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*INTEGRATION OF STIFF EQUATIONS**

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In the study of chemical kinetics, electrical circuit theory, and problems of missile guidance a type of differential equation arises which is exceedingly difficult to solve by ordinary numerical procedures. A very satisfactory method of solution of these equations is obtained by making use of a forward interpolation process. This scheme has the unusual property of singling out and approximating a particular solution of the differential equation to the exclusion of the manifold of other solutions. This behavior may be explained by a simple geometrical interpretation of the significance of the forward interpolation process. The differential equations to which this method applies are called "stiff."

A typical example of a stiff equation is the equation representing the rate of formation of free radicals in a complex chemical reaction. The free radicals are created and destroyed so rapidly compared to the time scale for the over-all reaction that to a first approximation the rate of production is equal to the rate of depletion. This is the notion of the pseudo-stationary state. In some cases such as the fast reactions occurring in flames or detonations, this approximation is not sufficiently accurate. The method described in the present paper provides a means for obtaining solutions to equations of this type to any degree of accuracy.

The numerical procedure described here can easily be extended to sets of simultaneous first-order differential equations. In any particular region, the differential equations can be uncoupled by introducing suitable linear combinations of the original dependent variables. Some of the uncoupled equations may be "stiff" in which case they can be integrated by the methods discussed here; whereas other uncoupled equations may be integrated by the more usual procedures.

1. Concept of Stiff Equations.—Consider the first-order differential equation,

$$\frac{dy}{dx} = [y - G(x)]/a(x, y). \qquad (1)$$

The right-hand side of this equation represents a general function of x and y which for each value of x has a root, $y = G(x)$. If Δx is the desired resolution of x or the interval which will be used in the numerical integration, the equation is "stiff" if

$$\left|\frac{a(x, y)}{\Delta x}\right| \ll 1 \qquad (2)$$

and $G(x)$ is well behaved [i.e., varies with x considerably more slowly

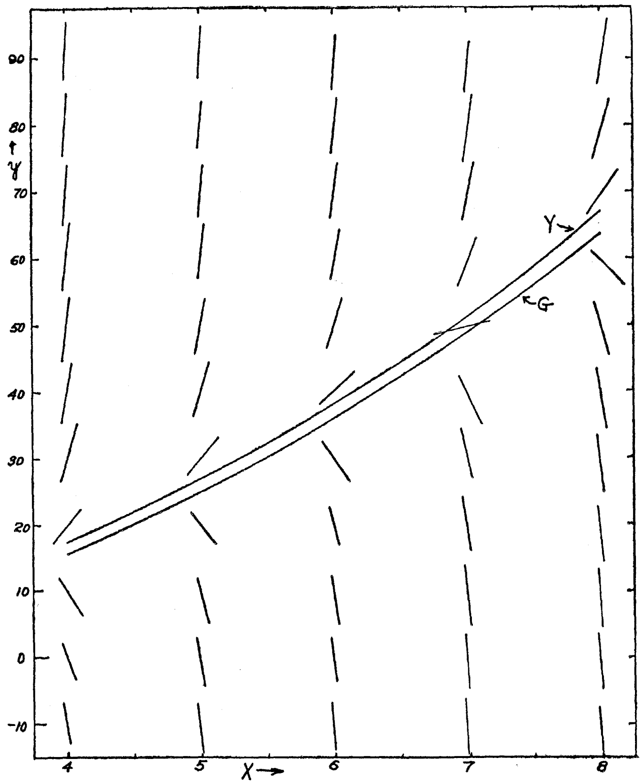

FIGURE 1

Slopes, dy/dx, for a Typical Stiff Equation, $dy/dx = 5(y - x^2)$.

than does exp $(x/a(x, G(x)))$]. The geometrical significance of the stiffness is shown in figure 1. Here the family of solutions horn out as one proceeds in the positive x direction. This can be chosen as the positive x direction without loss of generality. The slope, dy/dx, is drawn at regular intervals of x and y. For a particular value of x:· for large values of y the slope is very large and positive; for small values of y the slope is very large in the negative sense; in the vicinity of $y = G(x)$ the slope changes rapidly from large positive to large negative.

Looking at equation (1), it appears that if $a(x, y)$ is sufficiently small there is a special solution, $y = Y(x)$, which lies close to $y = G(x)$. To a first approximation, Y is given by $Y^{(1)}$,

$$Y^{(1)} = G + a(x, G)\frac{dG}{dx}. \tag{3}$$

The second approximation, $Y^{(2)}$, is obtained by substituting $Y^{(1)}$ for y in dy/dx and in $a(x, y)$,

$$Y^{(2)} = G + a(x, Y^{(1)})\frac{dY^{(1)}}{dx}. \tag{4}$$

In this manner, an arbitrary order of approximation of Y may be obtained in terms of the lower orders of approximation. If $a(x, y)$ does not depend upon y, we can write down the resulting expression for Y,

$$Y = \sum_{k=0}^{\infty} \frac{D^k G}{Dx^k} \tag{5}$$

where D/Dx is the differential operator, $a(x)d/dx$. Whereas the function $Y(x)$ remains close to $G(x)$, every other solution deviates exponentially. This can be seen by subtracting the differential equation for Y from equation (1). In the region about $Y(x)$ (assuming that $a(x, y)$ varies slowly with y),

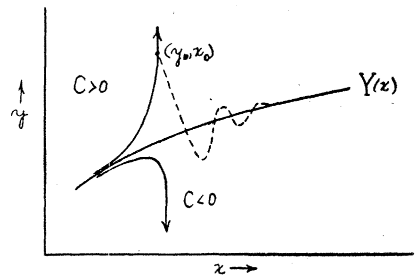

FIGURE 2

$$a(x, Y(x))\frac{d(y - Y)}{dx} = (y - Y). \tag{6}$$

This integrates to give

$$y - Y = C \exp\left[\int \frac{dx}{a(x, Y(x))}\right] \tag{7}$$

where C is a constant of integration. The qualitative appearance of this family of solutions is shown in figure 2.

2. *Numerical Solution of Stiff Equations Using Forward Interpolation.*—It is very difficult to integrate "stiff" equations by ordinary numerical methods. Small errors are rapidly magnified if the equations are inte-

grated in the direction such that the family of solutions horn out, whereas the numerical solutions oscillate violently about $Y(x)$ if the integration is carried out in the opposite direction.

We have discovered a method of numerically integrating "stiff" equations which has the desirable property that regardless of the starting conditions and regardless of the direction of integration, a solution is generated which rapidly converges to $Y(x)$. Thus for example, in figure 2, if we use this system of integration starting at the point (x_0, y_0) we obtain

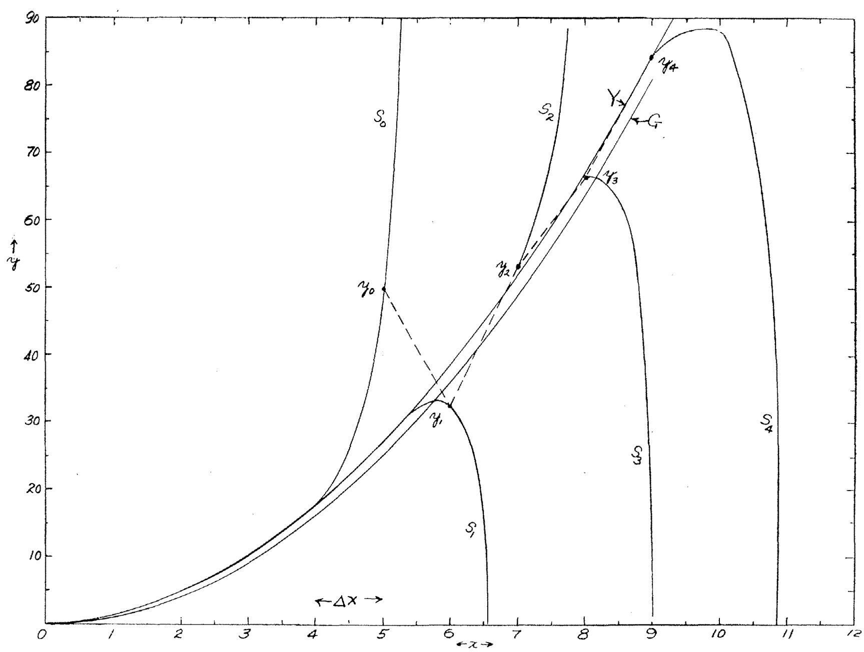

FIGURE 3

Integration of $dy/dx = 5(y - x^2)$ in the positive x direction from $(x = 5, y = 50)$. Here $a/\Delta x = 1/5$, $G(x) = x^2$, $Y(x) = 0.08 + 0.4x + x^2$.

the function indicated by the dotted line rather than the solution to the original differential equation which passes through this point and rapidly approaches infinity.

Let $x_0, x_1, \ldots, x_n, \ldots$ be a set of values of x spaced a distance Δx between successive points. Then the subscript on any quantity indicates that it is evaluated at the corresponding value of x. We wish to evaluate y_n from a knowledge of y at the previous points. Suppose, for example, that $y(x)$ can be approximated locally by a straight line passing through y_n and y_{n-1}. Then this straight line has the slope;

$$\left(\frac{dy}{dx}\right)_n = \frac{y_n - y_{n-1}}{\Delta x}. \tag{8}$$

Now, using this expression for the slope in evaluating the terms of the differential equation, equation (1), at the forward point one obtains:

$$\left(\frac{dy}{dx}\right)_n = \frac{y_n - y_{n-1}}{\Delta x} = \frac{y_n - G_n}{a(y_n, x_n)}. \tag{9}$$

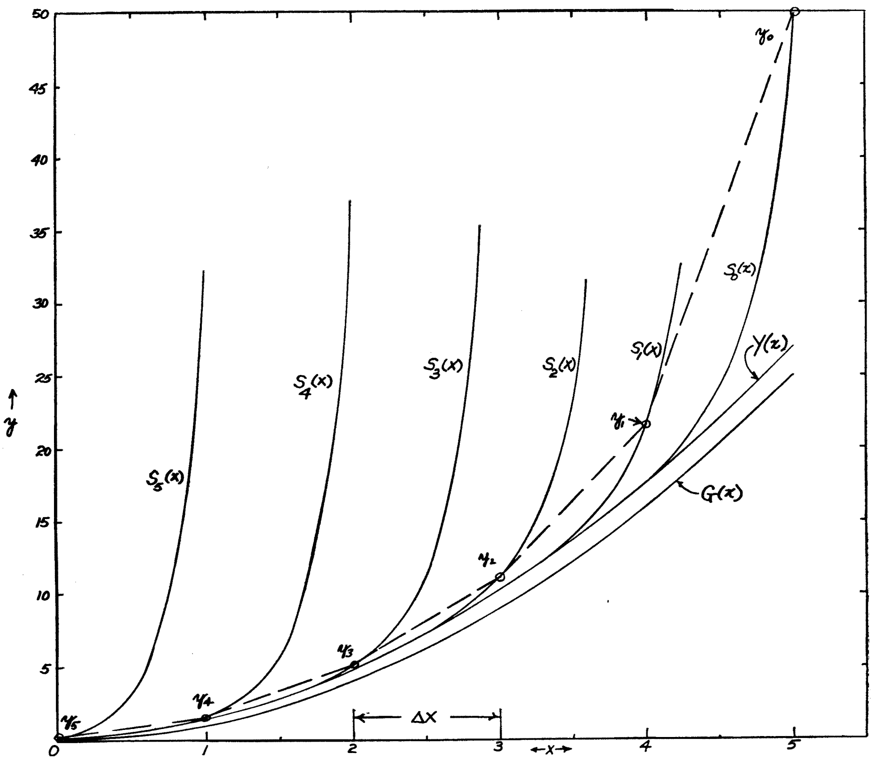

FIGURE 4

Integration of $dy/dx = 5(y - x^2)$ in the negative direction from $(x = 5, y = 50)$. Here $a/\Delta x = -1/5$, $G(x) = x^2$, $Y(x) = 0.08 + 0.4x + x^2$.

Thus,

$$y_n = \frac{G_n - \dfrac{a(x_n, y_n)}{\Delta x} y_{n-1}}{1 - \dfrac{a(x_n, y_n)}{\Delta x}}. \tag{10}$$

If $a(x, y)$ does not depend upon the value of y, equation (10) gives an explicit solution for y_n in terms of y_{n-1}; otherwise, equation (10) gives an implicit relationship between y_n and y_{n-1}. Thus starting from a point (x_0, y_0), equation (10) provides a numerical solution to the differential equation, equation (1). The curious fact is that quite regardless of the starting point, thus numerical solution seeks and approximates $Y(x)$ in the manner shown by the dotted curve in figure 2. The reason for this behavior may be seen geometrically from figure 3. Here y_0 lies on the curve $y = S_0(x)$ where $S_0(x)$ is a solution to the original differential equation. Equating $(dy/dx)_1$ from equations (8) and (9) is equivalent to asking what solution to equation (1), $y = S_1(x)$, has a tangent at the point x_1 which passes through the point (x_0, y_0). Similarly in passing from x_1 to x_2, etc. Since the slope for a stiff equation has a reasonable value (neither tremendously large in the positive or negative sense) only in the vicinity of $G(x)$ or $Y(x)$, it is clear that this numerical integration scheme limits us to approximating $Y(x)$.

It is interesting to notice that this method of integration may be used in either direction. An integration in the negative direction so that Δx is negative (i.e., in the direction of convergence of the manifold of solutions) is illustrated in figure 4. In this case the solution approaches the asymptote without oscillations. The integration in the two directions is not reversible since the definition of the forward point depends upon the direction of integration. This fact may be used numerically to hunt the special solution by first integrating in one direction and then reversing the direction.

3. *The Asymptotic Form.*—If $a(x, y)$ is a function only of x, it is easy to see how the numerical procedure leads to an approximation of Y. Since

$$G_n = Y_n - a(x_n)(dY/dx)_n, \tag{11}$$

equation (10) can be rewritten in the form

$$y_n - Y_n = -\left(\frac{\dfrac{a(x_n)}{\Delta x}}{1 - \dfrac{a(x_n)}{\Delta x}}\right)[y_{n-1} - Y_{n-1} + \epsilon] \tag{12}$$

where

$$\epsilon = -Y_n + Y_{n-1} + \Delta x \left(\frac{dY}{dx}\right)_n. \tag{13}$$

Expanding Y and (dY/dx) in Taylor series about the point, x_{n-1}, it follows that

$$\epsilon = \frac{1}{2}(\Delta x)^2\left(\frac{d^2Y}{dx^2}\right)_{n-1} + \frac{1}{3}(\Delta x)^3\left(\frac{d^3Y}{dx^3}\right)_{x_{n-1}} + \ldots. \tag{14}$$

Looking at equation (12) it appears that there are two reasons why y_n differs from Y_n. The rate of convergence of y toward Y is measured by the factor

$$b = \frac{\dfrac{a(x_n)}{\Delta x}}{1 - \dfrac{a(x_n)}{\Delta x}}. \tag{15}$$

The larger the interval size Δx, the smaller the value of b and the more rapidly y_n converges toward Y_n. The series converges for values of b less than unity and approaches an asymptote given approximately by

$$y = Y + a(x)\left[\frac{1}{2}(\Delta x)\frac{d^2Y}{dx^2} + \frac{1}{3}(\Delta x)^2\frac{d^2Y}{dx^3} + \ldots\right]. \tag{16}$$

This discrepancy between y and Y is due to the poorness of the fit of Y by successive linear segments. The smaller the intervals, Δx, the smaller this error.

The error in the asymptote of the series may be reduced by using a three-point formula for $(dy/dx)_n$ in which y is fit to a quadratic passing through y_n, y_{n-1} and y_{n-2}. Since the slope is evaluated at x_n, the same sort of forward interpolation is used as in the linear approximation. In place of equation (10), one obtains the following relation:

$$y_n = \frac{G_n - 2\dfrac{a(x_n, y_n)}{\Delta x}y_{n-1} + \dfrac{1}{2}\dfrac{a(x_n, y_n)}{\Delta x}y_{n-2}}{1 - \dfrac{3}{2}\dfrac{a(x_n, y_n)}{\Delta x}}. \tag{17}$$

In this case the difference between y_n and Y_n is given by[1]

$$y_n - Y_n = \left(\frac{\dfrac{a(x_n)}{\Delta x}}{1 - \dfrac{3}{2}\dfrac{a(x_n)}{\Delta x}}\right) \times \left[\begin{array}{l} -2(y_{n-1} - Y_{n-1}) + \dfrac{1}{2}(y_{n-2} - Y_{n-2}) \\ -\dfrac{1}{3}(\Delta x)^3\left(\dfrac{d^3Y}{dx^3}\right)_{n-1} - \dfrac{1}{12}(\Delta x)^4\left(\dfrac{d^4Y}{dx^4}\right)_{n-2} + \ldots \end{array}\right] \tag{18}$$

Hence the asymptotic form is approximately

$$y = Y + a(x)\left[\frac{2}{9}(\Delta x)^2\frac{d^3Y}{dx^3} + \frac{1}{18}(\Delta x)^3\frac{d^4Y}{dx^4} + \ldots\right]. \tag{19}$$

A geometrical argument of why y_n approximates Y_n follows the same line as for the linear case.

The use of a cubic to fit y leads to the expression

$$y_n = \frac{G_n + \dfrac{a(x_n, y_n)}{\Delta x}\left(-3y_{n-1} + \dfrac{3}{2}y_{n-2} - \dfrac{1}{3}y_{n-3}\right)}{1 - \dfrac{11}{6}\dfrac{a(x_n, y_n)}{\Delta x}} \tag{20}$$

with a discrepancy between y_n and Y_n given by[2]

$$y_n - Y_n = \left(\frac{\dfrac{a(x_n)}{\Delta x}}{1 - \dfrac{11}{6}\dfrac{a(x_n)}{\Delta x}}\right)\times$$

$$\left[\begin{array}{l} -3(y_{n-1} - Y_{n-1}) + \dfrac{3}{2}(y_{n-2} - Y_{n-2}) - \dfrac{1}{3}(y_{n-3} - Y_{n-3}) \\ - \dfrac{1}{4}(\Delta x)^4\left(\dfrac{d^4Y}{dx^4}\right)_{n-1} + \dfrac{1}{20}(\Delta x)^5\left(\dfrac{d^5Y}{dx^5}\right)_{n-1} + \ldots \end{array}\right]. \tag{21}$$

The use of a quartic leads to

$$y_n = \frac{G_n + \dfrac{a(x_n, y_n)}{\Delta x}\left(-4y_{n-1} + 3y_{n-2} - \dfrac{4}{3}y_{n-3} + \dfrac{1}{4}y_{n-4}\right)}{1 - \dfrac{25}{12}\dfrac{a(x_n, y_n)}{\Delta x}} \tag{22}$$

with the discrepancy between y_n and Y_n given by

$$y_n - Y_n = \left(\frac{\dfrac{a(x_n)}{\Delta x}}{1 - \dfrac{25}{12}\dfrac{a(x_n)}{\Delta x}}\right)\left[\begin{array}{l} -4(y_{n-1} - Y_{n-1}) + 3(y_{n-2} - Y_{n-2}) \\ - \dfrac{4}{3}(y_{n-2} - Y_{n-2}) + \dfrac{1}{4}(y_{n-4} - Y_{n-4}) \\ - \dfrac{1}{5}(\Delta x)^5\left(\dfrac{d^5Y}{dx^5}\right)_{n-1} + \ldots \end{array}\right]. \tag{23}$$

Thus by taking higher order polynomials to fit y at a large number of points, it is possible to obtain progressively more excellent fits of Y. In all cases, the use of forward interpolation in the evaluation of $(dy/dx)_n$ in terms of y_n, y_{n-1}, ... is the mathematical operation which forces y_n to seek out and approximate Y_n.

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[1] Assuming the value of $a(x, y)$ to be independent of y.

THE ELEMENTARY BASIC PRINCIPLES OF THE UNIFIED THEORY OF RELATIVITY*

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1. *Introduction.*—The unified theory of relativity exposed recently by Einstein[1] is based on three principles: (A) The introduction of a non-symmetric tensor $g_{\lambda\mu}$ in the space X_4 of the relativity; (B) the introduction of a non-symmetric connection $\Gamma_{\lambda\mu}^{\nu}$ by means of

$$\frac{\partial}{\partial x^{\lambda}} g_{\omega\mu} = \Gamma_{\omega\lambda}^{\nu} g_{\nu\mu} + \Gamma_{\lambda\mu}^{\nu} g_{\omega\nu} \tag{1}$$

and finally (C) the introduction of a (seemingly) overdetermined system of conditions imposed on the $\Gamma_{\lambda\mu}^{\nu}$, which yields $g_{\lambda\mu}$.

In the subsequent sections we will deal with each of these basic principles. However, we confine ourselves to results only. The corresponding detailed proofs will be given in a subsequent series of three papers in the *Journal of Rational Mechanics and Analysis.*

2. *Principle A.*—Denote by $h_{\lambda\mu}(k_{\lambda\mu})$ the symmetric (the skew symmetric) part of $g_{\lambda\mu}$ and by g, h, k the corresponding determinants. Throughout this paper we assume $h \neq 0$. If $n = 4$ and if $h_{\lambda\mu}$ is of the signature $+++-$ then there are in general two sets of bivectors B_1, B_2 totally perpendicular, which are privileged in the sense that they are polar conjugate with respect to the cone $h_{\lambda\mu}$ as well as with respect to the linear complex $k_{\lambda\mu}$ of bivectors. Closely connected with them are four sets of (imaginary) bivectors each of them being polar self conjugate with respect to $h_{\lambda\mu}$ and $k_{\lambda\mu}$.

Projecting this configuration from an arbitrary point P of our space X_4 into the ideal space H_3 of the tangent space $T_4(P)$ of X_4 at P, one obtains a linear line complex K containing a linear line congruence C (whose axes