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A COMPARISON OF FINITE DIFFERENCE METHODS FOR SOLVING LAPLACE'S EQUATION ON CURVILINEAR COORDINATE SYSTEMS

By

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Transformation of Two and Three-Dimensional Regions of Elliptic Systems

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COORDINATE GENERATION BY CONFORMAL AND QUASICONFORMAL MAPPINGS*

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Abstract

Many recent advances in the solution of elliptic equations have been limited to regions whose boundary contours coincide with coordinate lines of the Cartesian coordinate system. The reason for this lies in the fact that when an arbitrary curvilinear coordinate system is used, the original elliptic equation becomes much more complex. For example, Poisson's equation is transformed to an equation with variable coefficients and a mixed derivative term. There is no added complexity, or additional computer storage needed for the coefficients, if an orthogonal coordinate system is generated from a conformal mapping. Many numerical schemes are available for constructing conformal mappings. Several steps are generally required to find the mapping between an arbitrary region and a rectangular region. A simple finite difference scheme will be presented for constructing a conformal mapping of a rectangular region onto a simply or doubly-connected region. The procedure determines the module of the region, the boundary correspondence, and the position of the interior coordinate lines. The coordinate generation requires the solution of a nonlinear elliptic system with oblique derivative boundary conditions, but is easily solved by any of the standard iterative techniques.

Any study of second order linear elliptic equations will introduce the notion of quasiconformal mappings which transform the elliptic equation to canonical form (i.e., the principal part of the differential operator reduces to the Laplacian). Quasiconformal mappings have been studied extensively by complex analysts, but little work has been done on the numerical construction of quasiconformal mappings. Some preliminary theoretical and numerical results indicate that the above procedure for conformal mappings can be generalized to construct quasiconformal mappings. This would allow one to simultaneously fit the boundary contours with coordinate lines and simplify the original equation when transforming to the new coordinate system. The equation, in canonical form, could possibly be solved by methods which would not be applicable to the original equation.

Examples of coordinate systems generated from conformal and quasiconformal mappings will be presented and the accuracy of the numerical scheme will be discussed. For quasiconformal mappings there is need for improvement in both the rate of convergence of the iterative procedure and the accuracy of the converged solution.

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ABSTRACT

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ABSTRACT

Finite difference methods have been widely used in solving partial differential equations by numerical methods. In this paper is a comparison of different finite difference techniques used to solve Laplace's equation. Curvilinear coordinate systems are used on two-dimensional regions with irregular boundaries -- specifically, regions around circles and airfoils.

In Chapter II, truncation errors are analyzed for three different finite difference methods. A comparison of the false boundary method and two-point and three-point extrapolation schemes, used when having the Neumann boundary condition, is included in Chapter III. In the concluding chapter, the effects of spacing and nonorthogonality in the coordinate systems are studied.
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TRANSFORMATION OF TWO AND THREE-DIMENSIONAL REGIONS BY ELLIPTIC SYSTEMS

The previous status reports have emphasized progress in the analysis of coordinate generation methods and error in solving problems on curvilinear coordinate systems. Recent emphasis has been on the application of this analysis to study the errors resulting in numerical computations. A compilation of numerical examples involving the solution of Laplace's equation on various coordinate systems is contained in a Thesis by M. J. McCoy. An extension of this work to solutions of the stream function-vorticity equations is in progress. In the numerical examples, the coefficients of the transformed equations have been computed both analytically and numerically. The analysis and numerical results were presented at a recent SIAM Meeting.

An extension of the results on conformal mappings can also be reported. For years quasiconformal mappings have been of interest to mathematicians because they share many properties with conformal mappings and also can be used to reduce linear elliptic partial differential equations to canonical form. Applications to physical problems have been limited because there was no known method for constructing a quasiconformal mapping. It is now possible to modify the numerical scheme used for generating coordinates by elliptic systems to construct quasiconformal mappings. This new discovery, along with previously reported results on conformal mappings, will be presented at the Conference on Elliptic Problem Solvers in Santa Fe on June 30, 1980. The method should be of special interest to people working on the direct solution of elliptic problems since mixed derivative terms can be eliminated by quasiconformal mappings. An abstract of the talk is attached. The final manuscript is being prepared and will appear later in the proceedings of the Conference.
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I. INTRODUCTION

Finite difference meshes have been widely used in solving partial differential equations by numerical methods. In finite difference techniques, partial derivatives in the equation are replaced by difference quotients. For example, given a differentiable function \( U(x,y) \), the first partial derivative of \( U \) with respect to \( x \) may be replaced by the difference of \( U \) evaluated at two neighboring points, divided by the distance between these two points. This method requires that the region first be divided into a grid, or mesh, as shown for the case of a rectangle.

The intersection of the lines in the grid are called nodes or grid points or mesh points. At these points we try to approximate values of the solution to the problem.

For example, consider Laplace's equation

\[
\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0
\]

on the above rectangle whose lines are of unit width apart in each direction. Assume boundary conditions are specified. By replacing the partial derivatives in the equation by difference quotients at the point \( P \), the equation is approximated by
\[ \phi(P) - \frac{1}{4} ( \phi(N) + \phi(S) + \phi(E) + \phi(W) ) = 0 \]

where \( \phi(P) \), \( \phi(N) \), \( \phi(S) \), \( \phi(E) \), and \( \phi(W) \) represent approximations to the function \( \phi \) at \( P \) and its neighboring points in the grid.

The collection of all such equations for all nodes gives a system of equations whose unknowns approximate the solution of the problem at the interior nodes. We may, then, set up an iterative scheme in order to compute an approximate value of the function at each point. See [1] and [2].

We encounter a problem, however, if we use a rectangular grid on an arbitrary two-dimensional region with irregular boundaries.

The grid points, or computational nodes, may not fall on the boundary so that we may not be able to make full use of the boundary conditions. When solving an equation on such a region it may be possible to construct a curvilinear coordinate system such that certain coordinate lines coincide with the boundaries of the region. A curvilinear system
is defined to be a finite difference grid having the property that each neighborhood of a node is topologically equivalent to a rectangular grid in the plane, that is, the coordinate lines may be considered as level curves of a one-to-one transformation. We can then solve our problem by computing a solution to the transformed equation in the rectangular region.

For an example of a curvilinear coordinate system, consider the transformation from rectangular to polar coordinates:

\[
\begin{align*}
    x &= r \cos \theta, \\
    y &= r \sin \theta.
\end{align*}
\]

Define the function \( T \) by \( (x, y) = T(r, \theta) \). If \( r > 0 \) and \( 0 < \theta < 2\pi \), \( T \) is one-to-one except when \( r = 0 \) and onto the \( xy \)-plane.

\( T \) maps the box \( 0 < r < a, 0 < \theta < \theta_0 \cdot 2\pi \) onto a sector of a disc in the \( xy \)-plane.
The level lines $r = \text{constant}$ are mapped onto circles in the $xy$-plane and the lines $\theta = \text{constant}$ are mapped onto spokes.

We shall consider different types of curvilinear coordinate systems by defining $r$ and $\theta$ as functions of $\xi$ and $\eta$. Define $S$ as a one-to-one mapping of $1 \leq \xi \leq N, \ 2 \leq \eta \leq M$ onto $1 \leq r \leq 10, \ 0 \leq \theta \leq 2\pi$. 
Then $T \circ S$ is one-to-one and onto.

The level lines $\xi = \text{constant}$ and $\eta = \text{constant}$ are mapped as follows.
The Jacobian matrix of the transformation $T \circ S$ is

$$
\begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{bmatrix}
= \begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{bmatrix}
$$

and the Jacobian is $J = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi}$. As long as $J \neq 0$, the level lines do not intersect; and since the mapping is one-to-one in the region, the inverse of the transformation exists. Further, by the Inverse Function Theorem, the Jacobian matrix of the inverse of the transformation is the inverse of the matrix of the transformation. See [3].

When using curvilinear systems certain difficulties may arise. The coordinate system can have considerable effect on the error in the numerical solution to the problem. Crowder and Dalton [4] and Blottner and Roache [5] have demonstrated this for the one-dimensional case. E. de Rivas [6] gives a study of truncation errors in the use of nonuniform grids. We may readily see that coordinate line spacing rapidly changes or if we use an extremely nonorthogonal system, the second order differences of the $x$ and $y$ coordinate functions may become quite large. Therefore, when we consider the chain rule and Taylor series expansions, as we will do in this study, we see that our truncation
errors can become much worse when using such systems. See [7].

In our study we shall compare several different coordinate systems, methods for finding values on the boundary when having the Neumann boundary condition, and various finite difference schemes. Lau [8] has developed a finite difference method, in a manner similar to that to be used in this study, for the three-dimensional case. Also see [9].
II. FINITE DIFFERENCE METHODS AND ERROR ANALYSIS

We wish to solve the partial differential equation

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

on a two-dimensional, doubly-connected region $D$, with boundary components $\Gamma_1$ and $\Gamma_2$, and a cut along $\Gamma_3$ and $\Gamma_4$ which are coincident. Refer to Figure 1. We have Dirichlet boundary conditions on $\Gamma_2$ and either

(i) Dirichlet boundary conditions on $\Gamma_1$, or
(ii) Neumann boundary conditions on $\Gamma_1$.

In order to solve this problem what we have done is to transform our problem from the $xy$-plane to the $\xi\eta$-plane by a one-to-one mapping, where our transformed plane $D^*$ is a rectangular region and the boundaries correspond to constant coordinate lines. Since $\Gamma_3$ and $\Gamma_4$ are coincident in $D$, $\Gamma_3^*$ and $\Gamma_4^*$ are reentrant values in $D^*$. Refer to Figure 2. We are, then, able to solve our problem in the $\xi\eta$-plane.

In this study we wish to compare the accuracy of several finite difference methods of solving the problem, as well as to study the effects of nonorthogonality and rate of change of spacing of coordinate lines in the region.

First we shall consider the chain rule method. Suppose a coordinate system is given in a region $D$ of the $xy$-plane and $f$ is a function in $C^2(D)$. Difference expressions for the first and second order partial derivatives of $f$ can be obtained by transforming the region $D$ to a rectangular region $D^*$ and applying the chain rule. The relationship
between the derivatives of $f$ in the $xy$-plane and those in the $\xi\eta$-plane are given below:

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

$$\frac{\partial f}{\partial \eta} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \eta}.$$

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

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

The derivatives with respect to the $xy$-variables may be expressed in terms of derivatives with respect to the $\xi\eta$-variables provided the Jacobian of the transformation, $J = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi}$, does not vanish.

For example, we may solve the first two equations in (1) for $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$.

Higher derivatives may then be obtained by repeated applications of these expressions for $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$:

$$\frac{\partial f}{\partial x} = \left( \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} - \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} \right) / J,$$

$$\frac{\partial f}{\partial y} = \left( -\frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial y} \right) / J.$$

(2) $$\frac{\partial^2 f}{\partial x^2} = \left[ \left( \frac{\partial^2 f}{\partial \xi \partial \eta} \right)^2 - 2 \frac{\partial^2 f}{\partial \xi \partial \eta} \frac{\partial^2 f}{\partial x^2} \right] / J^2 + \left( \frac{\partial^2 f}{\partial \eta \partial \xi} \right)^2 / J^2 + \left( \frac{\partial^2 f}{\partial \eta \partial \eta} \right)^2 / J^2$$

$$- \frac{\partial^2 f}{\partial x \partial y} \left[ \left( \frac{\partial^2 f}{\partial \xi \partial \eta} \right)^2 - \left( \frac{\partial^2 f}{\partial \eta \partial \xi} \right)^2 \right] / J^2 + \left( \frac{\partial^2 f}{\partial \eta \partial \eta} \right)^2 / J^2.$$
All derivatives with respect to the \( \xi, \eta \)-variables may be approximated using difference operators, so we define the following expressions which replace the corresponding derivatives in the above equations.

\[
\begin{align*}
\frac{\partial^2 f}{\partial x \partial y} &= \left[ \frac{\partial f}{\partial \eta} \right] \left( \frac{\partial^2 f}{\partial \xi^2} - 2 \frac{\partial x}{\partial \xi} \frac{\partial^2 f}{\partial \xi \partial \eta} + \left( \frac{\partial x}{\partial \xi} \right)^2 \frac{\partial^2 f}{\partial \eta^2} \right] / \left( \frac{\partial^2 f}{\partial \xi \partial \eta} \right) \\
\frac{\partial^2 f}{\partial y^2} &= \left[ \frac{\partial f}{\partial \eta} \right] \left( \frac{\partial^2 f}{\partial \xi^2} - 2 \frac{\partial x}{\partial \xi} \frac{\partial^2 f}{\partial \xi \partial \eta} + \left( \frac{\partial x}{\partial \xi} \right)^2 \frac{\partial^2 f}{\partial \eta^2} \right] / \left( \frac{\partial^2 f}{\partial \xi \partial \eta} \right)
\end{align*}
\]

These are merely the second order central differences on a square mesh of unit width in the \( \xi, \eta \)-plane. See Figure 3. The coordinates \( x \) and \( y \) are also functions of \( \xi \) and \( \eta \), and their partial derivatives may also be approximated by difference expressions in a similar manner.

From (1) and the above method of obtaining the central differences, then we may set up a matrix equation.
\[
\begin{bmatrix}
  f_x & f_y \\
  f_z & f_n \\
  f_{\xi\xi} & f_{\eta\eta} \\
  f_{\xi\eta} & f_{\eta\eta}
\end{bmatrix} = A 
\begin{bmatrix}
  \frac{\partial f}{\partial x} \\
  \frac{\partial f}{\partial y} \\
  \frac{\partial^2 f}{\partial x^2} \\
  \frac{\partial^2 f}{\partial x\partial y} \\
  \frac{\partial^2 f}{\partial y^2}
\end{bmatrix}, \text{ where}
\]
\[
A = \begin{bmatrix}
  x_\xi & y_\xi & 0 & 0 & 0 \\
  x_\eta & y_\eta & 0 & 0 & 0 \\
  x_{\xi\xi} & y_{\xi\xi} & x_\xi^2 & 2x_\xi y_\xi & y_\xi^2 \\
  x_{\xi\eta} & y_{\xi\eta} & (x_\xi y_\eta + x_\eta y_\xi) & y_\xi y_\eta & y_\eta^2 \\
  x_{\eta\eta} & y_{\eta\eta} & x_\eta^2 & 2x_\eta y_\eta & y_\eta^2
\end{bmatrix}
\]

We may solve this by
\[
\begin{bmatrix}
  \frac{\partial f}{\partial x} \\
  \frac{\partial f}{\partial y} \\
  \frac{\partial^2 f}{\partial x^2} \\
  \frac{\partial^2 f}{\partial x\partial y} \\
  \frac{\partial^2 f}{\partial y^2}
\end{bmatrix} = A^{-1} \begin{bmatrix}
  f_x \\
  f_y \\
  f_{\xi\xi} \\
  f_{\xi\eta} \\
  f_{\eta\eta}
\end{bmatrix}, \text{ provided } \det A \neq 0.
\]

The determinant of A will not vanish in our case because J \neq 0.

Next we consider a Taylor series expansion of f about P. Using this and the difference expressions we have already developed, we get the following matrix equation:
\[
\begin{bmatrix}
  f_{\xi} \\
  f_{\eta} \\
  f_{\xi\xi} \\
  f_{\xi\eta} \\
  f_{\eta\eta}
\end{bmatrix}
= A
\begin{bmatrix}
  \frac{\partial^2 f}{\partial x^2} \\
  \frac{\partial^2 f}{\partial x \partial y} \\
  \frac{\partial^2 f}{\partial x^2} \\
  \frac{\partial^2 f}{\partial x \partial y} \\
  \frac{\partial^2 f}{\partial y^2}
\end{bmatrix}
\]
where
\[
A = \begin{bmatrix}
  x_{\xi} & y_{\xi} & \frac{1}{2}x_{\xi} & \frac{1}{2}y_{\xi} & \frac{1}{2}y_{\xi} \xi \\
  x_{\eta} & y_{\eta} & \frac{1}{2}x_{\eta} & \frac{1}{2}y_{\eta} & \frac{1}{2}y_{\eta} \\
  x_{\xi}\xi & y_{\xi}\xi & \left(\frac{1}{2}x_{\xi}\xi + \frac{1}{2}y_{\xi}\xi \right) & \left(\frac{1}{2}x_{\xi}\xi + \frac{1}{2}y_{\xi}\xi \right) & \left(\frac{1}{2}x_{\xi}\xi + \frac{1}{2}y_{\xi}\xi \right) \\
  x_{\xi}\eta & y_{\xi}\eta & \left(\frac{1}{2}x_{\xi}\eta + \frac{1}{2}y_{\xi}\eta \right) & \left(\frac{1}{2}x_{\xi}\eta + \frac{1}{2}y_{\xi}\eta \right) & \left(\frac{1}{2}x_{\xi}\eta + \frac{1}{2}y_{\xi}\eta \right) \\
  x_{\eta}\eta & y_{\eta}\eta & \left(\frac{1}{2}x_{\eta}\eta + \frac{1}{2}y_{\eta}\eta \right) & \left(\frac{1}{2}x_{\eta}\eta + \frac{1}{2}y_{\eta}\eta \right) & \left(\frac{1}{2}x_{\eta}\eta + \frac{1}{2}y_{\eta}\eta \right)
\end{bmatrix}
\]
the error terms are \(O(h^3)\), \(h\) the maximum distance between \(P\) and its neighbors, and
\[
\begin{align*}
(x^2)_{\xi\eta}(P) &= \frac{1}{2}(x(v)^2 + x(w)^2 - x(x)^2 - x(v)^2) \\
(xy)_{\xi\eta}(P) &= \frac{1}{2}(x(v)y(u) + x(w)y(w) - x(x)y(x) - x(v)y(v)) \\
(y^2)_{\xi\eta}(P) &= \frac{1}{2}(y(v)^2 + y(w)^2 - y(x)^2 - y(v)^2).
\end{align*}
\]
We may solve by
\[
\begin{bmatrix}
  \frac{\partial f}{\partial x} \\
  \frac{\partial f}{\partial y} \\
  \frac{\partial^2 f}{\partial x^2} \\
  \frac{\partial^2 f}{\partial x \partial y} \\
  \frac{\partial^2 f}{\partial y^2}
\end{bmatrix}
= A^{-1}
\begin{bmatrix}
  f_{\xi} \\
  f_{\eta} \\
  f_{\xi\xi} \\
  f_{\xi\eta} \\
  f_{\eta\eta}
\end{bmatrix}
\]
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When we compare the chain rule method with the Taylor series method, we consider the system \((4)\) for Taylor series and the system \((1a)\) for the chain rule, both of which use central difference approximations for the partial derivatives of \(x\) and \(y\) with respect to the \(\xi, \eta\)-variables. In the Taylor series expressions from \((4)\), only the first and second order terms are retained, and the truncation error is \(O(h^3)\) for each expansion. In the expressions for \(f_\xi\) and \(f_\eta\), if only the first order terms are retained, the truncation error is \(O(h^2)\). These expressions, though, are precisely those of the chain rule method. We see then that for our chain rule method, the error terms of \(f_\xi\) and \(f_\eta\) are \(O(h^2)\).

If we compare the last three equations in the Taylor series method and the chain rule method, we note that, in order to reproduce the Taylor series expressions from the chain rule expressions, some second order terms in \((4)\) would have to be added, as well as the error term which is \(O(h^3)\). Hence, considering the second order terms, the error in these chain rule expressions is \(O(h^2)\).

Therefore, in all five equations using the chain rule, the errors are \(O(h^2)\). The errors for the Taylor series method, retaining only first and second order terms, are all \(O(h^3)\). It appears then that, when we use central difference expressions for the coefficients in these systems, the Taylor series expansions should give better results than the chain rule.

The third scheme we consider uses the chain rule in the same manner as before, but the difference lies in our method of finding

\[
\frac{\partial x}{\partial \xi}, \frac{\partial x}{\partial \eta}, \frac{\partial^2 x}{\partial \xi^2}, \frac{\partial^2 x}{\partial \xi \partial \eta}, \frac{\partial^2 x}{\partial \eta^2}, \text{ etc.}
\]

Instead of approximating these partial derivatives by finite difference expressions as before, we compute these
values analytically. The accuracy of this method can also be evaluated from Taylor series expansions.

For the first order central differences in the computational region,

\[ f_{\xi} = \frac{3f}{3\xi} + \frac{1}{6} \frac{3f}{3\xi^2} \]

\[ = \left( \frac{2f}{3\xi} + \frac{1}{6} \frac{3f}{3\xi^2} \right) \frac{2f}{3\xi} \left( \frac{2f}{3\xi} + \frac{1}{6} \frac{3f}{3\xi^2} \right) + \frac{1}{2} \left( \frac{2f}{3\xi} + \frac{1}{6} \frac{3f}{3\xi^2} \right) \frac{2f}{3\xi} \frac{2f}{3\xi} + \frac{1}{2} \frac{2f}{3\xi} \frac{2f}{3\xi} \frac{2f}{3\xi} \frac{2f}{3\xi} , \]

where only the first and second order terms are retained.

Approximations for the second order differences are obtained in a similar way. If \( f_{\xi^2} = \frac{3f}{3\xi^2} + \frac{1}{12} \frac{4f}{3\xi^4} \) and \( f_{\xi^2} = \frac{3f}{3\xi^2} - \frac{1}{6} \left( \frac{4f}{3\xi^4} + \frac{4f}{3\xi^4} \right) \)
then, dropping all but the first and second order terms, we get the following estimates:

\[ f_{\xi^2} = \left( \frac{2f}{3\xi^2} + \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{2f}{3\xi^2} + \left( \frac{2f}{3\xi^2} + \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{2f}{3\xi^2} + \left( \frac{2f}{3\xi^2} + \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{2f}{3\xi^2} + \left( \frac{2f}{3\xi^2} + \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{2f}{3\xi^2} , \]

\[ f_{\xi^2} = \left( \frac{3f}{3\xi^2} - \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{3f}{3\xi^2} + \left( \frac{3f}{3\xi^2} - \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{3f}{3\xi^2} + \left( \frac{3f}{3\xi^2} - \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{3f}{3\xi^2} + \left( \frac{3f}{3\xi^2} - \frac{1}{6} \frac{4f}{3\xi^4} \right) \frac{3f}{3\xi^2} , \]

\[ f_{\xi^2} = \left( \frac{2f}{3\xi^2} + \frac{1}{12} \frac{4f}{3\xi^4} \right) \]
Here we observe that the difference formulas, arrived at via the chain rule, for the derivatives of \( f \) are accurate only if the higher order derivatives of the coordinate functions \( x \) and \( y \) become progressively smaller.

A comparison of the Taylor series expansion about \( P \) and the analytic derivatives suggests (and our study bears this out) that the numerical computation would be preferred due to the appearance of error in the first derivative terms when the coefficients are computed analytically.
III. ITERATION SCHEMES AND BOUNDARY TECHNIQUES

From both the chain rule and the Taylor series, we have, for 

\[ \nabla^2 \phi = 0, \]

\[ \begin{bmatrix} 
\phi_x \\
\phi_y \\
\phi_{xx} \\
\phi_{yy} \\
\phi_{xy} \\
\phi_{yx} 
\end{bmatrix} = A \begin{bmatrix} 
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y} \\
\frac{\partial^2 \phi}{\partial x^2} \\
\frac{\partial^2 \phi}{\partial y^2} \\
\frac{\partial^2 \phi}{\partial x \partial y} \\
\frac{\partial^2 \phi}{\partial y \partial x} 
\end{bmatrix}, \quad A = [A_{ij}]. \]

Then from \( x, y, \) and \( \phi \) we compute

\[ A^{-1} \begin{bmatrix} 
\phi_x \\
\phi_y \\
\phi_{xx} \\
\phi_{yy} \\
\phi_{xy} \\
\phi_{yx} 
\end{bmatrix} \]

to find \( \frac{\partial^2 \phi}{\partial x^2} \) and \( \frac{\partial^2 \phi}{\partial y^2} \).

Our transformed equation is 

\[ \nabla^2 \phi = a_1 \phi_x + a_2 \phi_y + a_3 \phi_{xx} + a_4 \phi_{yy} + a_5 \phi_{xy} = 0, \]

where \( A^{-1} = [B_{ij}] \) and \( a_j = B_{3j} + B_{5j} \). Using central differences to
approximate \( \nabla^2 \psi \) above in terms of the \( i, n \)-variables, we get

\[
L \psi = c_1 \psi(\xi, n) + c_2 \psi(\xi+1, n) + c_3 \psi(\xi-1, n) + c_4 \psi(\xi, n+1) + c_5 \psi(\xi, n-1) \\
+ c_6 \psi(\xi+1, n+1) + c_7 \psi(\xi+1, n-1) + c_8 \psi(\xi-1, n+1) + c_9 \psi(\xi-1, n-1)
\]

\( \psi = 0. \)

We will use the Successive Overrelaxation iteration scheme to approximate \( \psi \):

\[
\phi(s)(\xi, n) = -\frac{\omega}{c_1} \left( c_1 \psi(\xi, n) + c_2 \psi(\xi+1, n) + c_3 \psi(\xi-1, n) + c_4 \psi(\xi, n+1) \\
+ c_5 \psi(\xi, n-1) + c_6 \psi(\xi+1, n+1) + c_7 \psi(\xi+1, n-1) \\
+ c_8 \psi(\xi-1, n+1) + c_9 \psi(\xi-1, n-1) \right) + \phi(s-1)(\xi, n)
\]

\[
= -\frac{\omega}{c_1} L \psi + \phi(s-1)(\xi, n)
\]

\[
= \phi(s-1)(\xi, n) - \frac{\omega L \psi}{c_1}
\]

where \( c_1 = -2a_x - 2a_y \) and \( \omega \) is the relaxation factor. So we have, then,

\[
\phi(s) = \phi(s-1) + \frac{\omega L \psi}{2(a_x a_y)}.
\]

We have compared several techniques for finding values on the boundary. When we have the Neumann condition, \( \frac{\partial \psi}{\partial n} = 0 \), on the boundary, we go through an iteration scheme obtained in a manner similar to that of the scheme for the interior points. First \( \frac{\partial \psi}{\partial n} = 0 \) is computed by the expression

\[
\frac{\partial \psi}{\partial n} = V \phi \cdot \frac{V n}{|V n|} = 0 \quad \text{on} \quad n = \text{constant}.
\]

In the first two equations of (2), if we apply the relations for \( \frac{\partial f}{\partial x} \) and \( \frac{\partial f}{\partial y} \) with \( f = n \), we obtain

\[
\frac{\partial n}{\partial x} = -\frac{3y}{\partial \xi} J \quad \text{and} \quad \frac{\partial n}{\partial y} = \frac{2x}{\partial \xi} J
\]

so that

\[
\frac{V n}{|V n|} = \left( -\frac{3y}{\partial \xi}/\sqrt{a}, \frac{2x}{\partial \xi}/\sqrt{a} \right), \quad \nu \phi = \left( \frac{3y}{\partial x} \frac{3y}{\partial y} \right) = \left( \frac{3y}{\partial x}, \frac{3y}{\partial y} \right) \quad \text{where} \quad \sigma = \left( \frac{3y}{\partial x} \right)^2 + \left( \frac{3y}{\partial y} \right)^2.
\]
Since we have \(-\frac{\partial^2 \phi}{\partial x \partial y} + \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial y} = 0\). From

\[
\begin{bmatrix}
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y} \\
\frac{\partial^2 \phi}{\partial x^2} \\
\frac{\partial^2 \phi}{\partial x \partial y} \\
\frac{\partial^2 \phi}{\partial y^2}
\end{bmatrix}
= A^{-1}
\begin{bmatrix}
\phi_{\xi} \\
\phi_{\eta} \\
\phi_{\xi \xi} \\
\phi_{\xi \eta} \\
\phi_{\eta \eta}
\end{bmatrix},
\]

we get the equations

\[
\frac{\partial \phi}{\partial x} = B_{11} \phi_{\xi} + B_{12} \phi_{\eta} + B_{13} \phi_{\xi \xi} + B_{14} \phi_{\xi \eta} + B_{15} \phi_{\eta \eta}
\]

\[
\frac{\partial \phi}{\partial y} = B_{21} \phi_{\xi} + B_{22} \phi_{\eta} + B_{23} \phi_{\xi \xi} + B_{24} \phi_{\xi \eta} + B_{25} \phi_{\eta \eta},
\]

then from these equations and our boundary condition \(-\frac{\partial v}{\partial x} + \frac{\partial x}{\partial x} \frac{\partial v}{\partial y} = 0\),

we have

\[
\left(\frac{\partial x}{\partial \xi} B_{21} - \frac{\partial y}{\partial \xi} B_{11}\right) \phi_{\xi} + \left(\frac{\partial x}{\partial \xi} B_{22} - \frac{\partial y}{\partial \xi} B_{12}\right) \phi_{\eta} + \left(\frac{\partial x}{\partial \xi} B_{23} - \frac{\partial y}{\partial \xi} B_{13}\right) \phi_{\xi \xi} + \left(\frac{\partial x}{\partial \xi} B_{24} - \frac{\partial y}{\partial \xi} B_{14}\right) \phi_{\xi \eta} + \left(\frac{\partial x}{\partial \xi} B_{25} - \frac{\partial y}{\partial \xi} B_{15}\right) \phi_{\eta \eta} = 0,
\]

or

\[
d_1 \phi_{\xi} + d_2 \phi_{\eta} + d_3 \phi_{\xi \xi} + d_4 \phi_{\xi \eta} + d_5 \phi_{\eta \eta} = 0,
\]

where \(d_j = \frac{\partial x}{\partial \xi} B_{2j} - \frac{\partial y}{\partial \xi} B_{1j}\). The interior boundary component will be

\(n = 1\) a false boundary used for implementing the Neumann boundary condition as indicated in Figure 4.

So on the false boundary \(n = 1\), in a manner similar to that used in obtaining a scheme for the interior points, we have the iteration scheme

\[
\phi(n)_{(\xi, 1)} = \phi(n-1)(\xi, 1) + \frac{1}{d_2/2 - d_5} \left(d_1 \phi_{\xi} + d_2 \phi_{\eta} + d_3 \phi_{\xi \xi} + d_4 \phi_{\xi \eta} + d_5 \phi_{\eta \eta}\right)
\]
We have also studied the effects of using forward difference schemes for approximating values on the boundary. One method we considered uses the expressions

\[
\frac{\partial \phi}{\partial n}(\xi, n) = \left( -\phi(\xi, n+2) + 4\phi(\xi, n+1) - 3\phi(\xi, n) \right) / 2
\]

where we still have the boundary condition \( \frac{\partial \phi}{\partial n} = 0 \). For \( \frac{\partial \phi}{\partial x} \) and \( \frac{\partial \phi}{\partial y} \), the chain rule formula is used and the Neumann condition \( \frac{\partial \phi}{\partial n} = 0 \) is approximated by \( d_1 \phi + d_2 \phi_n = 0 \). Then we get the three-point extrapolation formula

(5) \( \phi(\xi, n) = \frac{4\phi(\xi, n+1) - \phi(\xi, n+2)}{3} + 2d_1 \phi(\xi, n) / d_2 \) at \( n = 2 \).

Another method used was \( \frac{\partial \phi}{\partial n}(\xi, n) = \phi(\xi, n+1) - \phi(\xi, n) \). Then we get the two-point extrapolation expression

(6) \( \phi(\xi, n) = \phi(\xi, n+1) + d_1 \phi(\xi, n) / d_2 \) at \( n = 2 \).

Because of the difficulty in getting the partial derivatives at the trailing edge of the airfoil necessary in approximating values of \( \phi \) there, we have used a three-point extrapolation on the trailing edge at \( n = 2 \), and \( \xi = 1 \) and \( \xi = N \).

(7) \( \phi(1, 2) = 3\phi(2, 2) - 3\phi(3, 2) + \phi(4, 2) \)

\( \phi(N, 2) = 3\phi(N-1, 2) - 3\phi(N-2, 2) + \phi(N-3, 2) \)

These formulas were obtained by fitting a parabola through the three known values in order to approximate the points \( \phi(1, 2) \) and \( \phi(N, 2) \) on it.
IV. COORDINATE SYSTEMS AND RESULTS

Different coordinate systems have been used in our region in order to compare the results when using grids with properties such as equal spacing, continuous changes in spacing, or an abrupt jump in spacing, and orthogonality or nonorthogonality. In our study we have used $1 \leq \xi \leq N = 40$ and $2 \leq \eta \leq M = 50$ on both circles and airfoils.

In each case, we have taken a known solution to the problem and compared values of this function on the grid to those of the approximated function which we have computed. Here we provide figures illustrating the coordinate systems and a graph for each comparison of the errors of the particular methods used for the systems. The graphs were plotted along either $\xi$ or $\eta$ equal to a constant.

The first coordinate system we will consider is an orthogonal one in which we have a jump in the coordinate line spacing. The lines close to the body are equally spaced before the jump, from radius 1 to 2.294. After the jump, from radius 2.294 to 10.0, though the distance between consecutive coordinate lines is again uniform, this distance has been increased to five times that between the lines before the jump. This coordinate system is generated by the following formulas:

We will denote $r$ at $\eta = \text{constant}$ by $r(\eta)$. Then

$$r(2) = 1$$
$$r(\eta+1) = r(\eta) + 2.7/(M-2) \quad \text{for} \ 2 \leq \eta \leq M/2$$
$$r(\eta+1) = r(\eta) + 13.5/(M-2) \quad \text{for} \ M/2 \leq \eta \leq M.$$

$$\theta = 2\pi \left( (\xi-1)/(N-1) \right).$$
Refer to Figures 5 and 6. In Figure 6, we have the same system as in 5, except on a larger scale, and we have only shown the first 29 coordinate lines close to the body.

In this comparison, we consider different methods for two different functions:

(i) \( \psi(x,y) = x \left( 1 + \frac{1}{x^2 + y^2} \right) \)

(ii) \( \psi(x,y) = \frac{1}{2} \log(x^2 + y^2) \), where \( x = r \cos \theta \) and \( y = r \sin \theta \).

For (i) we compare the results of chain rule and Taylor series, using central differences for the approximated values of the \( \xi_\eta \)-partial derivatives of \( x \) and \( y \), and the Neumann boundary condition on \( \Gamma_1 \), creating a false boundary at \( \eta = 1 \). For a graph of these errors along \( \xi = 1 \), refer to Figure 7. The results using Taylor series were better than those using the chain rule.

In (ii) we compare the chain rule and Taylor series using central differences for the coefficients, and the Dirichlet boundary condition. For a graph comparing the errors plotted along the line \( \xi = 1 \), refer to Figure 8. Again Taylor series gives better results.

Next we will compare a nonorthogonal system with an orthogonal one, using the function \( \phi(x,y) = \frac{1}{2} \log(x^2 + y^2) \), where \( x = r \cos \theta \) and \( y = r \sin \theta \). In the orthogonal system,

\[
\begin{align*}
\xi &= 1 + g \left( \frac{(n-2)/(M-2)}{ } \right) \\
\theta &= 2 \pi \frac{ (\xi-1)/(N-1) }{ }.
\end{align*}
\]

Refer to Figure 9.

For the nonorthogonal system we use

\[
\begin{align*}
\xi &= 1 + g \left( \frac{(n-2)/(M-2)}{ } \right) \quad \text{and} \quad \theta_{\text{max}} = \pi/6, \theta_{\text{min}} = \pi/6, \\
\theta &= \theta_{\text{min}} + \frac{\pi-1}{2} (\theta_{\text{max}} + \theta_{\text{min}}) + 2 \pi \left( \frac{ (\xi-1)/(N-1) }{ } \right),
\end{align*}
\]

Refer to Figure 10.
On each of these systems we have used the chain rule method, central differences for the coefficients, and the Dirichlet boundary condition on $\Gamma_1$. For a comparison of the error curves along $\zeta = 1$, see Figure 11. The errors were constant on each circular coordinate line, and the results using the orthogonal system were better.

For the function $\phi(x,y) = x\left(1 + \frac{1}{x^2+y^2}\right)$, we will again use the nonorthogonal system described above (see, Figure 10). We will compare the accuracy when using a false boundary with that when using the two-point and three-point extrapolation formulas, (6) and (5), respectively, for values on $\Gamma_1$ where we have the Neumann boundary condition. In each case we have used the chain rule method with central difference expressions for the coefficients.

At $n = 1$, we have taken for the $x$ and $y$ values,

\[
x(\zeta, 1) = 2x(\zeta, 2) - x(\zeta, 3)
y(\zeta, 1) = 2y(\zeta, 2) - y(\zeta, 3)
\]

when using the false boundary. For a graph along $n = 2$ comparing the errors when using these methods, refer to Figure 12. Since the error curves in each of these are symmetric about the line $\zeta = 20$, we have only shown the points for $1 < \zeta < 20$. We see that both the false boundary and the three-point extrapolation methods give much better results than the two-point extrapolation.

The next coordinate system we consider is generated by $x = r \cos \theta,$ $y = r \sin \theta,$ $\theta = 2\pi ( (\zeta-1)/(N-1) ),$ and $r = 1 + 10\left(\frac{M-n+2}{20}\right)\text{tanh}\left(\frac{M-n+2}{20}\right)$. Refer to Figures 13 and 14. Figure 14 is a plot of the same coordinate system as 13 on a larger scale, so we only show the 24 lines closest to the body. Again we use $\phi(x, y) = x\left(1 + \frac{1}{x^2+y^2}\right)$.
In this coordinate system we compare the results obtained using
the numerically approximated values of the $\xi$-partial derivatives of
$x$ and $y$, or the coefficients, in both the chain rule and Taylor series
methods with the chain rule method using the analytic derivatives of $x$
and $y$. In each case we use the Dirichlet boundary condition on $\Gamma_1$.

With both the chain rule and Taylor series where we use the
numerical coefficients we get good results. However, when using the
analytic derivatives with the chain rule, the errors were much larger.
Refer to Figure 15 for a graph of the errors along $\xi = 1$.

In the previous cases, we have considered coordinate systems and
functions on regions around circles. Now we move to the airfoil,

obtained by the following transformation:

\[
x = r \cos \theta, \quad y = r \sin \theta
\]

\[
x_1 = x(1-b), \quad y_1 = y(1-b)
\]

\[
x_2 = x_1 + b, \quad y_2 = y_1
\]

\[
\bar{x} = x_2 + \left( \frac{x_2}{x_2^2 + y_2^2} \right), \quad \bar{y} = y_2 - \left( \frac{y_2}{x_2^2 + y_2^2} \right).
\]

The transformation from $(x_2, y_2)$ to $(\bar{x}, \bar{y})$ is the classical Joukowski
transformation which is a conformal mapping. For this study we have
taken $b = -1$ and used the coordinate system generated by

\[
r = 1 + 9\left( \frac{(n-2)/(n-2)}{2n((\xi-1)/(n-1))} \right)
\]

with the function $f(x, y) = \frac{1}{x^2 + y^2}$. Refer to Figure 16. In each
of the methods we will compare, we have used the three-point extrapolation
formulas (7), discussed earlier, for approximating values on the
trailing edge.

First we compare the chain rule and the Taylor series using
numerical coefficients with the chain rule using analytically computed
coefficients. In each of these, we have used the Neumann boundary condition, with a false boundary. For a graph of the error curves along the line $\xi = 1$, see Figure 17. For the curves graphed along $\eta = 2$, see Figure 18. Note that these error curves are symmetric about $\xi = 20$, so that in Figure 18, we have only shown these curves for $1 \leq \xi \leq 20$. In both figures, we see that at most points, the Taylor series and the chain rule methods using approximated derivatives both give better results than the chain rule with analytic derivatives.

Finally, for the same coordinate system and function $\phi$ as in the immediately preceding comparison, we have used the chain rule method with numerically approximated derivatives in comparing the false boundary method with the three-point extrapolation of $\phi$ on $\Gamma_1$ where we have the Neumann boundary condition. Refer to Figure 19 for a graph of the error curves along $\eta = 2$. Again, since these curves are symmetric about $\xi = 20$, we have plotted them for $1 \leq \xi \leq 20$. These methods give equally satisfactory results.
V. CONCLUSION

The objective of this study was to determine the most accurate method, of several considered, used to solve numerically the partial differential equation $\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$. We have looked at several different coordinate systems on circles and on airfoils. In the comparison of the nonorthogonal system with the orthogonal one, we found that the orthogonal system gave better results.

We have also compared different schemes on the systems. When we compare Taylor series with the chain rule we see that, in general, Taylor series is more accurate. When considering these two methods, which use numerical coefficients, versus the chain rule with analytical coefficients, we see that the errors when using the analytical derivatives may be much greater than either of the first two methods.

Also considered in this study were the false boundary, two-point extrapolation, and three-point extrapolation methods used when having the Neumann boundary condition. We found that both the false boundary and the three-point extrapolation techniques give satisfactory results, each being more accurate than the two-point extrapolation method.
Figure 1
Figure 2

Transformed Plane
Computational Molecule

Figure 3
Figure 4
Figure 7

\( s = 1 \)

- Chain Rule
- Taylor Series
\[ \frac{\partial f}{\partial x} = 1 \]

- Chain Rule
- Taylor Series

Figure 6
Figure 9
\[ \xi = 1 \]

--- Orthogonal System

--- Nonorthogonal System

Figure 11
$\xi = 1$

- Chain Rule - Numerical Coefficients
- Taylor Series - Numerical Coefficients
- Chain Rule - Analytical Coefficients

Figure 15
Figure 17

\( \xi = 1 \)
- Chain Rule - Analytical Coefficients
- Taylor Series - Numerical Coefficients
- Chain Rule - Numerical Coefficients
Figure 18

$n = 2$

- Chain Rule - Analytical Coefficients
- Taylor Series - Numerical Coefficients
- Chain Rule - Numerical Coefficients

Error $\times 10^{-3}$

$\xi$

Figure 18
Three-Point Extrapolation

False Boundary

\( n = 2 \)

\( \Delta \) Three-Point Extrapolation

■ False Boundary

Figure 19
BIBLIOGRAPHY


