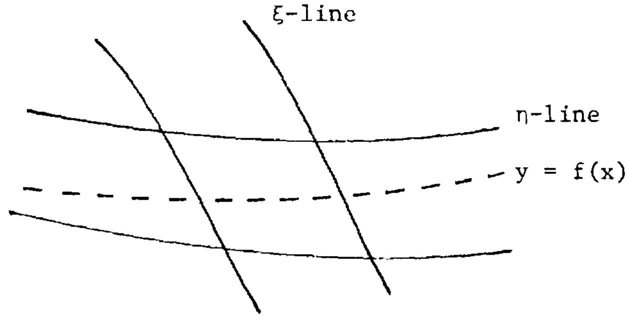
As discussed above for the control function Q, this idea can be carried over to the case of general boundaries to produce the same effect qualitatively. Thus in the general case, the control function P could be determined at each boundary from (43), and then values of P in the field could be taken from linear interpolation between the values at corresponding boundary points.

F. Attraction to Fixed Lines in Physical Space

As mentioned above, the attraction of coordinate lines to fixed lines and/or points in physical space, rather than to floating coordinate lines and/or points, requires further consideration. Recall that in the above discussion, η-lines are attracted to other η-lines, and ξ-lines are attracted to other ξ-lines. It is unreasonable, of course, to attempt to attract η-lines to ξ-lines, since that would have the effect of collapsing the coordinate system:



When, however, the attraction is to be to certain fixed lines in x-y space, defined by curves $y = f(x)$, care must be exercised to avoid attempting to attract η or ξ lines to specified curves that cut the η or ξ lines at large angles. Thus, in the figure below:



it is unreasonable to attract ξ lines to the curve $f(x)$, while it is natural to attract the η-lines to $f(x)$.

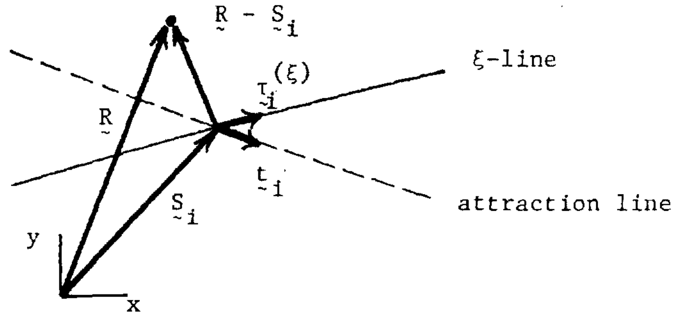
However in the general situation, the specified line $f(x)$ will not necessarily be aligned with either a ξ or η line along its entire length. Since it is unreasonable to attract a line parallel to itself, some provision is necessary to decrease the attraction to zero as the angle between the coordinate line and the given line $f(x)$ goes to zero. This can be accomplished by multiplying the attraction function by the cosine of the angle between the coordinate line and the line $f(x)$. It is also necessary to change the sign on the attraction function on either side of the line $f(x)$. This can be done by multiplying by the sine of the angle between the line $f(x)$ and the vector to the point on coordinate line.

These two purposes can be accomplished as follows. Let a general point (x, y) be located by the vector $\underset{\sim}{R}(x, y)$, and let the attraction line $y = f(x)$ be specified by the collection of points $\underset{\sim}{S}(x_i, y_i)$, $i = 1, 2, --, n$. Let the unit tangent to the attraction line be $\underset{\sim}{t}(x_i, y_i)$, and the unit tangent to a ξ-line be $\underset{\sim}{\tau}^{(\xi)}$. Then the sine and cosine of the angle between the ξ-line and the attraction line may be written as

$$\text{sine} = \frac{[\underset{\sim}{t}_i \times (\underset{\sim}{R} - \underset{\sim}{S}_i)] \cdot k}{|\underset{\sim}{R} - \underset{\sim}{S}_i|}$$

$$\text{cosine} = \mathbf{t}_i \cdot \boldsymbol{\tau}_i^{(\xi)}$$

where $\mathbf{k}$ is the unit vector normal to the two dimensional plane. These relations are evident from the figure



The control function P(x, y) may then be logically taken as

$$P(x,y) = -\sum_{i=1}^{n} a_i(\mathbf{t}_i \cdot \boldsymbol{\tau}_i^{(\xi)}) \frac{[\mathbf{t}_i \times (\mathbf{R} - \mathbf{S}_i)] \cdot \mathbf{k}}{|\mathbf{R} - \mathbf{S}_i|} \exp(-d_i|\mathbf{R} - \mathbf{S}_i|) \tag{44a}$$

with the analagous form for Q:

$$Q(x,y) = -\sum_{i=1}^{n} a_i(\mathbf{t}_i \cdot \boldsymbol{\tau}_i^{(\eta)}) \frac{[\mathbf{t}_i \times (\mathbf{R} - \mathbf{S}_i)] \cdot \mathbf{k}}{|\mathbf{R} - \mathbf{S}_i|} \exp(-d_i|\mathbf{R} - \mathbf{S}_i|) \tag{44b}$$

These functions depend on x and y through both $\mathbf{R}$ and $\boldsymbol{\tau}^{(\xi)}$ or $\boldsymbol{\tau}^{(\eta)}$ and thus must be recalculated at each point as the iterative solution of (36) proceeds. This form of coordinate control will therefore be more expressive than that based on attraction to other coordinate lines.

There is no real distinction between "line" and "point" attraction with this type of attraction. "Line" attraction here is simply attraction to a group of points that form a line f(x). If line attraction is specified, then the tangent to the line f(x) is computed from the adjacent points on the line. If point attraction is specified, then the "tangent" must be input for each point.

The tangents to the coordinate lines are computed from

$$\underset{\sim}{\tau}^{(\xi)} = \frac{1}{\sqrt{\alpha}}(\underset{\sim}{i}x_\eta + \underset{\sim}{j}y_\eta) \tag{45a}$$

$$\underset{\sim}{\tau}^{(\eta)} = \frac{1}{\sqrt{\gamma}}(\underset{\sim}{i}x_\xi + \underset{\sim}{j}y_\xi) \tag{45b}$$

G. Point Distribution on Boundary According to Curvature

One final technique to mention concerns the placement of points along the boundary according to the local boundary curvature. Let a boundary curve be described by the function $y = f(x)$. Then if s is arc length along the boundary we have

$$\frac{ds}{dx} = \sqrt{1 + f'^2}$$

Now take the rate of change of arc length with the curvilinear coordinate, ξ, along the boundary to be exponentially dependent on the local radius of curvature, r, of the boundary. Thus let

$$\frac{ds}{d\xi} = 1 - e^{-br}$$

where b is a free parameter. This function causes the arc length to change slowly with ξ where the curvature is large.

Then

$$\frac{d\xi}{dx} = \frac{ds}{dx}\Big/\frac{ds}{d\xi} = \frac{\sqrt{1 + f'^2}}{1 - e^{-br}}$$

Since f and r are known at each x, a normalized $\xi(x)$ may be determined from

$$\xi(x) = 1 + \frac{\displaystyle\int_0^x \frac{\sqrt{1 + f'^2}}{1 - e^{-br}}\, dx'}{\displaystyle\int_0^1 \frac{\sqrt{1 + f'^2}}{1 - e^{-br}}\, dx'}\, I \tag{46}$$

assuming x is normalized to vary from 0 to 1 and ξ to vary from 1 to I. The quadrature may be taken numerically if necessary.

Then for I number of ξ-points ξ = 1, 2, --, I on the boundary, the corresponding values of x can be determined by inversion of $\xi(x)$, done by interpolation of tabular values if necessary. The arc length between each of these points can then be calculated and the value of the free parameter b can be adjusted iteratively to produce, say, a specified maximum arc spacing along the boundary, or perhaps, to match a specified arc spacing at either end or, for that matter, at any given point. In application to airfoils, this procedure is applied to the upper surface with b chosen to match a specified maximum arc spacing. A separate application is then made to the lower surface with b there being chosen to match the arc spacing adjacent to the leading edge on the upper surface.

This procedure produces a smooth point distribution on the boundary, with points concentrated in regions of large curvature, yet free of the rapid spacing changes that lead to coordinate-system-introduced truncation error of the type discussed in an earlier section.

IV. SOME RECENT APPLICATIONS OF COORDINATE SYSTEMS

In addition to extensive application to airfoils, as illustrated in Fig. 4, in which the transformed plane is an empty rectangle, some more general configurations have recently been treated using a transformed plane that contains rectangular voids as discussed in Ref. 12. For example, a coordinate system used in a simulation of a nuclear reactor cooling system is shown in Fig. 5, taken from Ref. 13, and systems for Charleston harbor (Ref. 14) and a portion of Lake Ponchatrain are shown in Figs. 6 and 7.

V. CONCLUSION

Control of the spacing of coordinate lines so as to resolve large gradients in numerical solution of partial differential equations continues to be of paramount importance. Research has provided some means of control and of error estimation. The experience gained thus far has indicated the versatility of the coordinate systems generated from elliptic systems and the possibility of optimization of such systems in adaptation to the nature of particular partial differential systems and boundary configuration.

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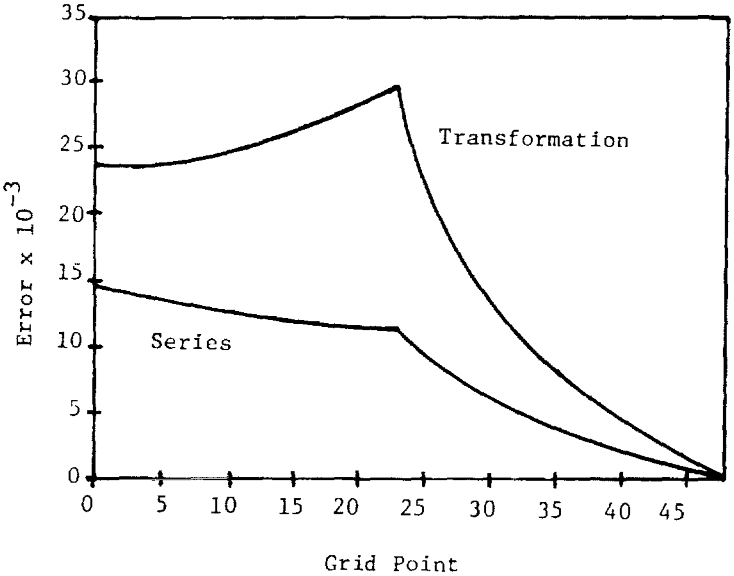

Figure 1.- Error at grid points on the coordinate line $1 \leq x \leq 10$, $y = 0$.

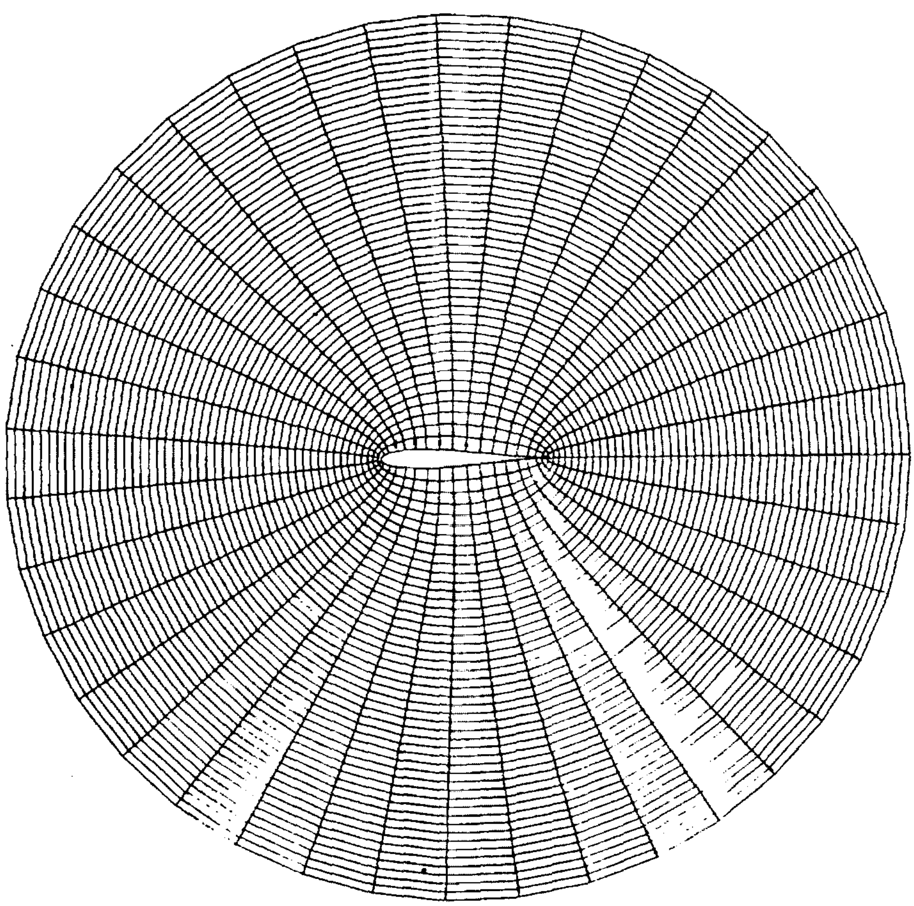

Figure 2.- Coordinate system about a Joukowski airfoil.

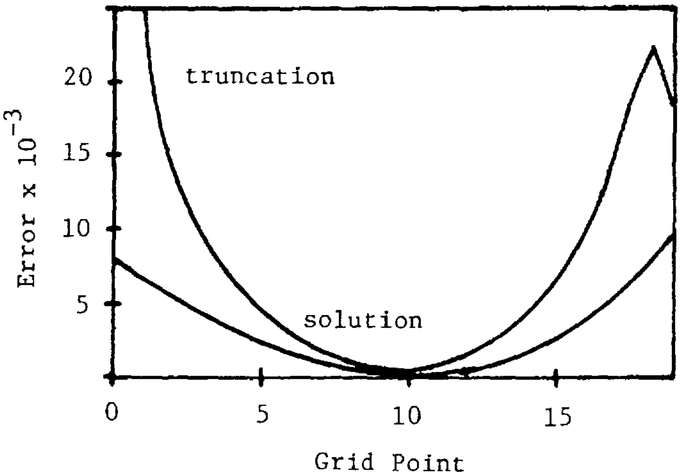

Figure 3.- Comparison of estimated truncation error in the Laplacian with the error in the solution of Laplace's equation.

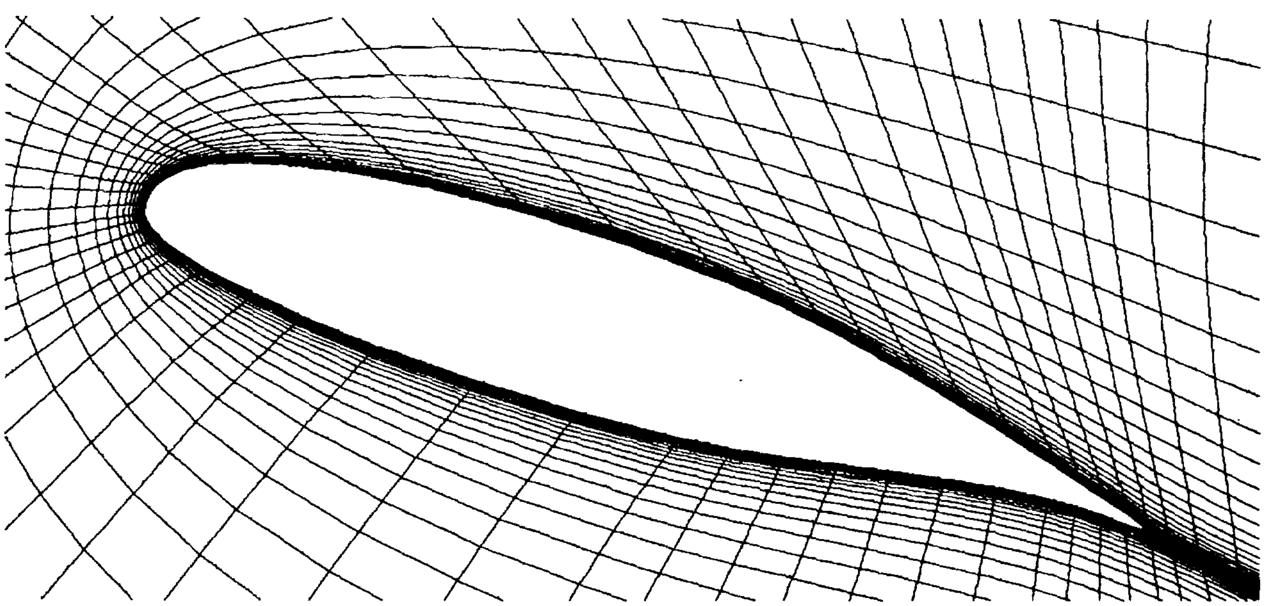

Figure 4.- Airfoil coordinate system with concentration of lines (supplied by Dr. Krishna Devarayalu of the Boeing Company).

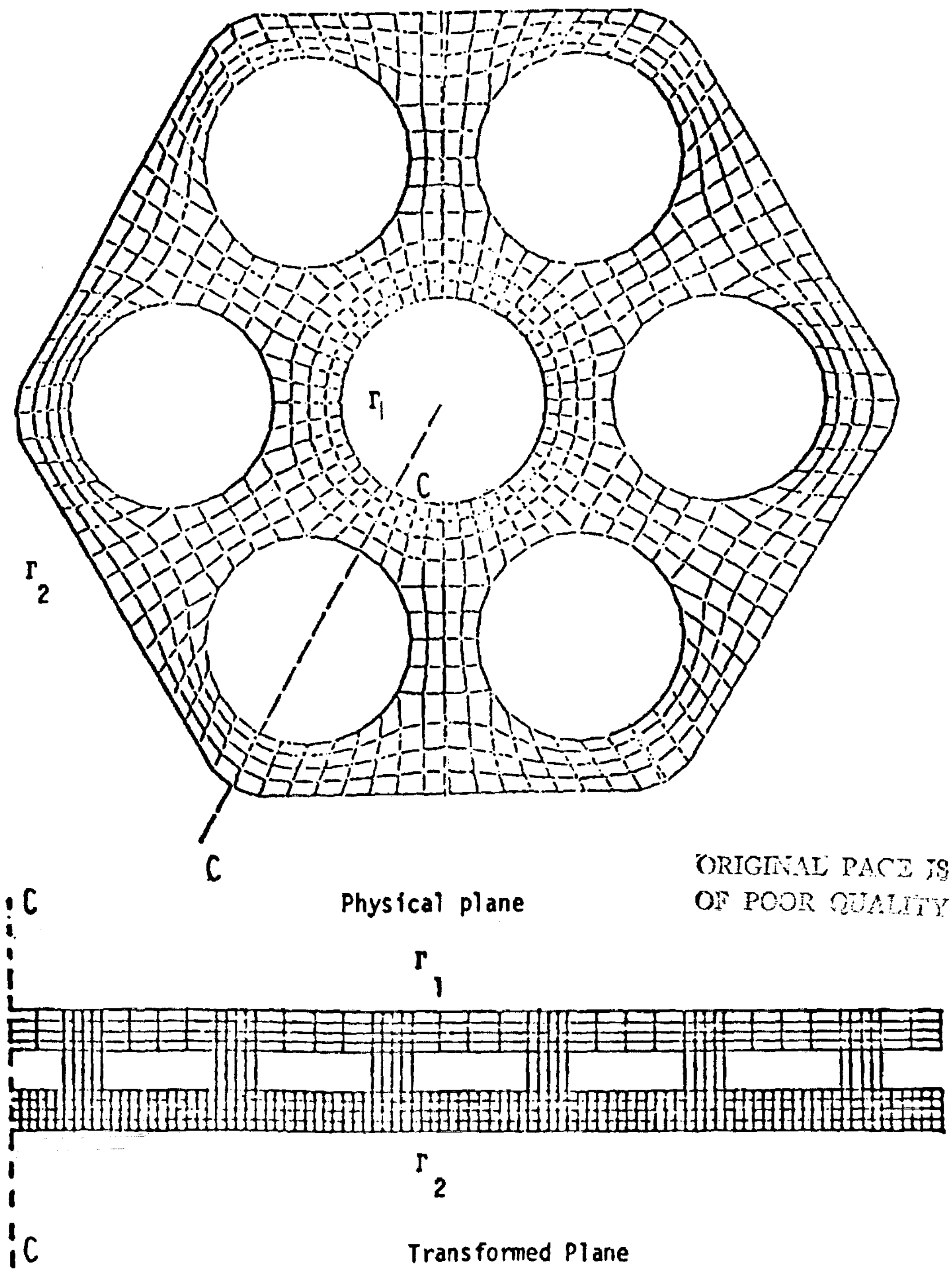

Figure 5.- Nuclear rod-bundle coordinate system (Ref. 13).

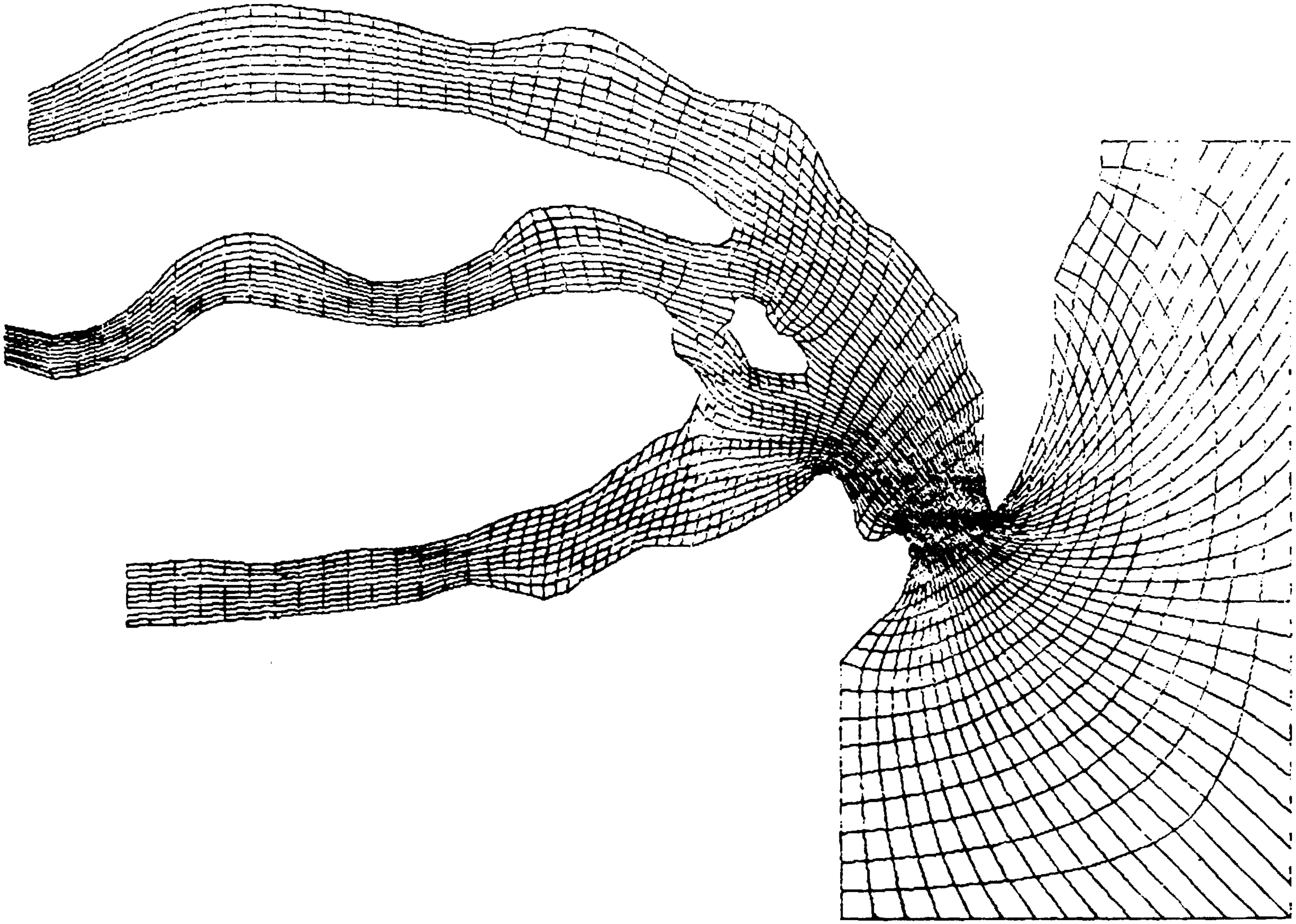

Figure 6.- Coordinate system for Charleston Harbor (Ref. 14).

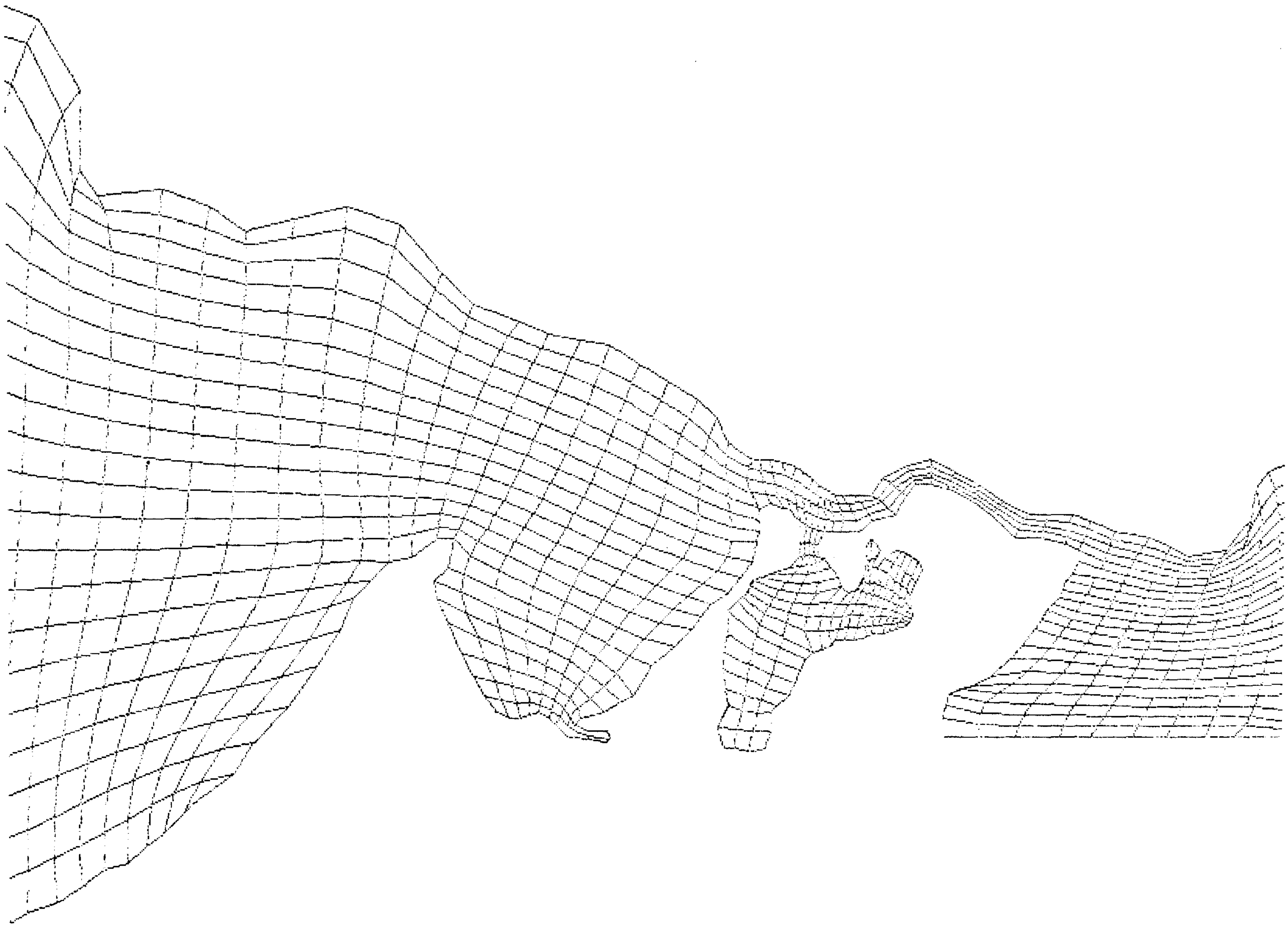

Figure 7.- Coordinate system for a portion of Lake Ponchatrain.