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NUMERICAL INTEGRATION OF FIRST-ORDER STIFF DIFFERENTIAL EQUATIONS

F. C. Loper and W. J. Phares

ARO, Inc.

February 1966

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FOREWORD

The work reported herein was sponsored by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), under Program Element 62405214, Project 6951, Task 695102.

The results of the research presented were obtained by ARO, Inc. (a subsidiary of Sverdrup and Parcel, Inc.), contract operator of the AEDC, AFSC, Arnold Air Force Station, Tennessee, under Contract AF40(600)-1200. The research was performed from January until June, 1965, under ARO Project No. RW2408, and the manuscript was submitted for publication on November 17, 1965.

The solution of the mathematical problem to which this report is addressed was stimulated by a requirement to solve a set of ordinary, first-order, nonlinear, stiff differential equations which describe chemical reaction rates applicable to hydrogen-air reactions. The authors wish to thank R. P. Rhodes, Jr., who proposed the problem which led to the development of this technique, and who worked jointly with the authors in solving the proposed problem.

This technical report has been reviewed and is approved.

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ABSTRACT

A method is presented for numerically integrating a system of stiff, first-order differential equations. This method is based on transforming the set of dependent variables so that the resulting system will not be stiff; the transformed system is then integrated by the Runge-Kutta method. The resulting procedure is often appreciably faster than classical methods in that a much larger step size is allowable with nominal increase in step computation time. Applications and results are discussed for systems of various order, including a system of six chemical rate equations.

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SECTION I
INTRODUCTION

Although systems of differential equations having the property of being stiff have been used as mathematical models of certain physical phenomena almost since the invention of the calculus, only in recent years have such systems been categorized according to this property and been formally recognized as a class of equations, the numerical solution of which often eludes the computer when sought by classical means. Since 1951, various works have been published on the subject (Refs. 1 through 5).

The primary reason that equations in this class present such difficulty is that an exceedingly small integration step size is sometimes required, making classical integration techniques impractical even on the most sophisticated computing machines.

The object of this presentation is to formulate a method that can be used efficiently on a high speed digital computer to obtain the solution of a system of first-order, ordinary, stiff differential equations. The method described is straightforward and practical when applied to stiff equations resulting from many physical problems.

The above objective may be realized by transforming the dependent variables in such a manner that the resulting system of equations will not be stiff in a neighborhood of the value of the independent variable at which the transformation was made. The Runge-Kutta method will be used to integrate the resulting system.

SECTION II
DEFINITIONS AND NOMENCLATURE

When presenting a similar technique, some authors develop their theory exclusively for a single equation with one dependent variable, and later state that the extension of their method to a system of such equations is "obvious". It is the contention of the authors of this presentation that any such extension is almost always ambiguous. It is also believed that with little or no sacrifice to clarity, the method can be developed in vector notation, leaving no doubt concerning how the method should be applied to the general case. Following these convictions, the nomenclature introduced below will be used throughout this document:

1. Roman characters will be used to denote real scalar quantities.
2. Greek characters will denote numbers which are, in general, complex scalars.
3. An $(\rightarrow)$ will indicate an $n \times 1$ column vector, and $\vec{\phi}$ denotes the null vector.
4. An $(\sim)$ will denote an $n \times n$ matrix; $\tilde{\phi}$ and $\tilde{I}$ denote the null matrix and identity matrix, respectively.
5. The notation Re (λ) will mean the real part of the complex number, λ.

Now consider the system of equations

$$\frac{dy_i}{dx} = F_i\,(x, y_1, y_2, \cdots, y_n)\,;\; y_i\,(x_0) = y_{i_0} \tag{1}$$

for $i = 1, \ldots, n$. More conveniently, Eq. (1) can be written

$$\frac{d\vec{y}}{dx} = \vec{F}\,(x, \vec{y})\,,\; \vec{y}\,(x_0) = \vec{y}_0 \tag{2}$$

where

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \quad \vec{F}\,(x, \vec{y}) = \begin{bmatrix} F_1\,(x, \vec{y}) \\ F_2\,(x, \vec{y}) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ F_n\,(x, \vec{y}) \end{bmatrix}$$

In order to get Eq. (2) in an applicable form, define the matrix

$$-\tilde{f}\,(x, \vec{y}) = \begin{bmatrix} \frac{\partial F_1}{\partial y_1}(x, \vec{y}) & \frac{\partial F_1}{\partial y_2}(x, \vec{y}) & \cdots & \frac{\partial F_1}{\partial y_n}(x, \vec{y}) \\ \frac{\partial F_2}{\partial y_1}(x, \vec{y}) & \frac{\partial F_2}{\partial y_2}(x, \vec{y}) & \cdots & \frac{\partial F_2}{\partial y_n}(x, \vec{y}) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \frac{\partial F_n}{\partial y_1}(x, \vec{y}) & \frac{\partial F_n}{\partial y_2}(x, \vec{y}) & \cdots & \frac{\partial F_n}{\partial y_n}(x, \vec{y}) \end{bmatrix} \tag{3}$$

It will be assumed throughout that $\tilde{f}(x, \vec{y})$ is nonsingular, this method being inapplicable at any point on the solution of Eq. (2) for which this is not true. Equation (2) can now be written

$$\frac{d\vec{y}}{dx} + \tilde{f}(x, \vec{y})\vec{y} = \vec{g}(x, \vec{y}) \quad , \quad \vec{y}(x_0) = \vec{y}_0 \tag{4}$$

where

$$\vec{g}(x, \vec{y}) = \vec{F}(x, \vec{y}) + \tilde{f}(x, \vec{y})\vec{y} \tag{5}$$

The form of Eq. (4) is now such that the definition of a stiff differential equation can be given. Definition: Let $x = x_1$ be a value of the independent variable in the region of interest, and let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of $\tilde{f}(x_1, \vec{y}(x_1))$. If

$$\mathrm{Re}(\lambda_i) >> 0$$

for any i, then Eq. (4) is said to be stiff at $x = x_1$.

SECTION III
DERIVATION OF THE TRANSFORMATION

It was mentioned previously that the dependent variable in Eq. (4), $\vec{y}(x_0)$, will be transformed so that if $|x - x_0| \leq h$, then the transformed equation will not be stiff. For the remainder of this paper, h is understood to be the integration step size for the Runge-Kutta method (fourth-order) on the transformed equations. The maximum allowable value of h will, of course, depend on the exact nature of the original differential equation; the transformation has allowed the value of h to be significantly increased in all test cases tried so far.

It is pointed out again that the validity of the method depends on the nonsingularity of $\tilde{f}(x, \vec{y})$.

It is convenient to define at this time the matrix

$$\tilde{u}(x) = \tilde{I} - \tilde{f}_0(x - x_0) + \frac{\tilde{f}_0^2(x - x_0)^2}{2!} - \frac{\tilde{f}_0^3(x - x_0)^3}{3!} + \cdots \tag{6}$$

which is sometimes referred to as

$$\tilde{u}(x) = \exp(-f_0(x - x_0))$$

for obvious reasons.

The following properties of the infinite matrix series, Eq. (6), can be readily verified independent of $\tilde{f}_0$ and $(x - x_0)$;

1. The series converges
2. $\tilde{u}(x)$ is nonsingular
3. $\tilde{u}(x)\,\tilde{f}_0 = \tilde{f}_0\,\tilde{u}(x)$

Note also that

$$\frac{d\,\tilde{u}(x)}{dx} + \tilde{f}_0\,\tilde{u}(x) = \tilde{\phi} \quad , \quad \tilde{u}(x_0) = \tilde{I} \tag{7}$$

Now, let $\vec{z}(x)$ be a solution of

$$\frac{d\vec{z}}{dx} + \tilde{f}_0\,\vec{z} = \vec{g}_0 \quad , \quad \vec{z}_0 = \vec{y}_0 \tag{8}$$

Hence

$$z = \tilde{u}(x)\,(\vec{y}_0 - \tilde{f}_0^{-1}\,\vec{g}_0) + \tilde{f}_0^{-1}\,\vec{g}_0 \tag{9}$$

Defining

$\vec{w}(x) = \vec{y}(x) - \vec{z}(x)$ one gets, by subtracting Eq. (8) from Eq. (4)

$$\frac{d\,\vec{w}(x)}{dx} + \tilde{f}\,(x, \vec{y})\,\vec{w}(x) = \vec{v}(x, \vec{y})\ ;\ \vec{w}_0 = \vec{\phi} \tag{10}$$

where

$$\vec{v}(x, \vec{y}) = \vec{g}(x, \vec{y}) - \vec{g}_0 + \left[\tilde{f}_0 - \tilde{f}(x, \vec{y})\right]\vec{z}(x) \tag{11}$$

Premultiplying Eq. (10) by $\tilde{u}(x)$ and postmultiplying Eq. (7) by $\vec{w}(x)$ gives

$$\tilde{u}(x)\,\frac{d\vec{w}}{dx} + \tilde{u}\,\tilde{f}(x, \vec{y})\,\vec{w} = \tilde{u}\,\vec{v}$$

and

$$\frac{d\tilde{u}}{dx}\,\vec{w} + \tilde{f}_0\,\tilde{u}(x)\,\vec{w} = \vec{\phi}$$

Subtracting,

$$\tilde{u}\,\frac{d\vec{w}}{dx} - \frac{d\tilde{u}}{dx}\,\vec{w} + \tilde{u}\,\tilde{f}(x, \vec{y})\,\vec{w} - \tilde{f}_0\,\tilde{u}(x)\,\vec{w} = \tilde{u}\,\vec{v}$$

$$(\tilde{u}^{-1})^2\left(\tilde{u}\,\frac{d\vec{w}}{dx} - \frac{d\tilde{u}}{dx}\,\vec{w}\right) + (\tilde{u}^{-1})^2\left[\tilde{u}\,\tilde{f}(x, \vec{y})\,\vec{w} - \tilde{f}_0\,\tilde{u}(x)\,\vec{w}\right] = (\tilde{u}^{-1})^2\,\tilde{u}\,\vec{v}$$

$$\frac{d}{dx}\,(\tilde{u}^{-1}\,\vec{w}) + \tilde{u}^{-1}\left[\tilde{f}(x, \vec{y}) - \tilde{u}^{-1}\,\tilde{f}_0\,\tilde{u}\right]\vec{w} = \tilde{u}^{-1}\,\vec{v} \tag{12}$$

Defining

$$\vec{t} = \tilde{u}^{-1}\,\vec{w}$$

$$\tilde{m} = \tilde{u}^{-1}\left[\tilde{f}\,(x,\vec{y}) - \tilde{f}_c\right]\tilde{u}$$

Eq. (12) becomes

$$\frac{d\vec{t}}{dx} + \tilde{m}\,\vec{t} = \tilde{u}^{-1}\,\vec{v}\,; \qquad \vec{t}\,(x_0) = \vec{\phi} \tag{13}$$

Equation (13) is the desired transformed equation, the relation between $\vec{t}$ and $\vec{y}$ being

$$\vec{y} = \tilde{u}\,(x)\,\vec{t}\,(x) + \tilde{f}_0^{-1}\left[\tilde{I} - \tilde{u}\,(x)\right]\vec{F}_0 + \vec{y}_0 \tag{14}$$

Setting

$$\vec{G}\,(x,\vec{t}) = \tilde{u}^{-1}\,\vec{v} - \tilde{m}\,\vec{t} = \tilde{u}^{-1}\left[\vec{F}\,(x,\vec{y}) - \vec{F}_0 + \tilde{f}_0\,(\vec{y} - \vec{y}_0)\right] \tag{15}$$

Eq. (13) can be written as

$$\frac{d\vec{t}}{dx} = \vec{G}\,(x,\vec{t})\,; \qquad \vec{t}\,(x_0) = \vec{\phi} \tag{16}$$

An interesting consequence of the transformation is observed if Eq. (2) is linear with constant coefficients. In that case

$$\tilde{f}\,(x,\vec{y}) \equiv \tilde{f}_0$$

$$\vec{g}\,(x,\vec{y}) \equiv \tilde{g}_0$$

$$\frac{d\vec{t}}{dx} \equiv \vec{\phi}$$

$$\vec{t}\,(x) \equiv \vec{\phi}$$

$$\vec{y}\,(x) = \tilde{f}_0^{-1}\,(\tilde{I} - \tilde{u})\,\vec{F}_0 + y_0 \tag{17}$$

Notice that Eq. (17) gives the exact solution of the linear equation with constant coefficients.

The fundamental question to be explored at this point, the transformation having been obtained, is whether, and to what extent, Eq. (16) is stiff. Basic to this question is the matrix

$$\left(\frac{\partial G_i}{\partial t_j}\right)$$

which is associated with Eq. (16) in the same manner that $\tilde{f}$ is associated with Eq. (2). On the assumption that all the necessary partial derivatives exist, it can be shown after some manipulation that

$$\left(\frac{\partial G_i}{\partial t_j}\right) = -\tilde{m}$$

As

$$\tilde{m} = \tilde{u}^{-1}\left[\tilde{f}(x,\vec{y}) - \tilde{f}_0\right]\tilde{u}$$

it follows that the eigenvalues of m are the same as the eigenvalues of

$$\tilde{f}(x,\vec{y}) - \tilde{f}_0$$

Thus, the spectral radius of $\tilde{m}$ can be made as small as desired simply by choosing an x sufficiently close to x_0. It is assumed here, of course, that $\tilde{f}(x,\vec{y})$ is continuous at $x = x_0$. According to the definition of a stiff equation given earlier, it follows that Eq. (16) is not a stiff equation at $x = x_0 + h$ provided the value of h is not too large. Any failure in the Runge-Kutta integration of Eq. (16) will, therefore, be the result of some other undesirable phenomenon.

SECTION IV
APPLICATION TECHNIQUES

One method of applying the transformation to obtain the solution of Eq. (2) would be to solve the transformed Eq. (16) for $\vec{t}(x)$ by the Runge-Kutta method, compute the corresponding $\vec{y}(x)$, update the transformation, and continue in the same fashion on a new interval. While $\vec{t}(x)$ is piecewise discontinuous, this of course has no bearing on the solution of interest, $\vec{y}(x)$.

Having served its purpose, the transformation can now, in a computational sense, be entirely removed from the procedure. Thus, the technique can be thought of in a completely different way, that of solving the untransformed Eq. (2) by a method different from that of Runge-Kutta.

While the above two interpretations of the method would theoretically yield identical answers, the second version seems to be advantageous to the first in practice. This was experienced in actual test runs in which the two interpretations were compared on the basis of run time, accuracy, and simplicity of program logic.

As a result of Eqs. (14) and (16), and the classical fourth-order Runge-Kutta equations (Ref. 6, p. 122), the equations necessary for integrating Eq. (2) with the transformation removed are

for j = 0

$$x = x_0$$
$$\vec{y} = \vec{y}_0 \tag{18a}$$
$$\vec{k}_0 = \vec{\phi}$$

for j = 1

$$x = x_0 + \frac{h}{2}$$
$$\vec{y} = \tilde{f}_0^{-1}\left[\tilde{I} - \tilde{u}(x)\right]\vec{F}_0 + \vec{y}_0 \tag{18b}$$
$$\vec{k}_1 = \tilde{u}^{-1}(x)\left[\vec{F}(x,\vec{y}) - \vec{F}_0 + \tilde{f}_0(\vec{y} - \vec{y}_0)\right]$$

for j = 2

$$x = x_0 + \frac{h}{2}$$
$$\vec{y} = \frac{h}{2}\tilde{u}(x)\vec{k}_1 + \tilde{f}_0^{-1}\left[\tilde{I} - \tilde{u}(x)\right]\vec{F}_0 + \vec{y}_0 \tag{18c}$$
$$\vec{k}_2 = \tilde{u}^{-1}(x)\left[\vec{F}(x,\vec{y}) - \vec{F}_0 + \tilde{f}_0(\vec{y} - \vec{y}_0)\right]$$

for j = 3

$$x = x_0 + h$$
$$\vec{y} = h\,\tilde{u}(x)\vec{k}_2 + \tilde{f}_0^{-1}\left[\tilde{I} - \tilde{u}(x)\right]\vec{F}_0 + \vec{y}_0 \tag{18d}$$
$$\vec{k}_3 = \tilde{u}^{-1}(x)\left[\vec{F}(x,\vec{y}) - \vec{F}_0 + \tilde{f}_0(\vec{y} - \vec{y}_0)\right]$$

at

$$x = x_0 + h$$
$$\vec{y} = \frac{h}{6}\tilde{u}(x)(2\vec{k}_1 + 2\vec{k}_2 + \vec{k}_3) + \tilde{f}_0^{-1}\left[\tilde{I} - \tilde{u}(x)\right]\vec{F}_0 + \vec{y}_0$$

Notice that although the algebra is somewhat more involved, there is a close similarity between\Eq. (18) and the corresponding Runge-Kutta equations.

The problem that initially motivated the development of this technique is a system of six chemical rate equations (Ref. 7). However, the matrix $\tilde{f}(x,y)$ associated with this problem was found to be ill-conditioned; hence, a modified version of the method was developed.

Equation (18) in scalar form was applied to each of the six equations individually. In other words, the six equations were, for purposes of making the transformation only, assumed to be uncoupled.

In order to determine whether or not to make the transformation on the i th equation, $\frac{dy_i}{dx} = f_i(x, \vec{y})$, the number $-\frac{\partial f_i}{\partial y_i} \geq 0$ was examined to see if the equation was suitable for integration by the Runge-Kutta Method.

If

$$-\frac{\partial f_i}{\partial y_i} \Delta x \geq 0.5$$

then the i th equation was transformed. If the above inequality did not hold, the i th equation was considered suitable for integration without making the transformation (Ref. 8, p. 198, or Ref. 1). Thus the six equations were solved as a coupled system, but the integration method used on the individual equations was dictated by the above criterion. Also, the test was made at every integration step so that at one value of x, for example, Eqs. (1), (2), (5), and (6) were transformed while Eqs. (2) and (4) were integrated by the Runge-Kutta method. At another value of x, an entirely different combination might very well have prevailed.

SECTION V
DISCUSSION OF RESULTS

Several stiff systems for which the analytic solution is known were solved both by the Runge-Kutta method and by the method under consideration here. One such equation is

$$y' + ay = x^2 \; ; \qquad y(0) = 0$$

A comparison of the errors, the absolute value of the difference between the exact answer and the approximation, is shown in Fig. 1 for $a = 100$ and $a = 1000$.

Figure 2 shows a similar graph for the Euclidian norm of the error vector associated with the system.

$$-y_1' + a_{11} y_1 + a_{12} y_2 = b_1 x \; ; \qquad y_1(0) = y_1^0$$

$$-y_2' + a_{21} y_1 + a_{22} y_2 = b_2 x^2 \; ; \qquad y_2(0) = y_2^0$$

No analytic solution was available for analyzing the success of the method as applied to the chemical rate equations. Essentially, the same solution was found using both the Runge-Kutta method proper and the transformed method, a considerably larger Δx being admissible in the latter case. These answers were also compared with solutions from another source (Ref. 7) as further confirmation of their validity.

SECTION VI
CONCLUSIONS

The method discussed herein for integrating a system of stiff, first-order differential equations has been found to be practical and expedient in all cases on which the method has been tested. Answers comparable to those indicated by the Runge-Kutta method were obtained with a considerably larger integration step size.

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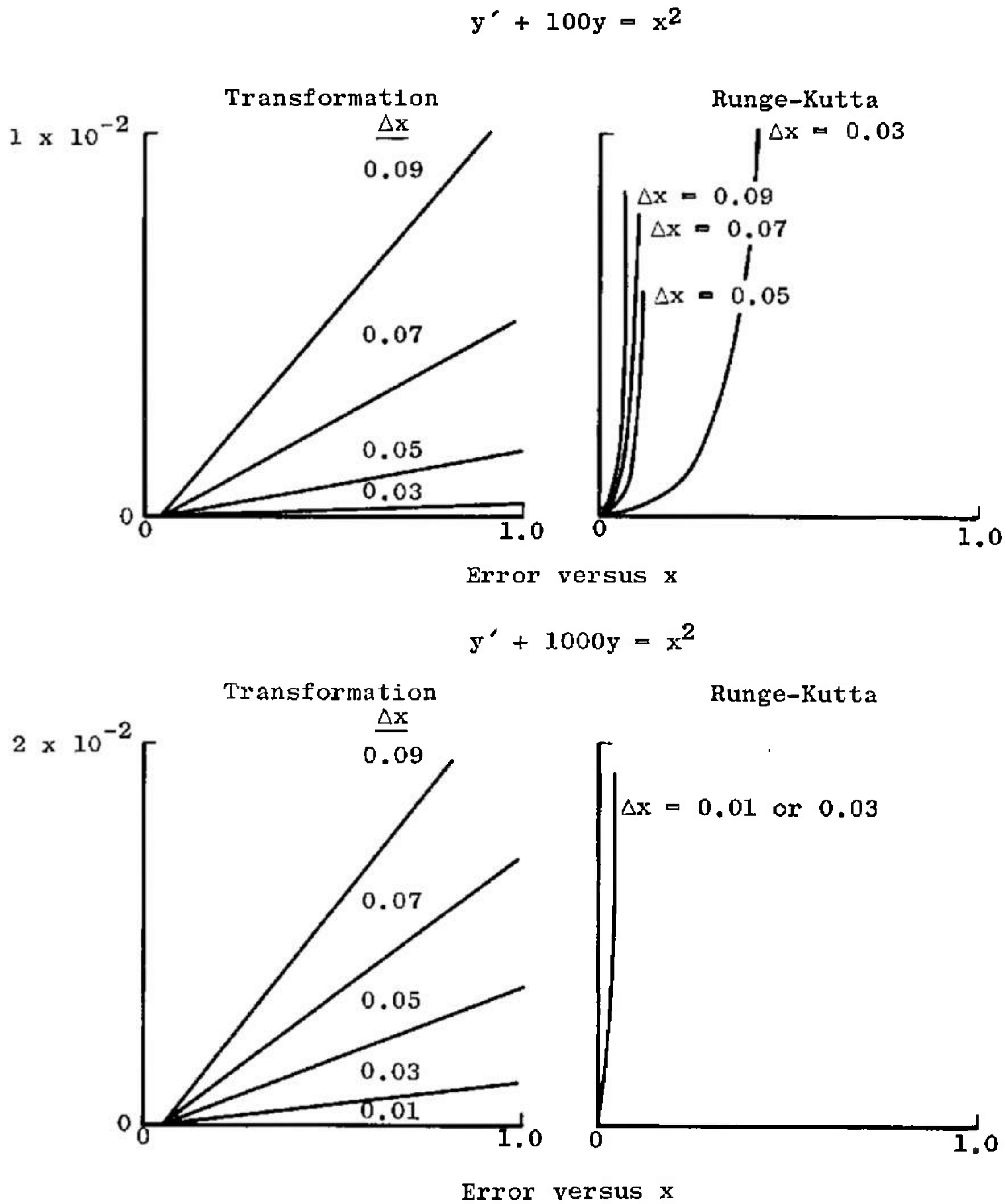

Fig. 1 Errors for a Single Equation

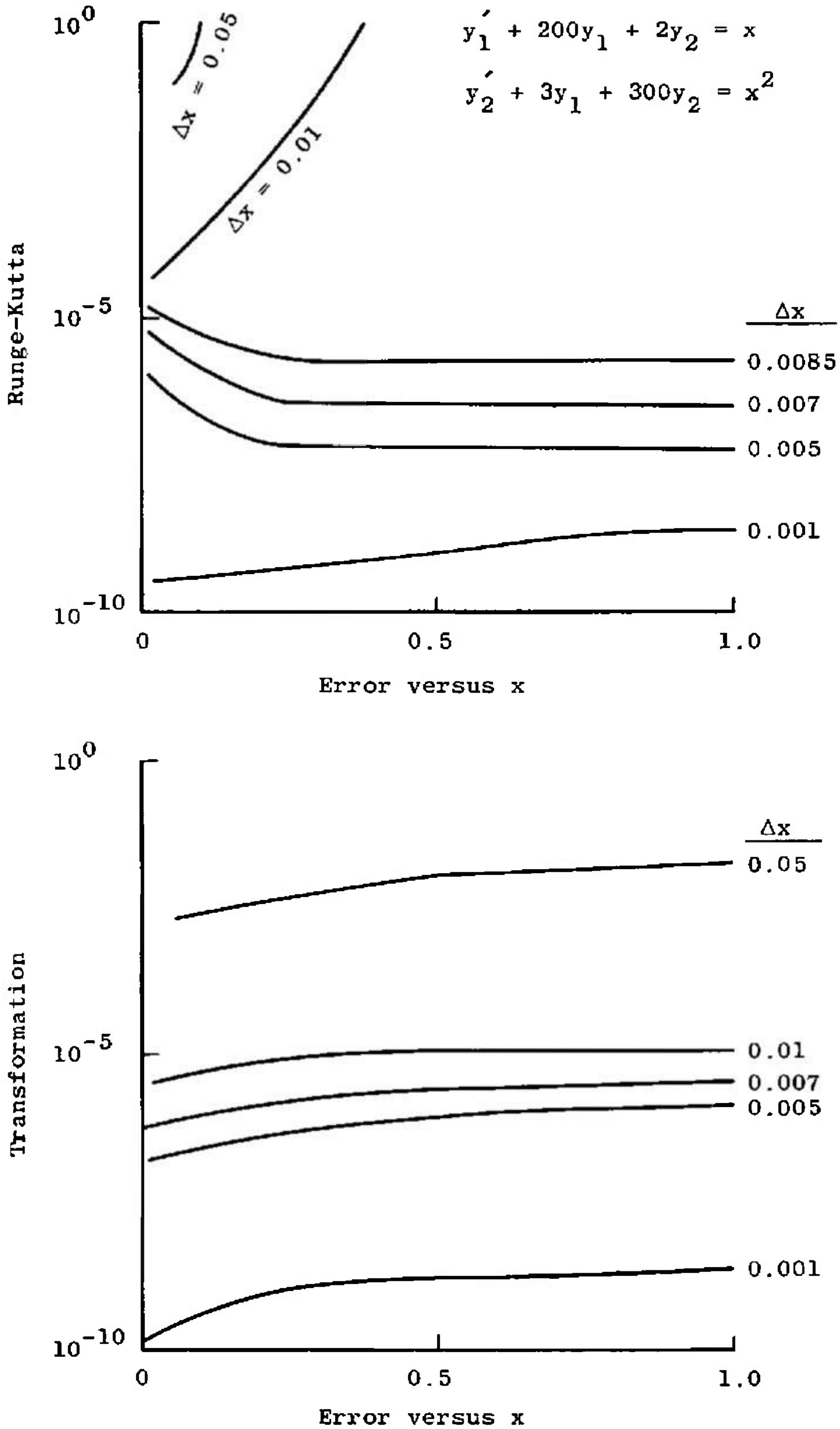

Fig. 2 Errors for a System of Two Equations

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13 ABSTRACT

A method is presented for numerically integrating a system of stiff, first-order differential equations. This method is based on transforming the set of dependent variables so that the resulting system will not be stiff; the transformed system is then integrated by the Runge-Kutta method. The resulting procedure is often appreciably faster than classical methods in that a much larger step size is allowable with nominal increase in step computation time. Applications and results are discussed for systems of various order, including a system of six chemical rate equations. (U)

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