Semi-Annual Status Report

for the period

November 15, 1982 through May 14, 1983

Submitted Under

NASA Grant NSG 1577

Entitled

Transformation of Two and Three-Dimensional Regions by Elliptic Systems

by

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May 16, 1983

TRANSFORMATION OF TWO AND THREE-DIMENSIONAL REGIONS BY ELLIPTIC SYSTEMS

The major effort during this contract period has been the analysis of finite-difference methods for composite grids. It was observed that linear interpolation between grids would suffice only where low order accuracy was required. In the context of fluid flow, this would be in regions where the flow was essentially free stream. Higher order interpolation schemes have also been investigated. The well-known quadratic and cubic interpolating polynomials would increase the formal accuracy of the overall numerical algorithm. However, it can also be shown that the stability of the algorithm may be adversely affected. Further numerical results are needed in order to assess the nature of this instability induced by the interpolation procedure. A complete report on composite grid schemes will be presented at the Conference on Large Scale Scientific Computation. A copy of that paper is attached to this report. One aspect of our work which is not discussed deals with the technical procedures in implementing interpolation schemes used on composite grids. Currently available software is not designed for repeated interpolation at the same points. Therefore, in order to maximize the efficiency of our programs, the location of the points used in the interpolation and the coefficients in the interpolation formula are computed only once. By storing these values, the cost of computing an interpolated value is comparable to the cost of applying the difference equation at an interior grid point.

The recent appearance of the paper by Hoffman (see attached reports) and personal communications with other researchers has motivated us to

take a closer look at the order of a numerical algorithm on a curvilinear coordinate system. The order of a method is, by definition, dependent on the manner in which the grid spacing is decreased. The grid spacing may be decreased by adding grid points or by moving existing grid points. A detailed analysis of order, including many commonly used mapping functions, appears in a paper to be presented at the ASME Applied Mechanics, Bioengineering, and Fluids Engineering Conference. A copy of that paper is also included in this report.

To be presented at the Conference on Large Scale Scientific Computation, Madison, May 1983 (to be published by Academic Press).

ERROR ANALYSIS AND DIFFERENCE EQUATIONS ON CURVILINEAR COORDINATE SYSTEMS

C. Wayne Mastin

1. INTRODUCTION.

A computational grid must be constructed when solving partial differential equations by finite-difference or finite element methods. Presently there are many grid generation algorithms. The choice of algorithm will depend on the users desire for control over properties such as orthogonality of coordinate lines, location of grid points, and smoothness of grid point distribution. All of these properties may affect the accuracy of the numerical solution. A survey of grid generation techniques may be found in the article by Thompson et. al [7]. This report will deal with methods for deriving difference equations on curvilinear coordinate systems and the effect of coordinate systems on the solution. Recent contributions dealing with the effect of the grid on truncation error for one-dimensional problems have been made by Hoffman [3] and Vinokur [8].

The motivation for this investigation can be seen by considering some current problems in computational fluid dynamics. Available computers can be used to model the flow about a wing-fuselage configuration. When additional components, such as fins, stores, and nacelles are added to the aircraft, the computational region becomes increasingly complicated. The grid can be extremely distorted and special difference formulas may be needed due to irregular neighborhood structures as encountered by by Lee et. al. [4] and Roberts [5]. In an attempt to limit grid distortion, overlapping grids have also been used for complicated regions. Each component is endowed with its own local coordinate system, and interpolation is used in the solution algorithm. Various interpolation procedures have been used by Atta [1], Atta and Vadyak [2], and Starius [6]. The

possible impact of the interpolation procedure on the solution algorithm will be investigated. It is noted that the interpolation technique may effect the local truncation error as well as the convergence rate of iterative algorithms and the stability of explicit algorithms.

2. FINITE-DIFFERENCE EQUATIONS.

A curvilinear coordinate system in the xy-plane is understood to be the image of a rectangular Cartesian coordinate system in a $\xi\eta$-plane. The induced grid is therefore composed of quadrilateral cells and difference equations may be derived by transforming the partial differential equation to the $\xi\eta$-plane.

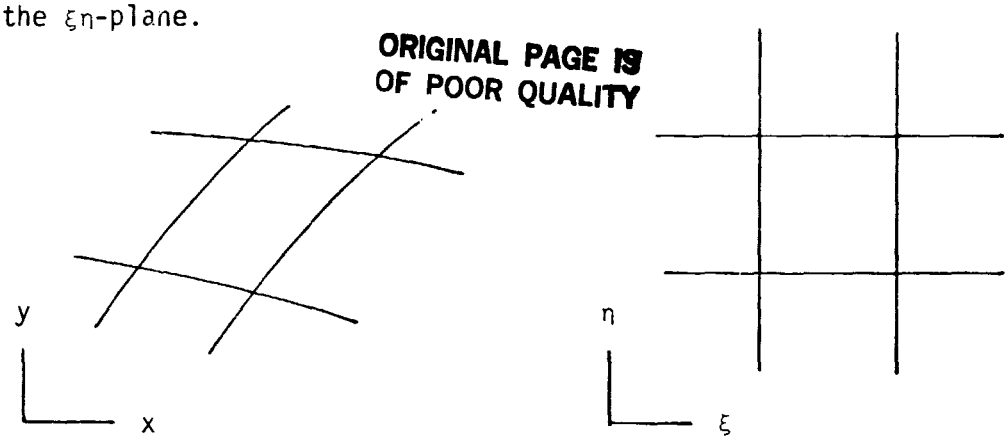

Figure 1.

A typical grid cell is indicated in Figure 1. This derivation gives no information on local truncation error, so an alternate derivation will be presented. Regardless of the derivation, the difference equations will involve derivatives of x and y with respect to ξ and η. Since the grid may be given only as a set at data points, it will be assumed that these derivatives are approximated using differences. It can be shown that the exact computation of these derivatives does not increase the accuracy of the method.

Second order central differences are commonly used in the numerical solution of partial differential equations. The truncation error depends on the grid spacing in the curvilinear coordinate system, and therefore, the corresponding grid spacing in the $\xi\eta$-plane will at present be assumed unity. The difference approximations with respect to ξ and η are then

$$
\begin{aligned}
f_{\xi} &= (f(\xi+1,\eta) - f(\xi-1,\eta))/2 \\
f_{\eta} &= (f(\xi,\eta+1) - f(\xi,\eta-1))/2 \\
f_{\xi\xi} &= f(\xi+1,\eta) + f(\xi-1,\eta) - 2f(\xi,\eta) \\
f_{\xi\eta} &= (f(\xi+1,\eta+1) + f(\xi-1,\eta-1) - f(\xi-1,\eta+1) - f(\xi+1,\eta-1))/4 \\
f_{\eta\eta} &= f(\xi,\eta+1) + f(\xi,\eta-1) - 2f(\xi,\eta).
\end{aligned}
\tag{1}
$$

The local truncation error in using these differences to approximate the derivatives with respect to x and y is revealed by examining a series expansion of the above differences at $(x(\xi,\eta), y(\xi,\eta))$. First derivative approximations are much simpler, and they will be considered first. After a little algebra, the difference expression f_ξ can be represented as

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

$$+ \frac{1}{2} y_\xi y_{\xi\xi} \frac{\partial^2 f}{\partial y^2} + \text{HOT}. \qquad (2)$$

The terms in this expansion can be separated into three categories. The first order terms are used in deriving the difference equations. The second order terms are due to the nonuniform spacing and curvature of the curvilinear coordinate systems. The remaining higher order terms (HOT) are proportional to the third power of the grid spacing, and terms of this order would appear even if a uniform rectangular grid were used. Clearly the same remarks can be made about the series expansion for f_η. From these comments it follows that one condition for the derived difference approximations to be second order, in the sense that the local truncation error is the same order as the square of the grid spacing, is the condition that the following quotients

$$\frac{x_{\xi\xi}}{|r_\xi|^2}, \quad \frac{y_{\xi\xi}}{|r_\xi|^2}, \quad \frac{x_{\eta\eta}}{|r_\eta|^2}, \quad \frac{y_{\eta\eta}}{|r_\eta|^2}, \quad r = (x,y) \qquad (3)$$

remain bounded as $|r_\xi| + |r_\eta|$ approaches zero. A second condition arises when examining the form of the truncation error in the approximation of $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$. From (2) it is seen that the truncation error for $\frac{\partial f}{\partial x}$ can be written

$$Tx = \frac{1}{J}(y_\eta T\xi - y_\xi T\eta)$$

where

$$J = x_\xi y_\eta - x_\eta y_\xi$$

and $T\xi$ and $T\eta$ are the second and higher order terms in (2) and the analogous expansion for f_η. Certainly some lower bound on the rate at which J approaches zero is necessary. Let θ be an approximation of the

angle between the coordinate lines measured by

$$\theta = \arctan\left(\frac{y_\xi}{x_\xi}\right) - \arctan\left(\frac{y_\eta}{x_\eta}\right).$$

If the degree of nonorthogonality is limited by the condition

$$|\cot\theta| \leq M, \tag{4}$$

then

$$J^2 \geq \frac{1}{M+1}|r_\xi|^2|r_\eta|^2$$

Once it is noted that each term in $T\xi$ has a factor of either x_ξ or y_ξ, it follows that when the quotients in (3) and cot θ remain bounded as $|r_\xi| + |r_\eta|$ approaches zero, the order of the difference approximations for first order derivatives is preserved on the curvilinear coordinate system.

The truncation error analysis is considerably more complicated for second order derivatives. The major conclusions will be derived without going into all the technical details. The series expansions for the second order differences are given.

$$f_{\xi\xi} = S^{(1)} + S^{(2)} + HOT$$

where

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

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

$$+ \frac{2}{3}x_{\xi\xi}x_\xi^2\frac{\partial^3 f}{\partial x^3} + \frac{1}{2}[x_\xi(x_\xi y_{\xi\xi} + y_\xi x_{\xi\xi}) + \frac{1}{4}x_{\xi\xi}$$

$$(x_\xi y_\xi + x_{\xi\xi}y_{\xi\xi})]\frac{\partial^3 f}{\partial x^2\partial y} + \frac{1}{2}[y_\xi(y_\xi x_{\xi\xi} + x_\xi y_{\xi\xi}) + \frac{1}{4}y_{\xi\xi}$$

$$(x_\xi y_\xi + x_{\xi\xi}y_{\xi\xi})]\frac{\partial^3 f}{\partial x\partial y^2} + \frac{2}{3}y_{\xi\xi}y_\xi^2\frac{\partial^3 f}{\partial y^3}.$$

The mixed derivative approximation involves diagonal neighbors and it is convenient to introduce the differences

$$f_s = (f(\xi+1,\eta+1) - f(\xi-1,\eta-1))/2\sqrt{2}$$

$$f_t = (f(\xi-1,\eta+1) - f(\xi+1,\eta-1))/2\sqrt{2}$$

$$f_{ss} = (f(\xi+1,\eta+1) + f(\xi-1,\eta-1) - 2f(\xi,\eta))/2$$

$$f_{tt} = (f(\xi-1,\eta+1) + f(\xi+1,\eta-1) - 2f(\xi,\eta))/2.$$

The series expansion has the form

$$f_{\xi\eta} = T^{(1)} + T^{(2)} + HOT$$

where

$$T^{(1)} = x_{\xi\eta}\frac{\partial f}{\partial x} + y_{\xi\eta}\frac{\partial f}{\partial y} + x_{\xi}x_{\eta}\frac{\partial^2 f}{\partial x^2} + (x_{\xi}y_{\eta} + x_{\eta}y_{\xi})\frac{\partial^2 f}{\partial x \partial y}$$

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

$$T^{(2)} = \frac{1}{2}x_{\xi\eta}(x_{ss} + x_{tt})\frac{\partial^2 f}{\partial x^2} + \frac{1}{2}(x_{\xi\eta}(y_{ss} + y_{tt}) + y_{\xi\eta}$$

$$(x_{ss} + x_{tt}))\frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2}y_{\xi\eta}(y_{ss} + y_{tt})\frac{\partial^2 f}{\partial y^2}$$

$$+ \frac{2}{3}(x_{ss}x_s^2 - x_{tt}x_t^2)\frac{\partial^3 f}{\partial x^3} + \frac{1}{2}[x_s(x_s y_{ss} + y_s x_{ss})$$

$$+ \frac{1}{4}x_{ss}(x_s y_s + x_{ss}y_{ss}) - x_t(x_t y_{tt} + y_t x_{tt})$$

$$- \frac{1}{4}x_{tt}(x_t y_t + x_{tt}y_{tt})]\frac{\partial^3 f}{\partial x^2 \partial y} + \cdots.$$

Once again the terms have been categorized into those used in the derivation of the difference equations, $S^{(1)}$ and $T^{(1)}$, the second and third order terms due to the curvilinear coordinates, $S^{(2)}$ and $T^{(2)}$, and the higher order terms which are representative of truncation error that would be present on a uniform rectangular grid. The two third order terms in $T^{(2)}$ which are omitted would be obtained by interchanging x and y in the two third order terms that are present. Now the differences with respect to s and t can be bounded by differences with respect to ξ and η. Therefore, the only additional conditions, other than those required for first derivatives, in order that the truncation error for second derivatives be the same order as the square of the grid spacing is that the

quotients

$$\frac{x_{\xi\eta}}{|r_\xi||r_\eta|}, \quad \frac{y_{\xi\eta}}{|r_\xi||r_\eta|}$$

remain bounded as $|r_\xi| + |r_\eta|$ approaches zero.

In the numerical solution of a partial differential equation, the truncation error may be decreased at a point by adding grid points or moving existing grid points. The technique used to decrease the grid spacing has a significant effect on the local truncation error as the above analysis indicates. This fact is further illustrated in the following one-dimensional examples. Let $x(\xi)$ be an arbitrary fixed grid point. Consider a sequence of grids where the distance between $x^{(n)}(\xi) = x(\xi)$ and its neighbors, $x^{(n)}(\xi-1)$ and $x^{(n)}(\xi+1)$, is decreased by a factor of 2 at each step. Then

$$\frac{x_{\xi\xi}^{(n)}}{(x_\xi^{(n)})^2} = 2\,\frac{x_{\xi\xi}^{(n-1)}}{(x_\xi^{(n-1)})^2} = 2^n\,\frac{x_{\xi\xi}^{(0)}}{(x_\xi^{(0)})^2}$$

and a reduction in the order of the local truncation error would occur unless the original grid was uniform; i.e., $x_{\xi\xi} = 0$. Now consider the case where the grid is defined by a mapping $x(\xi) = f(\zeta)$. Suppose the neighbors of $x(\xi)$ are $x(\xi-1) = f(\zeta-h)$ and $x(\xi+1) = f(\zeta+h)$. Then if $f'(\zeta) \neq 0$ and $f''(\zeta)$ exists

$$\lim_{h\to 0} \frac{x_{\xi\xi}}{x_\xi^2} = \frac{f''(\zeta)}{[f'(\zeta)]^2}$$

is finite. In this case the local truncation error is proportional to the square of the grid spacing or $O(h^2)$. It has been assumed that the function f and the image of $x(\xi)$, which is denoted by ζ, are fixed. This conclusion, that the order is preserved, would not necessarily hold if the function f changed as $h \to 0$.

It was noted above that the degree of skewness in a nonorthogonal coordinate system must be limited to maitain the order of the numerical algorithm. The effect of skewness can be further clarified by noting that

$$J = |r_\xi||r_\eta| \sin\theta.$$

Therefore, for first derivative approximations, the local truncation error varies inversely as the sine of the angle between the coordinate lines. It can also be shown that, for second derivative approximations, an increase in truncation error by a factor of $\sin^{-2}\theta$ is possible. If the skewness is accompanied by large variations in grid spacing, this factor increases to $\sin^{-3}\theta$. The general conclusion is that a moderate degree of skewness has little effect on truncation error. The principal disadvantage in using nonorthogonal coordinates is the added complexity of the difference equations.

Certainly this development does not cover all possible discretizations of a partial differential equation. However, similar conclusions hold for other commonly used difference approximations. In particular, the same conditions for maintaining the order of the difference approximation suffice when second order partial derivatives of the form

$$\frac{\partial}{\partial x}\left(a\frac{\partial f}{\partial x}\right)$$

are approximated by

$$\frac{1}{J}\left\{y_\eta\left[\frac{a}{J}(y_\eta f_\xi - y_\xi f_\eta)\right]_\xi - y_\xi\left[\frac{a}{J}(y_\eta f_\xi - y_\xi f_\eta)\right]_\eta\right\}.$$

Extreme distortions in grid cells can have an especially serious effect in the finite difference analogs of conservation laws. If the partial differential equation

$$f_x + g_y = s \tag{5}$$

is approximated by

$$(fy_\eta - gx_\eta)_\xi + (gx_\xi - fy_\xi)_\eta = Js,$$

then the consistency of the difference equation depends on the difference between

$$[(uv_\eta)_\xi - (uv_\xi)_\eta]/J$$

and

$$[u_\xi v_\eta - u_\eta v_\xi]/J$$

converging to zero where u and v are either of the coordinate variables x and y.

3. FINITE VOLUME EQUATIONS

An alternate method for approximating conservation laws has been widely used on curvilinear coordinate systems. Generally referred to as the finite volume method, it is derived by integrating the differential equation (5) over a grid cell and applying the Gauss Divergence Theorem.

Let C be an arbitrary grid cell with vertices $r(\xi,\eta)$, $r(\xi+1,\eta)$, $r(\xi,\eta+1)$, $r(\xi+1, \eta+1)$, where $r = (x,y)$. Let $f(\xi + \frac{1}{2}, \eta + \frac{1}{2})$ denote the values of the function f at the centroid of C. In the literature, the mean value over the cell is sometimes used rather than the value at the centroid. Since the difference in the two values is the same order as the truncation error, either definition may be assumed. Integrating equation (5) over C gives

$$\int_{\partial c} f\,dy - g\,dx = \int_{c} s\,dxdy.$$

A third order quadrature may be derived by using the values of f and g at the midpoints of the cell sides. In the usual finite volume formulation, this value on the cell side is approximated by the average of the values on the two cells having the given side in common. Thus the derived difference equation is of the form

$$\sum_{i=1}^{4} (\mu f)_i (\Delta y)_i - (\mu g)_i (\Delta x)_i = As \tag{6}$$

where A is the area of C and, for example,

$$(\mu f)_1 = \frac{1}{2}\left(f(\xi - \tfrac{1}{2},\eta + \tfrac{1}{2}) + f(\xi + \tfrac{1}{2},\eta + \tfrac{1}{2})\right)$$

$$(\Delta x)_1 = x(\xi,\eta) - x(\xi,\eta+1).$$

The effect of the curvilinear coordinate system can be analyzed by considering the difference between μf and the corresponding value of f at the midpoint of the common side. The Taylor series expansion of this difference is, for example,

$$\frac{1}{2}\left(f(\xi - \tfrac{1}{2},\eta + \tfrac{1}{2}) + f(\xi + \tfrac{1}{2},\eta + \tfrac{1}{2})\right) - f(\xi,\eta+\tfrac{1}{2}) = \tag{7}$$

$$\frac{1}{2}\frac{\partial f}{\partial x}(\xi,\eta+\tfrac{1}{2})\, x_{\xi\xi}(\xi,\eta+\tfrac{1}{2}) + \frac{1}{2}\frac{\partial f}{\partial y}(\xi,\eta+\tfrac{1}{2})\, y_{\xi\xi}(\xi,\eta+\tfrac{1}{2}) + \text{HOT}$$

where in this case

$$x_{\xi\xi}(\xi,\eta+\tfrac{1}{2}) = x(\xi+\tfrac{1}{2},\eta+\tfrac{1}{2}) + x(\xi-\tfrac{1}{2},\eta+\tfrac{1}{2}) - 2x(\xi,\eta+\tfrac{1}{2}),$$

with

$$x(\xi,\eta+\tfrac{1}{2}) = \tfrac{1}{2}\left(x(\xi,\eta+1) + x(\xi,\eta)\right).$$

Thus we again see that the order of the quadrature formula is preserved on the curvilinear coordinate system if the quotients in (3) remain bounded as the grid spacing decreases to zero. Here $|r_\xi|$ and $|r_\eta|$ are the distances between the cell centroids. The higher order terms, HOT, in (7) are the same order as the square of the grid spacing and hence do not decrease the third order accuracy that would exist with the midpoint rule.

Due to the simplicity of the equation (5) which was considered, several aspects of the finite volume method have not been mentioned. In practice, s is generally the temporal derivative of some physical quantity. When (6) is solved for s, it is apparent that some lower bound must be placed on A. This is again accomplished by limiting the nonorthogonality and is consistent with results for finite element methods where excessively thin elements are to be avoided. It is also noted that, in most finite volume methods, the equation (6) is implemented in a two-step algorithm to produce second order temporal accuracy.

Basically then, the finite volume methods also require restrictions on the grid to maintain the order of the algorithm. However they can be easier to implement in cases where many rectangular grids are patched together to fill a complicated region. In such cases it is not uncommon for a grid point to have more or less than four neighbors. This causes no problem in deriving finite volume equations, but special difference formulas must be derived when using the finite difference methods as described above. The same comment can be made for cases where triangular grids are produced by singularities in the curvilinear coordinate system.

4. PATCHED COORDINATE SYSTEMS

Thus far we have considered the curvilinear coordinate system at each point to be topologically equivalent to a rectangular cartesian coordinate system in the plane. As has been shown, a loss of accuracy in the numerical algorithm may occur if the grid is severely distorted. Therefore, when the region is too complicated, it may be advisable to partition the region and construct a separate curvilinear coordinate system for each subregion. Most grid generation techniques are flexible enough to permit

the smooth continuation of coordinate lines from one subregion into the next. However, at points where the boundaries of several subregions intersect, there may be greater than or less than four neighboring points. An inspection will reveal four grid points which have five neighbors in the grid of Figure 2. Special techniques must be applied to derive

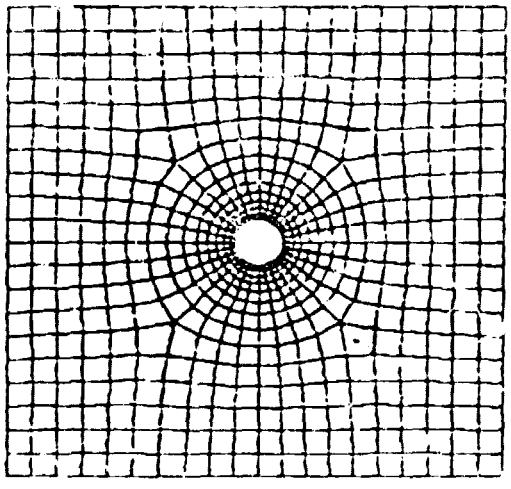

Figure 2.

difference equations at these points. One simple technique would be to select five nearby points and compute a Taylor series truncated after the second order terms. This would give a system of five equations which would be solved to obtain difference approximations for the first and second order derivatives. Unfortunately, the difference equation derived by this method would not resemble the difference equations at other points, which it is assumed would be derived by the usual change of variables formulas. Thus the effect of this differencing technique on numerical properties such as stability and iterative convergence would be uncertain.

A second method of dealing with special points caused by grid patching is more compatible with the usual differencing techniques. Basically it involves selecting nearby points to form a local curvilinear coordinate system. Let $r(\xi,\eta) = (x(\xi,\eta), y(\xi,\eta))$ be a grid point with an excess or deficiency of neighbors. Then four grid points, denoted by $r(\xi \pm 1,\eta)$ and $r(\xi, \eta \pm 1)$, are chosen to define the two coordinate directions through $r(\xi,\eta)$. Four additional points, denoted by $r(\xi \pm 1, \eta \pm 1)$ and $r(\xi \pm 1, \eta \mp 1)$, are chosen from the four quadrants of the new curvilinear coordinate system. The nine points to be used in deriving the difference equation at $r(\xi,\eta)$ have been defined. But the coordinate lines and grid cells may

be far from that of a uniform rectangular grid. Therefore, as has been discussed in Section 2, a loss of accuracy is to be expected when the usual finite difference equations are employed. In fact, the local truncation error for the first derivatives will be the same order as the grid spacing. Convergence of second derivative approximations cannot be guaranteed as the grid spacing decreases to zero. Despite this discouraging note, accurate results have been computed using this technique. The inconsistency of the difference approximation for second order equations motivated the search for a higher order approximation. A system of five equations in the five partial derivatives of the function f can be constructed by truncating the Taylor series expansions of the central differences in (1) after the second order terms. The system is written below with the notation of Section 2.

$$\begin{bmatrix} f_\xi \\ f_\eta \\ f_{\xi\xi} \\ f_{\xi\eta} \\ f_{\eta\eta} \end{bmatrix} = \begin{bmatrix} x_\xi & y_\xi & \frac{1}{2}x_\xi x_{\xi\xi} & \frac{1}{2}(x_\xi y_{\xi\xi} + y_\xi x_{\xi\xi}) \\ x_\eta & y_\eta & \frac{1}{2}x_\eta x_{\eta\eta} & \frac{1}{2}(x_\eta y_{\eta\eta} + y_\eta x_{\eta\eta}) \\ x_{\xi\xi} & y_{\xi\xi} & x_\xi^2 + \frac{1}{4}x_{\xi\xi}^2 & 2x_\xi y_\xi + \frac{1}{2}x_{\xi\xi}y_{\xi\xi} \\ x_{\xi\eta} & y_{\xi\eta} & x_\xi x_\eta + \frac{1}{2}x_{\xi\eta}(x_{ss}+x_{tt}) & x_\xi y_\eta + x_\eta y_\xi + x_{\xi\eta}(y_{ss}+y_{tt}) \\ x_{\eta\eta} & y_{\eta\eta} & x_\eta^2 + \frac{1}{4}x_{\eta\eta}^2 & 2x_\eta y_\eta + \frac{1}{2}x_{\eta\eta}y_{\eta\eta} \end{bmatrix}$$

$$\begin{bmatrix} \frac{1}{2}y_\xi y_{\xi\xi} \\ \frac{1}{2}y_\eta y_{\eta\eta} \\ y_\xi^2 + \frac{1}{4}y_{\xi\xi}^2 \\ y_{\xi\eta}(x_{ss}+x_{tt}) \quad y_\xi y_\eta + \frac{1}{2}y_{\xi\eta}(y_{ss}+y_{tt}) \\ y_\eta^2 + \frac{1}{4}y_{\eta\eta}^2 \end{bmatrix} \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial^2 f}{\partial x^2} \\ \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \qquad (8)$$

For a uniform rectangular grid, the usual difference approximations are produced. Although it cannot be guaranteed that the coefficient matrix is well-conditioned or at least nonsingular, this is suggested by the fact that the system (8) is a perturbation of the nonsingular system of equations which produces the usual difference equations. The later system has a coefficient matrix whose determinant is J^3. This technique generates a nine-point difference equation using the same differences on the local coordinate system that are used at the other points of the grid.

The local truncation error for first derivative approximations is the same order as the square of the grid spacing, whereas, the local truncation error for second derivative approximations is the order of the grid spacing. This result is valid regardless of the coordinate line spacing or curvature. It is only assumed that the coefficient matrix is not ill-conditioned.

While it is possible to generate consistent difference equations at special points encountered in grid patching, it should be noted that loss of accuracy is possible. The condition that grid lines pass smoothly from one region into the next also places a restriction on the number and location of grid points in each subregion. Coordinate lines which are discontinuous, or have discontinuous slopes, at subregion boundaries can be used, but this further complicates the problem of deriving accurate difference equations.

5. OVERLAPPING COORDINATE SYSTEMS

When dealing with complicated regions, especially multiply connected regions, there may be portions of the boundary where a curvilinear coordinate system can be easily constructed. For example, consider the region between a rectangle and a circle. A polar coordinate system is the obvious choice near the circle while a cartesian coordinate system would be best near the rectangle. Each of these coordinate systems can be extended into the region until they overlap and form a covering of the region by grid cells as illustrated in Figure 3. In general, there may be

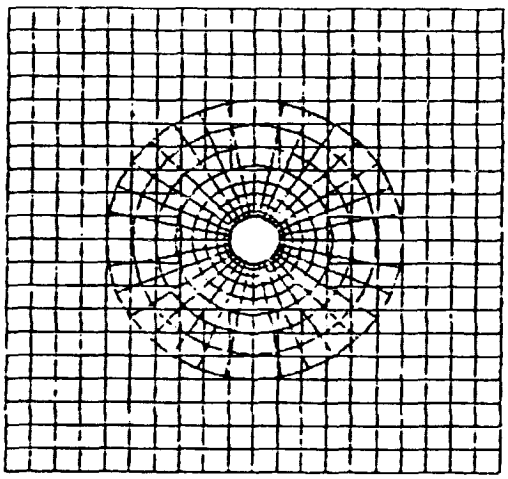

Figure 3.

several overlapping grid systems used to cover a particular region. The difference equations must couple the solution values on the various grid systems. This transmission of information is most frequently accomplished by interpolation at those grid boundary points which lie in the interior of the region. Several interpolation procedures will be examined along with their impact on finite difference methods.

Let $G^{(1)}$ be a grid with boundary point r_0 which is contained in some grid cell of the grid $G^{(2)}$. First, the general interpolation formula

$$f(r_0) = \sum_{j=1}^{k} \alpha_j f(r_j) \tag{9}$$

will be considered where r_j denotes a point in $G^{(2)}$. When the value of f at r_0 is replaced in a difference equation by the interpolated value, a new difference equation results which may have a different local truncation error. Conditions on the coefficients α_j which will preserve the order of the difference equation can be derived by examining the effect on a Taylor series at an interior neighbor r of r_0. If the value of f at r_0 is computed from the values at r_j by (9), then

$$\begin{aligned} f(r_0) = &\sum_{j=1}^{k} \alpha_j \, f(r) + \sum_{j=1}^{k} \alpha_j (x_j - x) \frac{\partial f}{\partial x}(r) \\ &+ \sum_{j=1}^{k} \alpha_j (y_j - y) \frac{\partial f}{\partial y}(r) \\ &+ \sum_{j=1}^{k} \alpha_j (x_j - x)^2 \frac{\partial^2 f}{\partial x^2}(r) \\ &+ 2 \sum_{j=1}^{k} \alpha_j (x_j - x)(y_j - y) \frac{\partial^2 f}{\partial x \partial y}(r) \\ &+ \sum_{j=1}^{k} \alpha_j (y_j - y)^2 \frac{\partial^2 f}{\partial y^2}(r) + \cdots . \end{aligned}$$

This series coincides with the actual Taylor series, computed at r_0, through first order terms if

$$\sum_{j=1}^{k} \alpha_j = 1, \quad \sum_{j=1}^{k} \alpha_j x_j = x_0, \quad \sum_{j=1}^{k} \alpha_j y_j = y_0, \tag{10}$$

and through second order terms if, in addition,

$$\sum_{j=1}^{k} \alpha_j (x_j)^2 = (x_0)^2, \quad \sum_{j=1}^{k} \alpha_j x_j y_j = x_0 y_0, \quad \sum_{j=1}^{k} \alpha_j (y_j)^2 = (y_0)^2. \tag{11}$$

It will be assumed that the conditions, indicated in Section 2, for preserving the order of first and second order difference equations hold for the individual grids $G^{(1)}$ and $G^{(2)}$. In that case, the local truncation error for first derivative approximations would be the same order as the grid spacing if (10) holds and the same order as the square of the grid spacing if both (10) and (11) hold. The order of the local truncation error for second order differences would be the same as the grid spacing if both (10) and (11) hold. The order would be the square of the grid spacing if an additional condition equating the coefficients of third order terms in the series was imposed. The condition which equates the p th order coefficients can be written as

$$\sum_{j=1}^{k} \alpha_j [x_j]^m [y_j]^{n-m} = [x_0]^m [y_0]^{n-m}, \tag{12}$$

$n + m = p$, $m = 0, 1, \cdots, p$.

Implicit schemes tend to be difficult to implement on regions which use several curvilinear coordinate systems. Therefore, most currently used algorithms involve the iterative solution of elliptic equations or the explicit solution of parabolic or hyperbolic equations. This naturally leads one to question the effect of the interpolation equation on iterative convergence in the first case and on stability in the later case. No detailed analysis will be given here, but a few obvious comments are worth noting. Diagonal dominance of the coefficient matrix of the difference equations is a sufficient, although not necessary, condition for the convergence of many iterative methods. A system of diagonally dominant difference equations will remain diagonally dominant when the interpolation equations (9) are appended if

$$\sum_{j=1}^{k} |\alpha_j| \leq 1. \tag{13}$$

However, when this condition is considered with the first equation in (10), which is necessary for consistency, it follows that diagonal dominance will be preserved whenever

$$\alpha_j \geq 0, \quad j = 1, 2, \cdots, k. \tag{14}$$

The stability properties of (9) can also be observed. Suppose the value at r_0 is computed at $t = (n+1)\Delta t$ by

$$f(r_0,(n+1)\Delta t) = \sum_{j=1}^{k} \alpha_j f(r_j,n\Delta t). \tag{15}$$

The von Neumann stability analysis is based on the behavior of an exponential solution of the form

$$f(x,y,t) = \exp(\lambda t)\exp(i\mu x)\exp(i\nu y).$$

Substituting in (15) gives the following

$$\exp(\lambda\Delta t) = \sum_{j=1}^{k} \alpha_j \exp(i\mu\Delta x_j)\exp(i\nu\Delta y_j),$$

where $\Delta x_j = x_j - x_0$ and $\Delta y_j = y_j - y_0$. For real μ and ν, the exponential solution will remain bounded as $n\to\infty$ provided (13) holds. Therefore, whenever (14) holds along with (10), the interpolation equations impose no additional stability restriction on the numerical algorithm.

Several different interpolation schemes will be reviewed in light of the above remarks. The first scheme is based on the approximation of a linear Taylor polynomial. For each boundary point r_0 of $G^{(1)}$, select a nearby point r_1 of $G^{(2)}$. The neighbors of r_1 in $G^{(2)}$ are indexed as in Figure 4 so that

$$f_\xi(r_1) = (f(r_3) - f(r_2))/2$$

$$f_\eta(r_1) = (f(r_5) - f(r_4))/2.$$

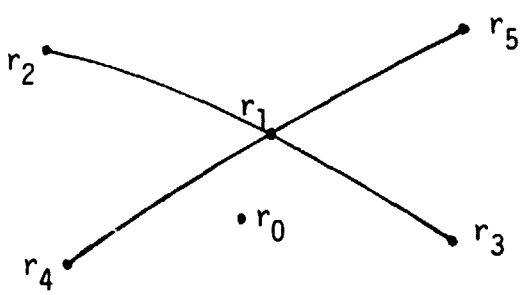

Figure 4.

These differences can be used to approximate the partial derivatives with respect to x and y. If the approximations are substituted in a Taylor series, truncated after the linear terms, then the resulting interpolation formula can be written

$$f(r_0) = \sum_{j=1}^{k} \alpha_j f(r_j),$$

where

$$\alpha_1 = 1$$

$$\alpha_2 = -\alpha_3 = ((x_0 - x_1)\, y_\eta - (y_0 - y_1)x_\eta)/2J$$

$$\alpha_4 = -\alpha_5 = ((y_0 - y_1)\, x_\xi - (x_0 - x_1)y_\xi)/2J.$$

In this case, it easily observed that equations (10) are valid, but (14) does not generally hold. Second degree Taylor polynomials have been used, but will not be considered here. It is doubtful that they would give better results since the approximation of second derivatives from the numerical solution may be very inaccurate. There are other interpolation schemes for which both (10) and (14) hold and these will be investigated next.

Let r_0 belong to a grid cell C of $G^{(2)}$ with vertices which will be denoted by r_j, j = 1, 2, 3, 4, as illustrated in Figure 5. There exists

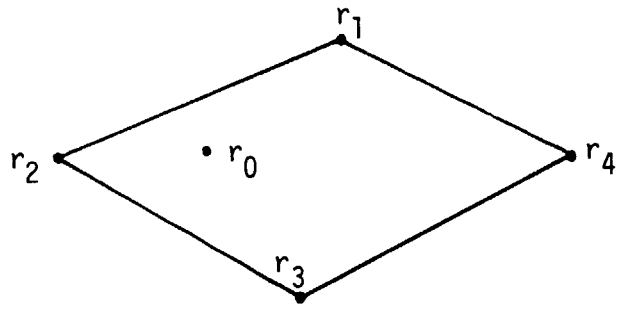

Figure 5.

a unique bilinear mapping of the unit square onto the cell C. The mapping can be given explicitly by

$$r = (1 - s)(1 - t)\, r_1 + s(1 - t)\, r_2 + t(1 - s)\, r_4 + st\, r_3,$$

where $0 \leq s, t \leq 1$. If we set $r = r_0$, then the system of two equations, in terms of the x and y coordinates, can be solved to determine the solution $s = s_0$, $t = t_0$. If f is also assumed to be a bilinear function of s and t, then

$$f(r_0) = (1 - s_0)(1 - t_0)\, f(r_1) + s_0(1 - t_0)\, f(r_2) + t_0(1 - s_0)\, f(r_4) + s_0 t_0\, f(r_3). \qquad (16)$$

It is immediately evident that this interpolation formula satisfies both (10) and (14). Although equations (11) would not be satisfied, this method can be modified to give higher order interpolants. Basically it involves constructing a bicubic mapping of a square grid in the st-plane onto the union of the nine cells consisting of C and the eight cells having an edge or vertex in common with C. This mapping can be expressed in terms of cubic Lagrange interpolating polynominals. The only additional difficulty is that the bicubic equations which determine s_0 and t_0 would now have to be solved numerically whereas the values of s_0 and t_0 in (16) can be computed exactly. By construction, the coefficients for the bicubic interpolation will satisfy (12) for $p = 0, 1, 2, 3$. Therefore the interpolation scheme would not increase the local truncation error. However, (14) would not be valid.

Interpolation on triangular regions is very popular in finite element analysis. Some of those ideas can be adapted to the present problem. Suppose each quadrilateral cell is divided into two triangular cells. Then r_0 will belong to a triangular cell with vertices r_1, r_2, r_3. Note that this would be the case in Figure 5 if the quadrilateral is partitioned by the diagonal from r_1 to r_3. Now the three equations in (10) determine the coefficients for the interpolation formula (9) which coincides with linear interpolation on the triangular cell. As long as r_0 is an interior or boundary point of the cell, the condition (14) will be satisfied. The accuracy of the interpolation formula can be increased by increasing the

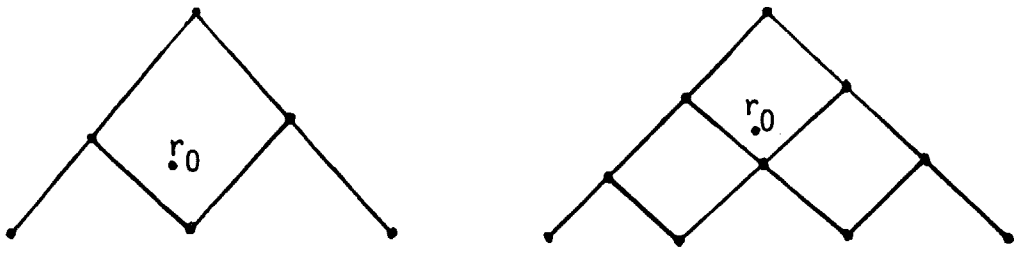

Figure 6.

number of interpolation points. Figure 6 indicates the grid points which could be used for quadratic and cubic interpolation. In each case, the coefficients in (9) can be calculated from the general equations in (12). The quadratic interpolant uses six coefficients obtained by setting $p = 0, 1, 2$ and the ten coefficients for the cubic interpolant are found by solving (12) with $p = 0, 1, 2, 3$. A few cautionary notes are in order. The linear interpolation polynomial always exists, but for severely distorted grids, the system in (12) may be singular and the interpolation polynomial may not exist in the quadratic and cubic case. Condition (14) is also not satisfied in the quadratic and cubic case.

Several interpolation schemes have been presented for use on overlapping coordinate systems. This does not include all techniques which are presently in use. In particular, we have not considered methods which interpolate normal derivatives at the boundary points of each grid. There is no reason why this analysis cannot be extended to cover that case. We would only need consider the formula (9) with some of the r_i in $G^{(1)}$ and the remaining r_i in $G^{(2)}$.

6. CONCLUSIONS.

The procedure for selecting a curvilinear coordinate system must necessarily involve a balance of certain requirements. The rate of change in coordinate line spacing and degree of skewness should be limited so that the formal accuracy of the difference equation is maintained. On the other hand, efficient use of grid points mandates the clustering of points in regions where the derivatives of the theoretical solution are large. If one must use a highly distorted coordinate system or is faced with the prospect of connecting many separate curvilinear coordinate systems in different subregions, it is generally possible to derive consistent difference approximations. While higher order approximations may exist, their use may not be necessary or advisable. The grid spacing is only one factor in the local truncation error. The other factor is the theoretical solution of the partial differential equation. In a region where all derivatives of the solution are negligible, the local truncation error will be small regardless of the order. Consequently, when solving fluid flow problems, the accuracy of the numerical algorithm is most likely to be maintained if irregularities in the grid can be confined to regions of free stream flow. There are multitudes of examples where the use of higher order methods produce inferior results for one reason or the other. In connection with the use of interpolation for overlapping coordinate systems, it should be recalled that Lagrange interpolating polynomials may be highly

oscillatory.

The analysis of error for nonlinear systems of partial differential equations solved numerically on large computational grids can never be precise. However the quality of a numerical solution can often be judged by examining the grid and the point-to-point variation in the numerical solution at the grid points and possibly by recomputing the solution on a properly refined grid.

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The author was supported by NASA Grant NSG 1577, Langley Research Center.

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To be presented at ASME Applied Mechanics, Bioengineering, and Fluids Engineering Conference, Houston, June 1983 (to be published by ASME).

Order of Difference Expressions for Curvilinear Coordinate Systems

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ABSTRACT

The order of finite difference representations on general curvilinear coordinate systems is considered in some detail. It is shown that the uniform grid order is formally preserved on the nonuniform, nonorthogonal grid in the sense of the error behavior with an increase in the number of points. However, the coefficients in the series expansion may become quite large for some point distributions. Several specific distributions are evaluated.

INTRODUCTION

Numerically-generated, boundary-conforming curvilinear coordinate systems have now become common in the numerical solution of partial differential equations, allowing very general codes to be constructed which are applicable to regions with arbitrarily-shaped boundaries. Surveys have been given in (1) and (2), and a source book with both basic exposition and state-of-the-art developments, (3), has recently become available.

Difference representations on curvilinear coordinate systems are constructed by first transforming derivatives with respect to cartesian coordinates into expressions involving derivatives with respect to the curvilinear coordinate and derivatives of the cartesian coordinates with respect to the curvilinear (the metric coefficients). The derivatives with respect to the curvilinear coordinates are then replaced with difference expressions on the uniform grid in the transformed region.

Considerable attention is appropriately now being focussed on evaluation of the truncation error of difference expressions on these curvilinear systems, but some misunderstandings have arisen regarding the identification of the true order of these expressions. The "order" of a difference representation refers to the exponential rate of decrease of the truncation error with the point spacing. On a uniform grid this concerns simply the behavior of the error with a decrease in the point spacing. With a nonuniform point distribution, there is some ambiguity in the interpretation of order, in that the minimum spacing may be decreased either by increasing the number of points in the field or by changing the distribution of a fixed number of points. Both of these could, of course, be done simultaneously, or the points could even be moved randomly, but to be meaningful the order of a difference representation must relate to the error behavior as the point spacing is decreased according to some pattern. This is a moot point with uniform spacing, but two senses of order on a nonuniform grid emerge: the behavior of the error as (1) the number of points in the field is increased while maintaining the same relative point distribution over the field, or (2) the point distribution over the field is changed so as to reduce the minimum spacing with a fixed number of points in the field.

On curvilinear coordinate systems, then, the definition of order of a difference representation is integrally tied to point distribution functions. The order is determined by the error behavior as the spacing varies with the points fixed in a certain distribution, either by increasing the number of points or by changing a parameter in the distribution, not simply by consideration of the points used in the difference expression as being unrelated to each other. This point is essentially what is noted by Hoffman in (4). Actually global order is meaningful only in the first sense, since as the minimum spacing is reduced with a fixed number of points in the field, the spacing somewhere else must certainly increase. This second sense of order on a nonuniform grid then is relevant only locally in regions where the spacing does in fact decrease as the point distribution is changed.

The question of order with nonuniform spacing has recently been considered by Vinokur (5), Hoffman (4), and by Thompson (2). Other studies of error on curvilinear coordinate systems have been reported in (6-7). The present discussion attempts to clarify this question.

ORDER ON NONUNIFORM SPACING

A general one-dimensional point distribution function can be written in the form

$$x(\xi) = g\left(\frac{\xi}{N}\right) \qquad (0 \leq \xi \leq N) \qquad (1)$$

In the following analysis, x will be considered to vary from 0 to 1. Any other range of x can be constructed simply by multiplying the distribution functions given here by an appropriate constant. With this form for the distribution function, the effects of increasing the number of points in a discretization of the field can be seen explicitly by defining the values of ξ at the points to be successive integers from 0 to N. In this form, N + 1 is then the number of points in the discretization, so that the dependence of the error expressions on the number of points in the field will be displayed explicitly by N. This form removes the confusion that can arise in interpretation of analyses based on a fixed ξ interval (0,1) where variation of the number of points is represented by variation of the interval $\Delta\xi$. The form of the distribution function, i.e., the relative concentration of points in certain areas while the total number of points in the field is fixed, is varied by changing parameters in the function.

The transformation of the first derivative is given by

$$f_x = \frac{f_\xi}{x_\xi} \tag{2}$$

if f_ξ is approximated by the second-order central difference expression we have, since $\Delta\xi = 1$ here,

$$f_\xi = \tfrac{1}{2}(f_{i+1} - f_{i-1}) + T_\xi \tag{3}$$

where T_ξ is the truncation error in this difference expression, and i±1 indicates points adjacent to the central point, i.e., indicates increments in ξ. A Taylor series expansion in ξ yields

$$T_\xi = f_\xi - \tfrac{1}{2}\sum_{n=0}^{\infty}\frac{1}{n!}f_{(n)} + \tfrac{1}{2}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}f_{(n)}$$

where $f_{(n)}$ represents the n^{th} ξ-derivative of f. The n = 0 and n = 1 terms lead to cancellations, so that T_ξ can be written

$$T_\xi = -\sum_{n=1}^{\infty}\frac{1}{(2n+1)!}f_{(2n+1)} \tag{4}$$

Using (3), the difference expression for f_x on this point distribution is

$$f_x = \frac{1}{2x_\xi}(f_{i+1} - f_{i-1}) + T_x \tag{5}$$

where now $T_x = \frac{1}{x_\xi}T_\xi$ is the truncation error in this difference representation of f_x. From (4) we have then

$$T_x = -\frac{1}{x_\xi}\sum_{n=1}^{\infty}\frac{1}{(2n+1)!}f_{(2n+1)} \tag{6}$$

Here the metric coefficient, x_ξ, is considered to be evaluated analytically, and hence has no error. (The case of numerical evaluation of the metric coefficients is considered in a later section.)

Now the series in (6) cannot be truncated without further consideration since the ξ-derivatives, $f_{(2n+1)}$, are dependent on the point distribution. Thus if the point distribution is changed, either through the addition of more points or through a change in the form of the disribution function, these derivatives will change. Since the terms of the series do not contain a power of some quantity less than unity, there is no indication that the successive terms become progressively smaller.

It is thus not meaningful to give the truncation error in terms of ξ-derivatives of f. Rather, it is necessary to transform these ξ-derivatives to x-derivatives, which, of course, are not dependent on the point distribution. The first ξ-derivative follows from (2):

$$f_\xi = x_\xi f_x \tag{7}$$

Now f_ξ, and the higher derivatives, depends on ξ explicitly through the ξ-derivatives of the metric derivatives, e.g., x_ξ, and implicitly through the x-dependence of f. Thus

$$\frac{d(f_\xi)}{d\xi} = \left(\frac{\partial(f_\xi)}{\partial\xi}\right)_x + \left(\frac{\partial(f_\xi)}{\partial x}\right)_\xi x_\xi \tag{8}$$

or, in operator form

$$\frac{d}{d\xi} = \frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x} \tag{9}$$

For example,

$$f_{\xi\xi} = \left(\frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x}\right)f_\xi = \left(\frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x}\right)(x_\xi f_x)$$

$$= x_{\xi\xi}f_x + x_\xi^2 f_{xx}$$

In general, then

$$f_{(n)} = \frac{d^n f}{d\xi^n} = \left(\frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x}\right)^n f \tag{10}$$

Note here that since f has no explicit ξ-dependence, we have

$$\left(\frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x}\right)f = x_\xi f_x = f_\xi$$

as expected.

The truncation error in f_x can then be written, using (10) in (6), as

$$T_x = -\frac{1}{x_\xi}\sum_{n=1}^{\infty}\frac{1}{(2n+1)!}\left(\frac{\partial}{\partial\xi} + x_\xi\frac{\partial}{\partial x}\right)^{2n+1} f \tag{11}$$

Note that the binomial theorem cannot be used to expand the power of the derivative operator here since $\frac{\partial}{\partial\xi}$ and $x_\xi\frac{\partial}{\partial x}$ do not commute, i.e.,

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

while

$$\left(x_\xi\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial\xi}\right) = x_\xi\frac{\partial^2}{\partial\xi\partial x}$$

Thus all permutations of the operator products of degree 2n+1 will occur in the expansion of the 2n+1 power of the derivative operator. For example, with 2n+1 = 3, the following eight operator products will occur:

$$\left(\frac{\partial}{\partial\xi}\right)^3,\ \left(\frac{\partial}{\partial\xi}\right)^2\left(x_\xi\frac{\partial}{\partial x}\right),\ \left(\frac{\partial}{\partial\xi}\right)\left(x_\xi\frac{\partial}{\partial x}\right)^2,\ \left(x_\xi\frac{\partial}{\partial x}\right)^3,$$

$$\left(\frac{\partial}{\partial\xi}\right)\left(x_\xi\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial\xi}\right),\ \left(x_\xi\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial\xi}\right)\left(x_\xi\frac{\partial}{\partial x}\right),$$

$$\left(x_\xi\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial\xi}\right)^2,\ \left(x_\xi\frac{\partial}{\partial x}\right)^2\left(\frac{\partial}{\partial\xi}\right)$$

But since f has no explicit ξ-dependence, all of these operator products having a $\frac{\partial}{\partial\xi}$ on the extreme right will make no contribution. Therefore, of the above eight-products for the 2n+1 power term, only four need to be

considered:

$$(\frac{\partial}{\partial\xi})^2(x_\xi\frac{\partial}{\partial x}),\ (\frac{\partial}{\partial\xi})(x_\xi\frac{\partial}{\partial x})^2,\ (x_\xi\frac{\partial}{\partial x})^3,\ (x_\xi\frac{\partial}{\partial x})(\frac{\partial}{\partial\xi})(x_\xi\frac{\partial}{\partial x})$$

Also since there is no explicit ξ-dependence in f, the following relations apply:

$$[(x_\xi\frac{\partial}{\partial x})^m]f = x_\xi^m\frac{d^mf}{dx^m}$$

$$[(\frac{\partial}{\partial\xi})^m(x_\xi\frac{\partial}{\partial x})]f = x_{(m+1)}\frac{df}{dx}$$

where $x_{(m+1)}$ indicates the m+1 ξ-derivative of x. Also

$$[(\frac{\partial}{\partial\xi})^\ell(x_\xi\frac{\partial}{\partial x})^m]f = (\frac{\partial}{\partial\xi})^\ell(x_\xi^m\frac{d^mf}{dx^m}) = \frac{d^\ell(x_\xi^m)}{d\xi^\ell}\frac{d^mf}{dx^m}$$

and,

$$[(x_\xi\frac{\partial}{\partial x})^\ell(\frac{\partial}{\partial\xi})^m(x_\xi\frac{\partial}{\partial x})^n]f = (x_\xi\frac{\partial}{\partial x})^\ell[\frac{d^m(x^n)}{d\xi^m}\frac{d^nf}{dx^n}]$$

$$= x_\xi^\ell\frac{d^m(x_\xi^n)}{d\xi^m}\frac{d^{\ell+n}f}{dx^{\ell+n}}$$

Other combinations appearing can be inferred from these.

From these relations it follows that $(\frac{\partial}{\partial x}+x_\xi\frac{\partial}{\partial x})^p$ will expand to the sum of products of ξ-derivatives of x, in each of which product the total number of ξ-differentiations is p. All possible combinations of ξ-derivatives appear in these products:

p = 1 x_ξ

p = 2 x_ξ^2, $x_{\xi\xi}$

p = 3 x_ξ^3, $x_{\xi\xi}x_\xi$, $x_{\xi\xi\xi}$

p = 4 x_ξ^4, $x_{\xi\xi\xi}x_\xi$, $x_{\xi\xi}{}^2$, $x_{\xi\xi}x_\xi^2$, $x_{\xi\xi\xi\xi}$

p = 5 x_ξ^5, $x_{\xi\xi\xi\xi}x_\xi$, $x_{\xi\xi\xi}x_{\xi\xi}$, $x_{\xi\xi\xi}x_\xi{}^2$, $x_{\xi\xi}{}^2x_\xi$, $x_{\xi\xi}x_\xi{}^3$, $x_{\xi\xi\xi\xi\xi}$

The n-term of the series in (11) then is of the form

$$\frac{1}{(2n+1)!}\sum_{m=1}^{2n+1}C_m\frac{d^mf}{dx^m}\prod_{i=1}^{2n+1}x_{(i)}^{a_{im}}\quad(m=1,2,\ldots2n+1)\qquad(12)$$

where the a_{im} are non-negative integers on the interval (0, 2n+1) such that

$$\sum_{i=1}^{2n+1} i\,a_{im} = 2n+1\quad(m=1,2,\ldots2n+1)\qquad(13)$$

Also

$$a_{i,1} = \delta_{i,2n+1},\quad a_{i,2n+1} = (2n+1)\delta_{i,1}$$

Neither the exponents, a_{im}, nor the numerical coefficients, C_m, depend on the point distribution. The first and last of the C_m coefficients are unity: $C_1 = C_{2n+1} = 1$. In (12), $x_{(i)}$ is the i^{th} ξ-derivative of x. As an example of (12), for n = 1 we have the term

$$\frac{1}{3!}(\frac{\partial}{\partial\xi}+x_\xi\frac{\partial}{\partial x})^3f$$

which expands to

$$\frac{1}{6}(x_{\xi\xi\xi}f_x + 3x_\xi x_{\xi\xi}f_{xx} + x_\xi^3f_{xxx})$$

Here m = 1,2,3, and $C_1 = C_3 = 1$, $C_2 = 3$, and $a_{13} = 3$, $a_{12} = a_{22} = a_{31} = 1$, with all the other a_{im} being zero. In the general case, as in this example, the 2n+1 products that are summed to construct the n-term of the series will each contain 2n+1 ξ-differentiations.

Order with Fixed Distribution Function

Now from the form of the distribution function (1), it is clear that

$$x_{(i)} = \frac{D_i}{N^i}\qquad(14)$$

where the coefficient D_i does depend on the point distribution function of (1), but not on the number of points, N. Therefore, in (12),

$$\prod_{i=1}^{2n+1}x_{(i)}^{a_{im}} = \prod_{i=1}^{2n+1}(\frac{D_i}{N^i})^{a_{im}} = \frac{\prod_{i=1}^{2n+1}D_i^{a_{im}}}{N^{\sum_{i=1}^{2n+1}i\,a_{im}}} = \frac{\prod_{i=1}^{2n+1}D_i^{a_{im}}}{N^{2n+1}}$$

by (14). The truncation error in the difference expression for f_x then is

$$T_x = -\sum_{n=1}^{\infty}\frac{1}{(2n+1)!N^{2n}}\sum_{m=1}^{2n+1}A_{mn}\frac{d^mf}{dx^m}\qquad(15)$$

where the coefficients, A_{mn}, given by

$$A_{mn} = \frac{C_m}{D_1}\prod_{i=1}^{2n+1}D_i^{a_{im}}\qquad(16)$$

depend on the distribution function, but not on the number of points. The series (15) is thus a power series in the inverse of the number of points in the field. It therefore is possible to truncate the series as the number of points in the field, N, increases, with the result

$$T_x = -\frac{1}{6N^2}\sum_{m=1}^{3}A_{m1}\frac{d^mf}{dx^m}\qquad(17)$$

where, from (16),

$$A_{m1} = \frac{C_m}{D_1}\prod_{i=1}^{3}D_i^{a_{im}}\quad(m=1,2,3)$$

and, as noted above,

$$C_1 = C_3 = 1,\ C_2 = 3,\ a_{13} = 3,\ a_{12} = a_{22} = a_{31} = 1$$

and all other a_{im} are zero. Thus

$$A_{11} = \frac{D_3}{D_1},\quad A_{21} = D_2,\quad A_{31} = D_1^2$$

The truncation error of the difference expression (5) can then be written, using (14), as

$$T_x = -\frac{1}{6}\frac{x_{\xi\xi\xi}}{x_\xi}f_x - \frac{1}{2}x_{\xi\xi}f_{xx} - \frac{1}{6}x_\xi^2f_{xxx}\qquad(18)$$

The first two terms arise from the nonuniform spacing, while the last term is the familiar term occuring with uniform spacing as well.

From (17) it is clear that the difference representation (5) is second-order regardless of the form of the point distribution function in the sense that the truncation error goes to zero as $1/N^2$ as the number or points increases. This means that the error will be quartered when the number of points is doubled in the same distribution function. Thus all difference representations maintain their order on a nonuniform grid with any distribution of points in the formal sense of the truncation error decreasing as the number of points is increased while maintaining the same relative point distribution over the field.

The critical point here is that the same relative point distribution, i.e., the same distribution function is used as the number of points in the field is increased. If this is the case, then the error will be decreased by a factor that is a power of the inverse of the number of points in the field as their number is increased. Random additions of points will, however, not maintain order. This point has also been noted by Hoffman in (4). In a practical vein this means that a solution made with twice the number of points as another solution will exhibit one-fourth of the error (for second-order representations in the transformed plane) when the two solutions use the same point distribution function. However if the number of points is doubled without maintaining the same relative distribution the error reduction will not be as great as one-fourth.

From the standpoint of formal order in this sense, then, there is no need for concern over the form of the point distribution. However, formal order in this sense relates only to the behavior of the truncation error as the number of points is increased, and the coefficients A_{mn} in the series (15) may become large as the parameters in the distribution are altered to reduce the minimum spacing with a given number of points in the field. Thus, although the error will be reduced by the same order for all point distributions as the number of points is increased, certain distributions will have smaller error than others with a given number of points in the field, since the coefficients in the series, A_{mn}, while independent of the number of points, are dependent on the distribution function.

Since the numerical coefficients, C_m, in (16) do not depend on the distribution function, the quantities of concern for the n-term of the series (15) are

$$\frac{A_{mn}}{C_m} \equiv \frac{1}{D_1} \prod_{i=1}^{2n+1} D_i^{a_{im}} \qquad (m = 1,2,\ldots,2n+1)$$

$$= \frac{1}{Nx_\xi} \prod_{i=1}^{2n+1} N^{ia_{im}} x_{(i)}^{a_{im}}$$

$$= (Nx_\xi)^{\sum_{i=1}^{2n+1} a_{im} - 1} \prod_{i=1}^{2n+1} \left(\frac{N^{i-1}x_{(i)}}{x_\xi}\right)^{a_{im}} \qquad (19)$$

Now at least one a_{im} must be greater than or equal to unity for each m, and therefore the exponent of Nx_ξ in the above expression is not negative. Since the a_{im} do not depend on the distribution function, we are led by (19) to compare distribution functions on the basis of behavior of the following quantities as the minimum value of x_ξ on the field goes to zero with fixed N:

$$Nx_\xi \quad \text{and} \quad \frac{N^{i-1}x_{(i)}}{x_\xi} \qquad (i = 1,2,\ldots, 2n+1) \qquad (20)$$

Now for uniform spacing we have $D_i = 0$ for $i \geq 2$, and then by (16), all A_{mn} are zero except $A_{2n+1,n}$, which is given by

$$A_{2n+1,n} = \frac{C_{2n+1}}{D_1} D_1^{a_{1,2n+1}} = D_1^{2n}$$

Thus the contribution to the truncation error that remains with uniform spacing arises from the $m = 2n+1$ term of (15). The ratio of the coefficients A_{mn} to the coefficient $A_{2n+1,n}$, corresponding to the uniform spacing error, is then, from (16) and (14).

$$\frac{A_{mn}}{A_{2n+1,n}} = \frac{C_m}{C_{2n+1}} \frac{\prod_{i=1}^{2n+1} D_i^{a_{im}}}{\prod_{i=1}^{2n+1} D_i^{a_{i,2n+1}}}$$

$$= \frac{C_m}{D_1^{2n+1}} \prod_{i=1}^{2n+1} D_i^{a_{im}} = C_m \prod_{i=2}^{2n+1} \left(\frac{x_{(i)}}{x_\xi^i}\right)^{a_{im}} \qquad (21)$$

Note that this ratio is the ratio of the coefficient of $d^m f/dx^m$ to that of f_x in the n-term, i.e., the $(\frac{1}{N})^{2n+1}$ term, of the series (15) for the truncation error. The ratios of the terms arising from the nonuniform spacing to that from the spacing itself in the n-term of the truncation error expansion (15) as a power series in the inverse of number of points are then

$$\frac{A_{mn}}{A_{2n+1,n}} \frac{\frac{d^m f}{dx^m}}{\frac{d^{2n+1} f}{dx^{2n+1}}} = C_m \frac{\frac{d^m f}{dx^m}}{\frac{d^{2n+1} f}{dx^{2n+1}}} \prod_{i=2}^{2n+1} \left(\frac{x_{(i)}}{x_\xi^i}\right)^{a_{im}} \qquad (22)$$

Order with Fixed Number of Points

The above considerations have been concerned with order in the formal sense of the truncation error being reduced by a factor equal to a power of N as the number of points in the field is increased, while maintaining the same relative point distribution. It has been shown that all point distributions maintain formal order in this sense, but that some distributions may be superior to others with a given total number of points in the field. Also, comparisons may be made on the basis of the magnitude of the series coefficients, ultimately through the quantities given in (20). All this was based on a series expansion of the error in ascending inverse powers of the number of points in the field, N.

An alternate sense of order for point distributions is based on expansion of the truncation error in a series in ascending powers of the spacing, x_ξ. This can be developed from the series given above as (15), but with D_i from (14) substituted in the expression for A_{mn} given by (15):

$$A_{mn} = \frac{C_m}{D_1} \prod_{i=1}^{2n+1} (N^i x_{(i)})^{a_{im}} = \frac{C_m}{D_1} \prod_{i=1}^{2n+1} \left[\left(\frac{D_1}{x_\xi}\right)^i x_{(i)}\right]^{a_{im}}$$

But, by (13),

$$\prod_{i=1}^{2n+1} D_1^{ia_{im}} = D_1^{\sum_{i=1}^{2n+1} ia_{im}} = D_1^{2n+1}$$

so that

$$A_{mn} = C_m D_1^{2n} \prod_{i=1}^{2n+1} \left(\frac{x_{(i)}}{x_\xi^i}\right)^{a_{im}} = C_m (Nx_\xi)^{2n} \prod_{i=1}^{2n+1} \left(\frac{x_{(i)}}{x_\xi^i}\right)^{a_{im}} \tag{23}$$

Then the series (15) becomes

$$T_x = - \sum_{n=1}^{\infty} \frac{(x_\xi)^{2n}}{(2n+1)!} \sum_{m=1}^{2n+1} B_{mn} \frac{d^m f}{dx^m} \tag{24}$$

where

$$B_{mn} = C_m \prod_{i=1}^{2n+1} \left(\frac{x_{(i)}}{x_\xi^i}\right)^{a_{im}} \tag{25}$$

Recall that the numerical coefficients, C_m, and the exponents, a_{im}, do not depend on the distribution function. However, in contrast to the series of (15), the coefficients, B_{mn}, may be dependent on the variation of the spacing, x_ξ, with a fixed number of points. The series here is therefore not a power series in x_ξ, and cannot be truncated unless the coefficients, B_{mn}, are bounded as the spacing goes to zero with a fixed number of points. A sufficient condition for this is that the quantities involved in the ratio of the coefficients to that arising with uniform spacing, i.e., (22),

$$\frac{x_{(i)}}{x_\xi^i} \qquad (i = 1,2,\ldots,\infty) \tag{26}$$

be bounded as x_ξ goes to zero with fixed N. Where this is the case, the order of the difference representation is maintained with the non-uniform point distribution in the sense that the truncation error is reduced by a factor equal to a power of the spacing as the spacing is decreased with a fixed number of points in the field.

In the specific distribution functions to be considered below, it will be seen that it is possible for the quantities of (20) to be larger than those of (26), but for most functions the reverse is true. The difference between these two approaches to order should be kept clear. The first approach concerns the behavior of the truncation error as the number of points in the field increases with a fixed relative distribution of points. The series here is a power series in the inverse of the number of points in the field, and formal order is maintained for all point distributions. The coefficients in the series may, however, become large for some distribution functions as the minimum spacing decreases for any given number of points. Evaluation of particular distribution functions in this approach is based on the quantities of (20). The other approach concerns the behavior of the error as the minimum spacing decreases with a fixed number of points in the field. Distribution functions satisfying the conditions (26) maintain order in this second sense and can be compared on the basis of these quantities. This second sense of order is thus more stringent. The conditions of (26) seem to be unattainable, however.

Conditions equivalent to those given in (20) for comparison of distribution functions were also obtained by Vinokur in (5) from consideration of appropriate length scales in regions of large gradients. (In that analysis the transformed variable, ξ, is normalized to the interval (0,1) so the number of points in the field does not appear explicitly. The correct interpretation of the results of (5) with the present form of distri- function is the conditions of (20) and not as given in (2) where the N^{i-1} factor was omitted.)

EVALUATION OF DISTRIBUTION FUNCTIONS

As an example of the application of the measures of order discussed above, ten distribution functions were analysed with specified spacing at $\xi = 0$. The functions and the coefficients discussed above are listed in Tables 1-3, using the following notation:

$$L_N^{(i)} \equiv N^{i-1} \frac{x_{(i)}}{x_\xi} \qquad L_S^{(i)} \equiv \frac{x_{(i)}}{x_\xi^i} \qquad S \equiv (x_\xi)_0$$

$$\bar{\xi} \equiv \frac{\xi}{N}$$

with the subscripts 0 and N indicating evaluation at $\xi = 0$ and N, respectively. The table both the values of the coefficients, L_N and L_S, at the points of minimum spacing, i.e., $\xi = 0$, and the maximum values, together with the location of the maximum. The relation of these coefficients to the produce NS as the minimum spacing S, approaches zero is also given. Plots of the coefficients at $\xi = 0$ and the maximum values of the coefficients against the minimum spacing are given in Figs. 1 and 2. The variation of the coefficients over the field is shown in Figs. 3 and 4. The first of these shows the entire field for a minimum spacing of 10^{-3}, while the second gives detail of the region near the minimum spacing ($\xi = 0$) for a minimum spacing of 10^{-6}. The behavior of the coefficients is qualitatively the same for different values of the minimum spacing. Finally, Fig. 5 shows the variation of ξ with x, i.e., the point distribution, the entire field being shown for minimum spacings of 10^{-3} and 10^{-6}, while detail of the region near the minimum spacing ($\xi = 0$) is shown for minimum spacings of 10^{-6} and 10^{-9}. Here the ordinate, ξ, can also be interpreted as the fraction of the total number of points that fall between $x = 0$ and the local value of x.

From Fig. 5b it is clear that, of the functions considered here, only the exponential, the hyperbolic sine, the hyperbolic tangent, and the error function are suitable as point distribution functions with very small minimum spacing. The quadratic and sine functions do not actually achieve the specified spacing of 10^{-6}, and the rest of the functions concentrate essentially all of the points at the left boundary. The error function gives the smoothest coverage of the field. The hyperbolic tangent is next in this regard, while the exponential and hyperbolic sine give about the same distributions in most of the field. Of the four suitable functions the hyperbolic sine concentrates more points near the minimum spacing, i.e., the left boundary. This function also gives the most nearly uniform point distribution in the region of high concentration, since the second derivative, and hence $L_N^{(2)}$ and $L_S^{(2)}$, vanishes at $\xi = 0$. This vanishing second derivative also occurs with the tangent and arctangent, but these functions concentrate too many of the points near the left boundary.

The plots of the coefficients over the field, Fig. 3 and 4, show $L_N^{(2)}$ for the hyperbolic sine rising rapidly from zero to quickly level off just above the uniform value for the exponential. The hyperbolic tangent, by contrast, falls from a value close to that at which the hyperbolic sine levels off. The error function starts a bit higher than the hyperbolic tangent but falls faster. All four of these functions give essentially uniform values of the coefficient $L_N^{(2)}$ in

the region extending 100 times the minimum spacing from the left boundary, cf. Fig. 4a, except for the initial rise from zero that occurs for the hyperbolic sine in the region extending 10 times the minimum spacing from the boundary. The value that occurs for the error function is about twice that for the others. Outside this boundary layer region near the left boundary, the hyperbolic tangent and the error function drop off to zero, while the exponential and hyperbolic sine remain uniform. Thus the hyperbolic sine has the best behavior very near the minimum spacing, while the error function, followed closely by the hyperbolic tangent, behaves best outside the boundary layer region. The error function is, however, a bit higher than the others within the boundary layer. Note that the exponential, although a suitable distribution function, maintains the uniform value near that from which the hyperbolic tangent drops off, and therefore the exponential is never as good as the hyperbolic tangent in regard to the coefficient $L_N^{(2)}$. The trends for $L_N^{(3)}$ are essentially the same as for $L_N^{(2)}$, except that now the value for the hyperbolic sine is uniform, so that this function has no advantage in regard to $L_N^{(3)}$.

For the coefficient $L_S^{(2)}$, all four functions give very nearly the same values within the boundary layer, except for the rapid initial rise from zero that occurs for the hyperbolic sine and a slightly larger initial value occurring for the error function. Outside the boundary layer the values for the error function and the hyperbolic tangent drop off to zero, the drop being a bit faster for the error function, while the values for the exponential and hyperbolic sine drop off together to a nonzero value. Again the behavior of $L_S^{(3)}$ is qualitatively the same.

It thus appears that the following conclusions can be reached on the basis of these coefficients:

(1) The exponential is not as good as the hyperbolic tangent and therefore should not be used.

(2) The hyperbolic sine is the best function in the lower part of the boundary layer. Otherwise this function is not as good as the hyperbolic tangent.

(3) The error function and the hyperbolic tangent are the best functions outside the boundary layer. Between these two the hyperbolic tangent is the better within the boundary layer, while the error function is the better outside.

(4) The logarithm, sine, tangent, arctangent, inverse hyperbolic tangent, quadratic, and also the inverse hyperbolic sine (not included in Table 1 or the figures) are not suitable.

Figs 1 and 2 show that the the variations of both $L_N^{(i)}$ and $L_S^{(i)}$ with the minimum spacing are essentially the same for all four of the suitable functions (except that $L_N^{(2)}$ and $L_S^{(2)}$ at $\xi = 0$ remain zero for the hyperbolic sine). These figures also show that consideration of the values at $\xi = 0$ only would be deceptive, leading incorrectly to preference for the tangent and arctangent, both of which are shown by the other figures to be unsuitable. Finally, Fig. 2 shows that the four suitable functions do in fact preserve order in the sense of variation of truncation error as the number of points in the field increases, since $L_N^{(i)}$ has only small variation with the minimum spacing. The same cannot be said, however, for order in the sense of variation of the error as the minimum spacing decreases with a fixed number of points. In fact, Figs. 2(c) and (d) show that the logarithmic slope of $L_S^{(i)}$ is near -1 for these functions, and hence the order is strictly only first in this sense (since the $L_S^{(i)}$ are the coefficients of the x_ξ^i term in the error expansion).

Vinokur (5) considered all of the functions included here, except the exponential, logarithm, and quadratic, and also considered the arcsine, which was found to be unsuitable. As noted above, the analysis of that reference is based on the quantities $L_N^{(i)}$. Vinokur also shows how to use a basic distribution function, with specified slope x_ξ at one boundary, to construct a distribution function that allows the slope to be specified at both boundaries. Forms that allow the slope to be specified at an interior point are also given.

Although, as has been shown, all distribution functions maintain order in the formal sense with nonuniform spacing as the number of points in the field is increased. The results obtained for these particular distribution functions show that considerable error can arise with nonuniform spacing in actual applications. Recal that the ratio of the coefficients from the nonuniform spacing in the series (15) to the coefficient arising from spacing itself is given by (22), which with the definitions of $L_S^{(i)}$ gives the following bound for this ratio:

$$\frac{A_{mn}}{A_{2n+1,n}} \frac{\dfrac{d^m f}{dx^m}}{\dfrac{d^{2n+1} f}{dx^{2n+1}}} \le C_m \frac{\dfrac{d^m f}{dx^m}}{\dfrac{d^{2n+1} f}{dx^{2n+1}}} \prod_{i=2}^{2n+1} (L_S^{(i)})^{a_{im}} \qquad (27)$$

The n=1 term then yields, for the coefficients involved in the leading term of the series (15):

$$\frac{A_{13}}{A_{31}} \frac{f_x}{f_{xxx}} = L_S^{(3)} \frac{f_x}{f_{xxx}}, \quad \frac{A_{23}}{A_{31}} \frac{f_{xx}}{f_{xxx}} = 3L_S^{(2)} \frac{f_{xx}}{f_{xxx}} \qquad (28)$$

Now a typical case involving a boundary layer might have 100 points with a minimum spacing of 10^{-6} relative to a maximum field extent of unity. Thus $N = 10^2$, $S = 10^{-6}$, and $NS = 10^{-4}$. Then for

$$L_S^{(i)} = \left(\frac{1}{NS}\right)^{i-1}$$

as for the best of the functions considered, we have

$$L_S^{(2)} = 10^4, \quad L_S^{(3)} = 10^8$$

and then the ratios of the error from the nonuniform spacing to that which arises from the spacing itself are, approximately,

$$10^8 \frac{f_x}{f_{xxx}} \quad \text{and} \quad 10^4 \frac{f_x}{f_{xxx}}$$

Since the error term from the spacing here is $S^2 f_{xxx} = 10^{-12} f_{xxx}$, the error terms due to the nonuniform spacing are

$$10^{-4} f_x \quad \text{and} \quad 10^{-8} f_{xx}$$

as compared with $10^{-12} f_{xxx}$ due to the spacing. Now for the same number of points with uniform spacing we would have a spacing of 10^{-2} and an error of $10^{-4} f_{xxx}$. Thus the error due to the nonuniform spacing in this case is well below what would occur on a uniform grid with the same number of points, except for the f_x term. (It will be shown below that this term can be eliminated from the truncation error by evaluating the coordinate derivatives numerically rather than analytically.)

This example shows that the contributions to the error from the nonuniform spacing are significant and must be considered. While the contribution form the spacing itself decreases with the spacing, the con-

tributions from the nonuniform spacing increase as the spacing decreases for very small spacings.

EFFECT OF NUMERICAL METRIC COEFFICIENTS

All of the above considerations have assumed that the derivatives of x with respect to ξ are evaluated exactly. If the coordinate derivative, x_ξ, in the difference expression (5) is evaluated numerically by the same central difference expression used for f we have, in place of (5):

$$f_x = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}} + T'_x \tag{29}$$

With x expanded in Taylor series we have

$$x_{i+1} - x_{i-1} = 2x_\xi + 2\sum_{n=1}^{\infty} \frac{x_{(2n+1)}}{(2n+1)!} \tag{30}$$

Using this and (5) in (29) we then have

$$f_x = \frac{f_x - T_x}{1 + \frac{1}{x_\xi}\sum_{n=1}^{\infty} \frac{x_{(2n+1)}}{(2n+1)!}} + T'_x \tag{31}$$

Now the f_x term of T_x corresponds to m = 1 in (15):

$$-\sum_{n=1}^{\infty} \frac{A_{1n}}{(2n+1)!N^{2n}}$$

and by (16),

$$A_{1n} = \frac{C_1}{D_1}\prod_{i=1}^{2n+1} D_i\, a_{i1}$$

But $C_1 = 1$ and $a_{i1} = \delta_{i,2n+1}$, as given above, so that, using (14),

$$A_{1n} = \frac{D_{2n+1}}{D_1} = \frac{N^{2n} x_{(2n+1)}}{x_\xi}$$

Then the coefficient of f_x in T_x is

$$-\frac{1}{x_\xi}\sum_{n=1}^{\infty} \frac{x_{(2n+1)}}{(2n+1)!}$$

and, for use in (31), we have

$$f_x - T_x = f_x\left(1 + \frac{1}{x_\xi}\sum_{n=1}^{\infty} \frac{x_{(2n+1)}}{(2n+1)!}\right) + \sum_{n=1}^{\infty} \frac{1}{(2n+1)!N^{2n}} \sum_{m=2}^{2n+1} A_{mn} \frac{d^m f}{dx^m}$$

But the coefficient of f_x on the right here is exactly the denominator in ( ), so that, using (14) in this denominator, we have the following expression for the truncation error in the difference representation (29):

$$T'_x = -\frac{\sum_{n=1}^{\infty} \frac{1}{(2n+1)!N^{2n}} \sum_{m=2}^{2n+1} A_{mn} \frac{d^m f}{dx^m}}{1 + \frac{1}{D_1}\sum_{n=1}^{\infty} \frac{D_{2n+1}}{(2n+1)!N^{2n}}} \tag{32}$$

The lead term of the error then is

$$T'_x = -\frac{1}{6N^2}\sum_{m=2}^{3} A_{m1} \frac{d^m f}{dx^m}$$

which is the same as (17), except that the lower limit of m is 2 in the present case. This can finally be written as

$$T'_x = -\frac{1}{2} x_{\xi\xi} f_{xx} - \frac{1}{6} x_\xi^2 f_{xxx} \tag{33}$$

Thus the use of numerical evaluation of the coordinate derivative, rather than exact analytical evaluation, eliminates the f_x term from the truncation error. Since this term is the most troublesome part of the error, being dependent on the derivative being represented, it is clear that numerical evaluation of the metric coefficients by the same difference representation used for the function whose derivative is being represented is preferable to exact analytical evaluation. It should be understood that there is no incentive, per se, for accuracy in the metric coefficents, since the object is simply to represent a discrete solution accurately, not to represent the solution on some particular coordinate system. The only reason for using any function at all to define the point distribution is to ensure a smooth distribution. There is no reason that the representations of the coordinate derivatives have to be accurate representatives of the analytical derivatives of that particular distribution function.

Two-Dimensions

The two-dimensional transformation of the first derivative is given by

$$f_x = \frac{1}{J}(y_\eta f_\xi - y_\xi f_\eta) \tag{34}$$

where the Jacobian of the transformation is

$$J = x_\xi y_\eta - x_\eta y_\xi$$

With two-point central difference representations for all derivatives, we have

$$f_x = \frac{\delta_\eta y\, \delta_\xi f - \delta_\xi y\, \delta_\eta f}{\delta_\xi x\, \delta_\eta y - \delta_\eta x\, \delta_\xi y} + T_x \tag{35}$$

where

$$\delta_\xi f \equiv f_{i+1,j} - f_{i-1,j} \qquad \delta_\eta f \equiv f_{i,j+1} - f_{i,j-1}$$

and T_x is the truncation error. After expansion of all quantities in Taylor series about the central point and considerable algebraic manipulation, we have for the leading term of the truncation error

$$T_x = \frac{1}{2J}(y_\xi x_\eta x_{\eta\eta} - x_\xi y_\eta x_{\xi\xi}) f_{xx} + \frac{1}{2J}(y_\xi y_\eta)(y_{\eta\eta} - y_{\xi\xi}) f_{yy} + \frac{1}{2J}[y_\xi y_\eta (x_{\eta\eta} - x_{\xi\xi}) + x_\eta y_\xi y_{\eta\eta} - x_\xi y_\eta y_{\xi\xi}] f_{xy} + \text{second-order terms in the spacing} \tag{36}$$

where the coordinate derivatives are understood to

represent central difference expressions, e.g.,

$$x_\xi = \frac{1}{2}(x_{i+1,j} - x_{i-1,j}) \; , \; x_\eta = \frac{1}{2}(x_{i,j+1} - x_{i,j-1})$$

$$x_{\xi\xi} = x_{i+1,j} - 2x_{ij} + x_{i-1,j}$$

$$x_{\eta\eta} = x_{i,j+1} - 2x_{ij} + x_{i,j-1}$$

These contributions to the truncation error arise from the nonuniform spacing. The familiar terms proportional to a power of the spacing occur in addition to these terms as noted.

Sufficient conditions can be stated for maintaining the order of the difference representations. First of all, as in the one-dimensional case, the ratios

$$\frac{x_{\xi\xi}}{x_\xi^2} \; , \; \frac{y_{\xi\xi}}{y_\xi^2} \; , \; \frac{x_{\eta\eta}}{x_\eta^2} \; , \; \frac{y_{\eta\eta}}{y_\eta^2}$$

must be bounded as x_ξ, x_η, y_ξ, y_η approach zero. A second condition must be imposed which limits the rate at which the Jacobian approaches zero. This condition can be met by simply requiring that $\cot\theta$ remain bounded, where θ is the angle between the ξ and η coordinate lines. The fact that this bound on the nonorthogonality imposes the correct lower bound on the Jacobian follows from the fact that

$$|\cot\theta| \leq M \qquad (37)$$

implies

$$J^2 \geq \frac{1}{M+1}[x_\xi^2 x_\eta^2 + x_\xi^2 y_\eta^2 + x_\eta^2 y_\xi^2 + y_\xi^2 y_\eta^2].$$

With these conditions on the ratios of second to first derivatives, and the limit on the nonorthogonality satisfied, the order of the first derivative approximations is maintained in the sense that the contributions to the truncation error arising from the nonuniform spacing will be second-order terms in the grid spacing.

The truncation error terms for second derivatives that are introduced when using a curvilinear coordinate system are very lengthy and involve both second and third derivatives of the function f. However, it can be shown the same sufficient conditions, together with the condition that

$$\frac{x_{\xi\eta}}{x_\xi x_\eta} \quad \text{and} \quad \frac{y_{\xi\eta}}{y_\xi y_\eta}$$

remain bounded, will insure that the order of the difference representations is maintained.

It was noted above that a limit on the nonorthogonality, imposed by (37), is required for maintaining the order of difference representations. The degree to which nonorthogonality effects truncation error can be stated more precisely. The truncation error for a first derivative f_x can be written

$$T_x = \frac{1}{J}(y_\eta T_\xi - y_\xi T_\eta)$$

where T_ξ and T_η are the truncation errors for the difference expressions f_ξ and f_η. Now all coordinate derivatives can be expressed using direction cosines of the angles of inclination, ϕ_ξ and ϕ_η of the ξ and η coordinate lines. After some simplification, the truncation error has the form

$$T_x = \frac{1}{\sin(\phi_\eta - \phi_\xi)}\left(\sin\phi_\eta\cos\phi_\xi \frac{T_\xi}{x_\xi} - \sin\phi_\xi\cos\phi_\eta \frac{T_\eta}{x_\eta}\right) \qquad (38)$$

Therefore the truncation error, in general, varies inversely with the sine of the angle between the coordinate lines. Note that there is also a dependence on the direction of the coordinate lines. To further clarify the effect of nonorthogonality, the following example is included. For simplicity, only the truncation error terms arising from nonuniform spacing are considered.

The contribution from nonorthogonality can be isolated by considering the case of skewed parallel lines with $x_\eta = x_{\eta\eta} = x_{\xi\eta} = y_{\xi\xi} = y_{\xi\eta} = 0$ as diagramed below:

Here (36) reduces to

$$T_x = -\frac{1}{2}x_{\xi\xi}f_{xx} + \frac{1}{2}\left(\frac{y_\xi}{x_\xi}\right) y_{\eta\eta}f_{yy} - \frac{1}{2}\left(\frac{y_\xi}{x_\xi}\right)x_{\xi\xi}f_{xy}$$

Since $\cot\theta = \dfrac{y_\xi}{x_\xi}$, this may be written

$$T_x = -\frac{1}{2}x_{\xi\xi}f_{xx} + \frac{1}{2}(y_{\eta\eta}f_{yy} - x_{\xi\xi}f_{xy})\cot\theta \qquad (39)$$

The first term occurs even on an orthogonal system and corresponds to the first term in (33). The last two terms arise from the departure from orthogonality. For $\theta < 45°$, these terms are no greater than those from the nonuniform spacing. Reasonable departure from orthogonality is therefore of little concern when the rate-of-change of grid spacing is reasonable. Large departure from orthogonality may be more of a problem at boundaries, where one-sided difference expressions are needed. Therefore, grids should probably be made as nearly orthogonal at the boundaries as is practical. Note that the contribution from nonorthogonality vanishes on a skewed uniform grid.

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Table 1

Coefficients at Minimum Spacing

FUNCTION	NS	$(L_N^{(2)})_0$	$(L_N^{(3)})_0$	$(L_S^{(2)})_0$	$(L_S^{(3)})_0$
Exponential: $\frac{e^{\alpha\bar{\xi}} - 1}{e^{\alpha} - 1}$	$\frac{\alpha}{e^{\alpha} - 1}$	α	α^2	$e^{\alpha} - 1$	$(e^{\alpha} - 1)^2$
Hyperbolic Tangent : $1 - \frac{\tanh \alpha(1 - \bar{\xi})}{\tanh \alpha}$	$\frac{2\alpha}{\sinh 2\alpha}$	$2\alpha\tanh \alpha$	$2\alpha^2(3\tanh^2\alpha - 1)$	$2\sinh^2\alpha$	$\frac{1}{2}(3\tanh^2\alpha - 1)\sinh^2 2\alpha$
Hyperbolic Sine : $\frac{\sinh \alpha\bar{\xi}}{\sinh \alpha}$	$\frac{\alpha}{\sinh \alpha}$	0	α^2	0	$\sinh^2\alpha$
Error Function : $1 - \frac{\operatorname{erf} \alpha(1 - \bar{\xi})}{\operatorname{erf} \alpha}$	$\frac{2}{\sqrt{\pi}} \frac{\alpha e^{-\alpha^2}}{\operatorname{erf} \alpha}$	$2\alpha^2$	$2\alpha^2(2\alpha^2 - 1)$	$\sqrt{\pi}\, \alpha e^{\alpha^2} \operatorname{erf}\alpha$	$\frac{\pi}{2}(2\alpha^2 - 1)(e^{\alpha^2}\operatorname{erf}\alpha)^2$
Tangent : $\frac{\tan \alpha\bar{\xi}}{\tan \alpha}$ $(0 \le \alpha \le \frac{\pi}{2})$	$\frac{\alpha}{\tan \alpha}$	0	$2\alpha^2$	0	$2\tan^2\alpha$
Arctangent : $1 - \frac{\tan^{-1}\alpha(1 - \bar{\xi})}{\tan^{-1}\alpha}$	$\frac{\alpha}{(1 + \alpha^2)\tan^{-1}\alpha}$	$\frac{2\alpha^2}{1 + \alpha^2}$	$\frac{2\alpha^2(3\alpha^2 - 1)}{(1 + \alpha^2)^2}$	$2\alpha\tan^{-1}\alpha$	$2(3\alpha^2 - 1)(\tan^{-1}\alpha)^2$
Sine : $1 - \frac{\sin \alpha(1 - \bar{\xi})}{\sin \alpha}$ $(0 \le \alpha \le \frac{\pi}{2})$	$\frac{\alpha}{\tan \alpha}$	$\alpha\tan \alpha$	α^2	$\tan^2\alpha$	$-\tan^2\alpha$
Log : $1 - \frac{\ell n[1 + \alpha(1 - \bar{\xi})]}{\ell n(1 + \alpha)}$	$\frac{\alpha}{(1 + \alpha)\ell n(1 + \alpha)}$	$\frac{\alpha}{1 + \alpha}$	$\frac{2\alpha^2}{(1 + \alpha)^2}$	$\ell n(1 + \alpha)$	$2[\ell n(1 + \alpha)]^2$
Inverse Hyperbolic Tangent : $\frac{\tanh^{-1}\alpha\bar{\xi}}{\tanh^{-1}\alpha}$ $(0 \le \alpha \le 1)$	$\frac{\alpha}{\tanh^{-1}\alpha}$	0	$2\alpha^2$	0	$2(\tanh^{-1}\alpha)^2$
Quadratic : $\alpha\bar{\xi} + (1 - \alpha)\bar{\xi}^2$ $(0 \le \alpha \le 1)$	α	$\frac{2(1 - \alpha)}{\alpha}$	0	$\frac{2(1 - \alpha)}{\alpha^2}$	0

Table 2

Maximum Coefficients

	$(L_N^{(2)})_{max}$	$(L_N^{(3)})_{max}$	$(L_S^{(2)})_{max}$	$(L_S^{(3)})_{max}$
Exponential:	same (uniform)	same (uniform)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)
Hyperbolic Tangent :	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)
Hyperbolic Sine :	$\alpha \tanh \alpha$ ($\bar{\xi} = 1$)	same (uniform)	$\frac{1}{2}\sinh \alpha$ ($\sinh \alpha\bar{\xi} = 1$)	same ($\bar{\xi} = 0$)
Error Function :	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)
Tangent :	$2\alpha\tan\alpha$ ($\bar{\xi} = 1$)	$2\alpha^2(3\tan^2\alpha + 1)$	$\tan \alpha$ ($\bar{\xi} = \frac{\pi}{4\alpha}$)	$\frac{9}{4}\tan^2\alpha$ ($\tan \alpha\bar{\xi} = \frac{1}{\sqrt{3}}$)
Arctangent :	$\frac{\sqrt{3}}{2}\alpha$ ($\bar{\xi} = 1 + \frac{1}{\sqrt{3}\,\alpha}$)	$\frac{9}{8}\alpha^2$ ($\bar{\xi} = 1 + \frac{\sqrt{5}}{3}\frac{1}{\alpha}$)	same	same
Sine :	same ($\bar{\xi} = 0$)	same (uniform)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)
Log :	α ($\bar{\xi} = 1$)	$2\alpha^2$ ($\bar{\xi} = 1$)	same (uniform)	same (uniform)
Inverse Hyperbolic Tangent :	$\frac{2\alpha^2}{1 - \alpha^2}$ ($\bar{\xi} = 1$)	$\frac{2\alpha^2(3\alpha^2 + 1)}{(1 - \alpha^2)^2}$ ($\bar{\xi} = 1$)	$2\alpha\tanh^{-1}\alpha$ ($\bar{\xi} = 1$)	$2(3\alpha^2 + 1)(\tanh^{-1}\alpha)^2$ ($\bar{\xi} = 1$)
Quadratic :	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)	same ($\bar{\xi} = 0$)

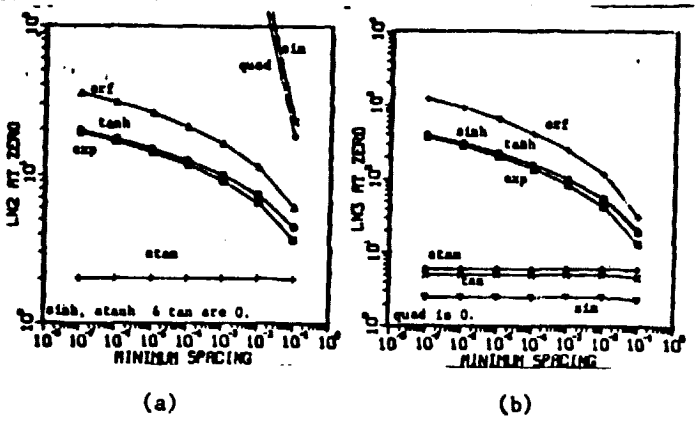
NOTE: 'Same' indicates maximum value is same as value at $\bar{\xi} = 0$.

Table 3

Coefficients as Minimum Spacing Approaches Zero

	$(L_N^{(2)})_0$	$(L_N^{(3)})_0$	$(L_S^{(2)})_0$	$(L_S^{(3)})_0$	$(L_N^{(2)})_{max}$	$(L_N^{(3)})_{max}$	$(L_S^{(2)})_{max}$	$(L_S^{(3)})_{max}$
Exponential:	$\ell n \frac{1}{NS}$	$(\ell n \frac{1}{NS})^2$	$\frac{1}{NS}$	$(\frac{1}{NS})^2$	same	same	same	same
Hyperbolic Tangent :	$\ell n \frac{1}{NS}$	$(\ell n \frac{1}{NS})^2$	$\frac{1}{NS}$	$(\frac{1}{NS})^2$	same	same	same	same
Hyperbolic Sine :	0	$(\ell n \frac{1}{NS})^2$	0	$(\frac{1}{NS})^2$	$\ell n \frac{1}{NS}$	same	$(\ell n \frac{1}{N})^2$	same
Error Function :	$2\ell n(\frac{1}{NS})$	$4(\ell n \frac{1}{NS})^2$	$\frac{\sqrt{\pi}}{2} \frac{1}{NS}$	$\frac{\pi}{4} (\frac{1}{NS})^2$	same	same	same	same
Tangent :	0	$\frac{\pi^2}{2}$	0	$\frac{\pi^2}{2} (\frac{1}{NS})^2$	$\frac{\pi^2}{2} \frac{1}{NS}$	$\frac{3\pi^4}{8} (\frac{1}{NS})^2$	$\frac{\pi}{2} \frac{1}{NS}$	$\frac{9\pi^2}{16} (\frac{1}{NS})^2$
Arctangent :	2	6	$\frac{2}{NS}$	$6(\frac{1}{NS})^2$	$\frac{\sqrt{3}}{\pi} \frac{1}{NS}$	$\frac{9}{2\pi^2} (\frac{1}{NS})^2$	same	same
Sine :	$\frac{\pi^2}{4} \frac{1}{NS}$	$\frac{\pi^2}{4}$	$\frac{\pi^2}{4} (\frac{1}{NS})^2$	$-\frac{\pi^2}{4} (\frac{1}{NS})^2$	same	same	same	same
Log :	1	2	$\frac{1}{NS}$	$2(\frac{1}{NS})^2$	$\frac{1}{NS}$	$2(e^{\frac{1}{NS}})^2$	same	same
Inverse Hyperbolic Tangent :	0	$2(1 - NS)$	0	$2(\tanh^{-1}\alpha)^2$	$\frac{2}{NS}$	$8(\frac{1}{NS})^2$	$\frac{2}{NS}$	$8(\frac{1}{NS})^2$
Quadratic:	$\frac{2}{NS}$	0	$2(\frac{1}{NS})^2$	0	same	same	same	same

NOTE: 'same' indicates maximum value is same as value at $\bar{\xi} = 0$.



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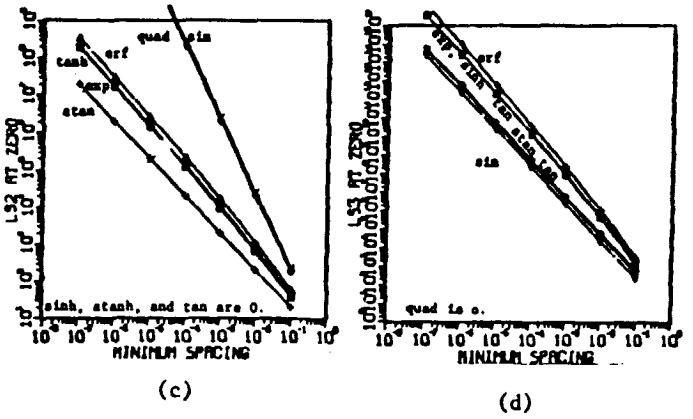
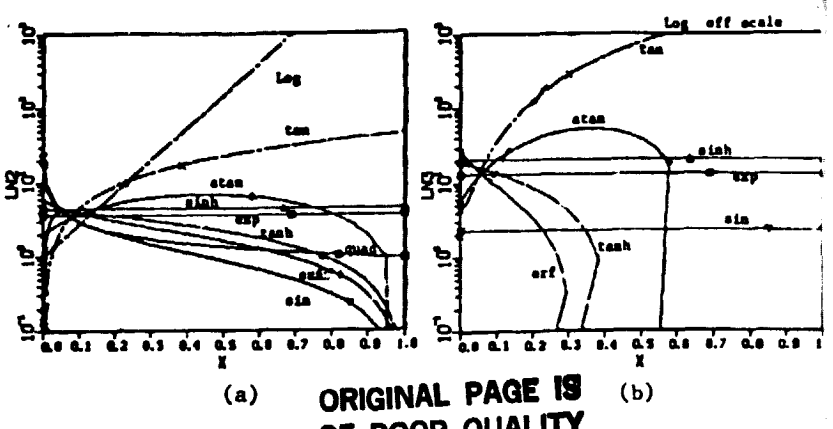


(c) (d)

Fig. 1 $L_N^{(i)}$ and $L_S^{(i)}$ ξ(i = 2,3) at Point of Minimum Spacing (ξ = 0).



(a) (b)

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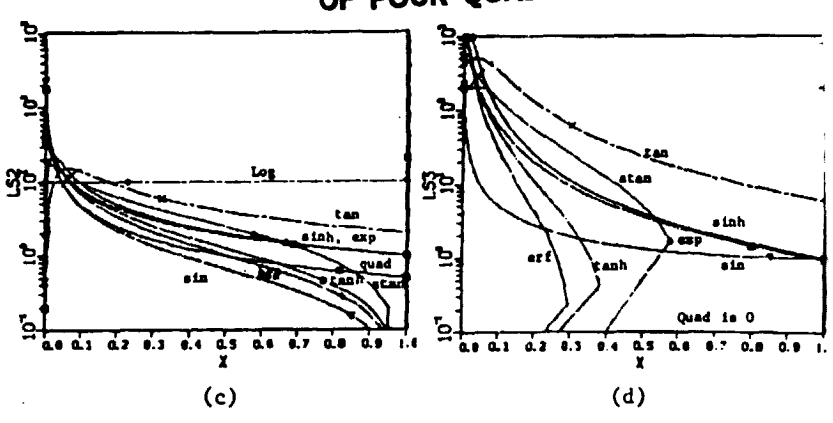
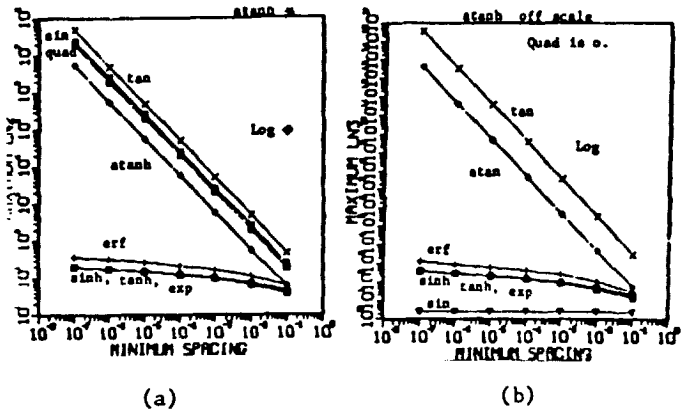
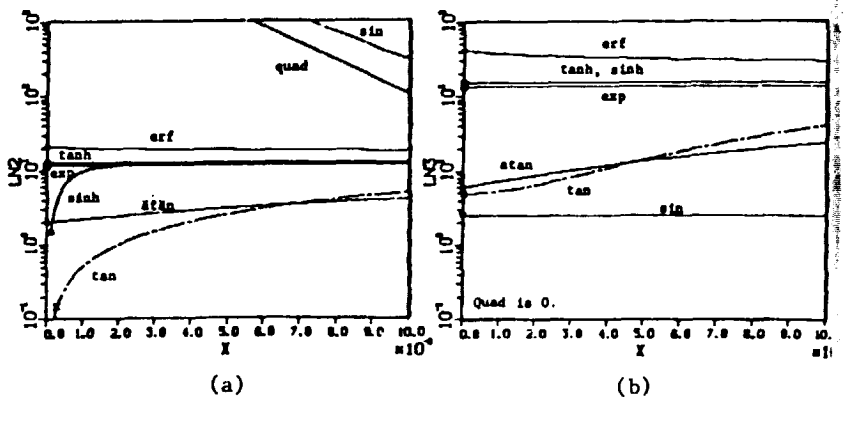


(c) (d)

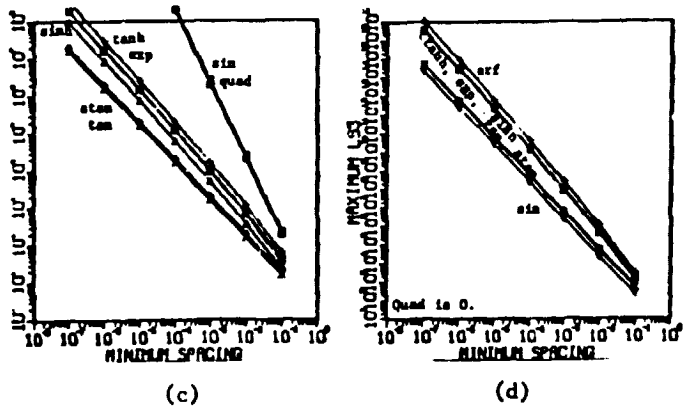
Fig. 3 Variation of $L_N^{(i)}$ and $L_S^{(i)}$ over the Field for Minimum Spacing of 10^{-3}.



(a) (b)

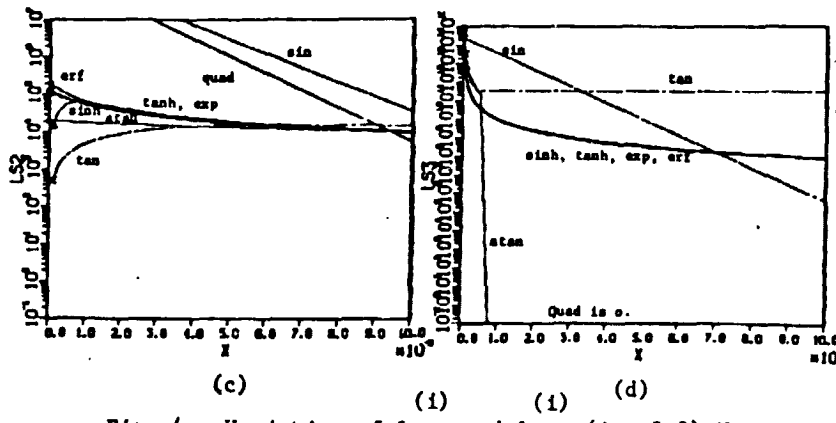


(a) (b)



(c) (d)

Fig. 2 Maximum Values of $L_N^{(i)}$ and $L_S^{(i)}$ (i = 2,3).



(c) (d)

Fig. 4. Variation of $L_N^{(i)}$ and $L_S^{(i)}$ (i = 2,3) Near Point Minimum Spacing (ξ = 0) for a Minimum Spacing of 10^{-6}.

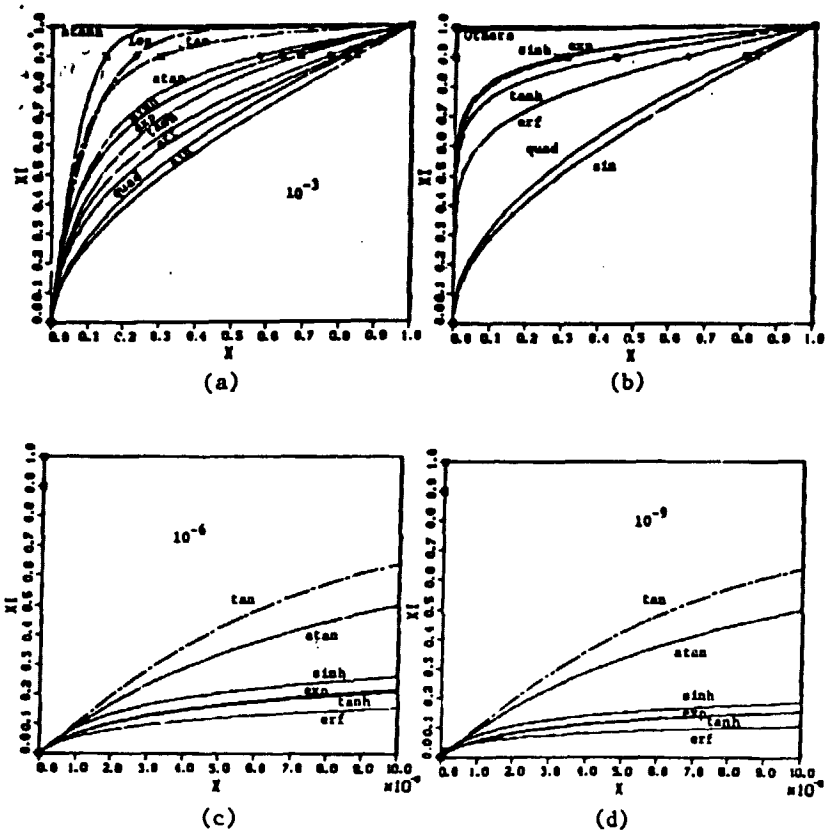


Fig. 5 Point Distribution

This research was partially supported under Air Force Contract F08635-82-K-0409, Eglin AFB, and under NASA Grant NSG 1577, Langley Research Center.