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# ON THE NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS OF THE FIRST ORDER*

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**Summary.** The difference methods for the numerical integration of ordinary differential equations of the first order are discussed by using operator calculus and symbolic expansions. A new straightforward central difference method is developed, which is based on a formula closely associated with Simpson's rule. The main features of the method are that, for each step of integration, the largest unknown term is determined by an algebraic equation and that the remaining difference correction is extremely small. The method can directly be applied even to systems of the first order with one-point boundary conditions. A numerical example is given.

**1. Introduction.** Different methods have been given in the literature for the numerical integration of the ordinary differential equation of the first order

$$\frac{dy}{dx} = F(x, y) \tag{1}$$

with the initial condition $y = y_0$ for $x = x_0$ . The purpose of this paper is to discuss only the methods based on the theory of finite differences, since they seem to combine simplicity with a large general applicability. The fundamental formulas are here of two types: central difference (CD) formulas and backward difference (BD) formulas. The central difference formulas, due to Gauss, are characterized by an extremely rapid convergence or semi-convergence and a small error-term, but in using them each step of the integration demands estimation and iteration. The use of estimations is avoided altogether in the integrations by means of the backward difference formulas, of which the first is due to Adams-Bashforth, but instead are these formulas slowly convergent and have relatively large error-terms. Both these methods have difficulties in knowing how to start, and in general it has been recommended to start the integration independently by means of a Taylor-series expansion.

By using operator calculus and symbolic expansions, the connection between the CD-formulas and the BD-formulas will here be investigated in greater detail. Utilizing the experience found in this way, we will show that it is possible to construct integration methods which combine the straightforwardness of the BD-methods with the simplicity and rapid convergence of the CD-methods. Even the starting problem will be simply solved.

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**2. Difference operators. The extrapolation principle.** Let $h$ be the interval, let $E$ be the step-operator defined by $Ef(x) = f(x + h)$, and let $f_n$ mean $f(x_0 + nh)$. We will then introduce the operators $\Delta$, $\nabla$, $\delta$, and $\mu$ for the formation of forward, backward, and central differences, and mean values, respectively, by

$$\Delta = E - 1, \qquad \nabla = 1 - E^{-1}, \tag{2}$$

$$\delta = E^{1/2} - E^{-1/2}, \qquad \mu = (E^{1/2} + E^{-1/2})/2. \tag{3}$$

From (3) one obtains directly

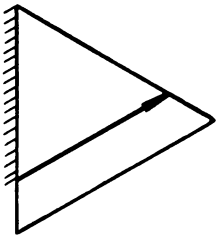
$$\mu^2 = 1 + \delta^2/4, \qquad \mu(1 + \delta^2/4)^{-1/2} = 1. \tag{4}$$

which relations often can be used in transforming CD-formulas into a suitable form. In the following we will use operator calculus and symbolic expansions[1] (Sheppard 1899; see also Michel 1946, Bickley 1948). If $D = d/dx$ is the differentiation operator, Taylor's series gives $E = \exp(hD)$, and from (3) we then get

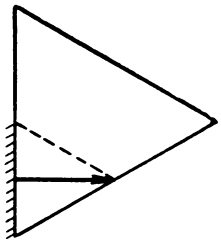
$$hD = 2 \sinh^{-1} \delta/2, \tag{5}$$

which is the basic CD-formula for numerical derivation and integration.[2]

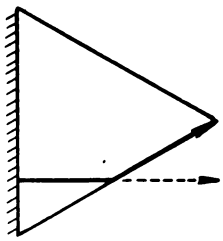
Among computers it is now a well-known fact that, in using pure CD-formulas or BD-formulas for some purpose, it is often impossible to utilize all the function values in a given material, which is illustrated by the first two figures below:



BD-formula



CD-formula



CD-formula with some CD extrapolated by means of available BD (or mixed CD-BD-formula)

The triangle indicates a function given numerically in equidistant points and its difference scheme. The full line shows the differences involved in a difference formula of a certain type; the part of the function values taken into account in this way is shaded. The dots in the last figure indicate CD extrapolated by means of available BD.

Bickley and Miller (1942) pointed out that there exist an infinite series of "mixed" CD-BD-formulas by means of which a given material could be taken into full account, and they have worked out extensive tables for the numerical derivation. As far as we

[1]The formulas obtained in this way have only symbolic character, but they can be rigorously derived and their remainder-term can be determined by starting from Newton's interpolation formula for unequal interval with Cauchy's remainder (see Nielsen 1908).

[2]For tables of coefficients, see e.g. Salzer (1943, 1944, and 1945).

know, corresponding tables for the numerical integration have not yet been published, nor is it necessary.

Here we will proceed in another way. From (2) we obtain

$$E = 1 + \nabla E = 1 + \nabla + \nabla^2 + \cdots + \nabla^p + \nabla^{p+1}E$$
$$= 1 + \nabla + \nabla^2 + \nabla^3 + \cdots = (1 - \nabla)^{-1}, \tag{6}$$

and according to (2) and (3) we then get the extrapolation formulas

$$\delta^{2m}F_n = \nabla^{2m}(1 - \nabla)^{r-m}F_{n+r} = \sum_{k=0}^{\infty} a_k^{(r-m)}\nabla^{2m+k}F_{n+r},$$

$$\delta^{2m+1}F_{n+1/2} = \nabla^{2m+1}(1 - \nabla)^{r-m-1}F_{n+r} = \sum_{k=0}^{\infty} a_k^{(r-m-1)}\nabla^{2m+1+k}F_{n+r},$$

$$2\mu\delta^{2m}F_{n+1/2} = \nabla^{2m}(2 - \nabla)(1 - \nabla)^{r-m-1}F_{n+r} = \sum_{k=0}^{\infty} b_k^{(r-m)}\nabla^{2m+k}F_{n+r}, \tag{7}$$

$$2\mu\delta^{2m+1}F_n = \nabla^{2m+1}(2 - \nabla)(1 - \nabla)^{r-m-1}F_{n+r} = \sum_{k=0}^{\infty} b_k^{(r-m)}\nabla^{2m+1+k}F_{n+r}$$

with the coefficients

$a_k^{(s)}$:

| $s$ \ $k$ | 0 | 1 | 2 | 3 | 4 | · |
|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 0 | 0 | 0 | · |
| −1 | 1 | 1 | 1 | 1 | 1 | · |
| −2 | 1 | 2 | 3 | 4 | 5 | · |
| −3 | 1 | 3 | 6 | 10 | 15 | · |
| −4 | 1 | 4 | 10 | 20 | 35 | · |
| · | · | · | · | · | · | · |

$b_k^{(s)}$:

| $s$ \ $k$ | 0 | 1 | 2 | 3 | 4 | · |
|---|---|---|---|---|---|---|
| 0 | 2 | 1 | 1 | 1 | 1 | · |
| −1 | 2 | 3 | 4 | 5 | 6 | · |
| −2 | 2 | 5 | 9 | 14 | 20 | · |
| −3 | 2 | 7 | 16 | 30 | 50 | · |
| −4 | 2 | 9 | 25 | 55 | 105 | · |
| · | · | · | · | · | · | · |

satisfying elementary recurrence relations. The formulas (6)-(7) form together an "extrapolation principle", by means of which CD-quantities in the horizontal lines $n$ and $(n + \frac{1}{2})$ can be expressed in terms of the BD in the backward line $(n + r)$. The series in (7) are only formally infinite; in the practical use they are always interrupted after a difference of the finite order $p$, corresponding to an extrapolation of the function under consideration by a *polynomial* of the degree $p$.

Instead of using the rather complicated "mixed" CD-BD formula of the Bickley-Miller type, we can now take a given material into full account simply *by using a pure CD-formula and by extrapolating as many additional CD as possible by means of the given BD in the last backward line available.* Since the coefficients in (7) are all integers, the extrapolations can be rapidly carried out on ordinary desk machines. The result will be

the same as obtained by using a "mixed" formula, and we have to remember that the error in our case is given by the sum of the remainder in the pure CD-formula and the remainders in (7).

**3. Gauss's formulas and the classical backward difference methods.** According to (4) and (5) the first order equation $y' = F(x, y)$ is equivalent with the CD-equation

$$\begin{aligned} hF &= \mu(1 + \delta^2/4)^{-1/2} 2 \sinh^{-1} \delta/2 \cdot y \\ &= \mu\, \delta y - \frac{1}{6}\mu\, \delta^3 y + \frac{1}{30}\mu\, \delta^5 y - \frac{1}{140}\mu\, \delta^7 y + -\cdots , \end{aligned} \tag{8}$$

from which $y$ can be solved by the inverse relation

$$\begin{aligned} h^{-1}y &= \mu(1 + \delta^2/4)^{-1/2}\{2 \sinh^{-1} \delta/2\}^{-1} \cdot F \\ &= \mu\, \delta^{-1}F - \frac{1}{12}\mu\, \delta F + \frac{11}{720}\mu\, \delta^3 F - \frac{191}{60480}\mu\, \delta^5 F + \frac{2497}{3628800}\mu\, \delta^7 F - \cdots . \end{aligned} \tag{9}$$

Here the symbol $\delta^{-1}F$ means the first sum of $F$, defined by $\delta(\delta^{-1}F) = F$; the "summation constants" included in this and other sums will here be determined by the condition that the integration formulas under consideration should be valid even in the starting point $x = x_0$ . Formula (9) forms the basis of a method of numerical integration[3] due to Gauss, which was first published by Encke (1837) and which has frequently been used in the celestial mechanics (see e.g. Charlier 1907).

Here we will study a slightly modified form. By applying the operator $\delta E^{1/2}$ on both members of (9) we get

$$h^{-1}\, \delta y_{n+1/2} = \mu F_{n+1/2} - \frac{1}{12}\mu\, \delta^2 F_{n+1/2} + \frac{11}{720}\mu\, \delta^4 F_{n+1/2} - \frac{191}{60480}\mu\, \delta^6 F_{n+1/2} + \cdots \tag{10}$$

a form used for instance by Hartree (1928). This is nothing but the *trapezoidal rule* with difference correction, and we note that, in integrating a given fix integrand $F = F(x)$, the whole material can be taken into full account by using the "extrapolation principle" developed in §2. In integrating the differential equation (1), we will now show that it is possible to avoid the use of estimations, characteristic for the earlier CD-methods, by using the same principle.

Let us assume that we have started the integration in some way and that we have computed $y$, $F = F(x, y)$, and the difference scheme for $F$ accurately up to the point $n$ given by $x = x_0 + nh$. Since we know the BD of $F$ in the backward line $n$, we can now extrapolate the CD in the horizontal line $(n + \frac{1}{2})$ in formula (10) according to (7), and in this way we find approximate values of $y_{n+1}$ and $F_{n+1}$ . Repeating the process we obtain approximate values of $y_{n+2}$ , $F_{n+2}$ , $y_{n+3}$ , $F_{n+3}$ , $\cdots$ . Going back to the point $(n + 1)$, we can then improve the accuracy of the solution by the repeated use of formula (10) and the extrapolation formulas (7), utilizing the CD found on later stages of the first approximate calculation and extrapolating some additional CD by means of the last BD-line available. By iterations it is in this way possible to obtain a pure CD-result in a straightforward manner.

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[3]The remainder was first derived by Nielsen (1908); see also Steffensen (1924) and Nyström (1926).

The connection between this method and the classical BD-methods is perhaps of some interest. Putting the expressions for the CD in (10), extrapolated according to (7) by means of the BD-lines $n$, $n + 1$, $n + 2$, $\cdots$, into formula (10) we get

$$\begin{aligned} h^{-1}y_{n+1} - h^{-1}y_n &= F_n + \frac{1}{2}\nabla F_n + \frac{5}{12}\nabla^2 F_n + \frac{3}{8}\nabla^3 F_n \\ &\quad + \frac{251}{720}\nabla^4 F_n + \frac{95}{288}\nabla^5 F_n + \cdots \\ &= F_{n+1} - \frac{1}{2}\nabla F_{n+1} - \frac{1}{12}\nabla^2 F_{n+1} - \frac{1}{24}\nabla^3 F_{n+1} \\ &\quad - \frac{19}{720}\nabla^4 F_{n+1} - \frac{3}{160}\nabla^5 F_{n+1} - \cdots = \cdots, \end{aligned} \tag{11}$$

which is nothing but the BD-formulas given first in another way by Adams-Bashforth (1883). The accuracy of the first formula is low,[4] corresponding to our first approximation above, and it is usually recommended to improve the accuracy by using one or more additional BD-formula, which may formally be obtained from the ground formula by letting the operator $1 = (1 - \nabla)E$ work repeatedly on its right-hand member.[5] A comparison between the formulas (11) and the simple formula (10) shows immediately that, from the point of view of the computer, it is considerably simpler to use the single CD-formula (10) together with the extrapolation formulas (7) than the corresponding classical BD-methods.

Let us now also consider formulas for taking a double step[6] from $(n - 1)$ to $(n + 1)$ by means of the values associated with $n$. Letting the operator $\mu\delta$ work on both members of (9) and using (4), we get in the point $n$

$$h^{-1}\mu\,\delta y_n = F_n + \frac{1}{6}\delta^2 F_n - \frac{1}{180}\delta^4 F_n + \frac{1}{1512}\delta^6 F_n - \frac{23}{226800}\delta^8 F_n + \cdots, \tag{12}$$

which is nothing but *Simpson's rule* with difference correction.[7] By combining (12) with the extrapolation formulas (7) and using iterations, we can again construct a straightforward CD-method in the same way as described in connection with formula (10) for taking a single step.

The connection between this method and the classical BD-methods is easily seen. By putting the expressions for the CD in (12), extrapolated according to (7) by means

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[4]The remainder was first derived by Nielsen (1908); the propagation of errors has been investigated by v. Mises (1930) and by Schulz (1932). The method has been further developed in Russian memoirs by Kryloff; a modification has been given by Falkner (1936).

[5]See also the note by Stohler (1943).

[6]The first method of this type was developed by Richardson (1911, 1927), who used approximate CD-expansions and afterwards improved the solutions by a certain process called the "$h^2$-extrapolation"; compare also Duncan (1948).

[7]The simple Simpson's rule has earlier been used for numerical integration by Bickley (1932) and by Collatz and Zurmühl (1942a).

of the BD-lines $n$, $n+1$, $n+2$, $\cdots$, into formula (12) we obtain

$$h^{-1}y_{n+1} - h^{-1}y_{n-1}$$

$$= 2F_n + \frac{1}{3}\nabla^2 F_n + \frac{1}{3}\nabla^3 F_n + \frac{29}{90}\nabla^4 F_n + \frac{14}{45}\nabla^5 F_n + \cdots \tag{13}$$

$$= 2F_{n+1} - 2\nabla F_{n+1} + \frac{1}{3}\nabla^2 F_{n+1} - \frac{1}{90}\nabla^4 F_{n+1} - \frac{1}{90}\nabla^5 F_{n+1} - \cdots = \cdots .$$

The first formula (13) was derived by Nyström (1926), and later a slightly modified form was given by Lindelöf (1939); his correction term can here be obtained by taking the remainder terms in (7) into account.[8] The second formula (13) has been treated by Levy-Baggot (1934) and by Sibagaki (1936). Again we find that it is simpler to use the single CD-formula (12) together with the extrapolation formulas (7) than the corresponding classical BD-methods.

The main conclusion in this section is therefore that, from the computer's point of view, it is considerably simpler to use a fundamental CD-formula in combination with the extrapolation principle (7) than any of the classical BD-methods. However, if high accuracy is desired, the numerical integrations based on (10) or on (12) are rather laborious to carry out, since each step of the integration demands iterations of the whole difference scheme. In the next section we will therefore try to modify the basic CD-formula in order to find a still simpler and more straightforward integration method.

**4. A new central difference method.** I) *THE BASIC FORMULA.* Let us first try to derive a new formula of the Gaussian type (9), but having a much smaller difference correction. According to (3) and (12) we have

$$h^{-1}\mu\,\delta y = F + \frac{1}{3}(\mu\,\delta F - \nabla F) - \frac{1}{180}\delta^4 F + \frac{1}{1512}\delta^6 F - \frac{23}{226800}\delta^8 F + \cdots . \tag{14}$$

Letting the operator $(\mu\delta)^{-1}$ work on both members of this equation, using (4) in treating the difference correction, and transforming the $F$-term to the left member, we get the integration formula

$$h^{-1}y - \frac{1}{3}F(x, y) = (\mu\delta)^{-1}\{F - \frac{1}{3}\nabla F\}$$
$$- \frac{1}{180}\mu\,\delta^3 F + \frac{31}{15120}\mu\,\delta^5 F - \frac{557}{907200}\mu\,\delta^7 F + \cdots , \tag{15}$$

which forms the basis for our method. The sum in the right member is dominating and will be called the main term:

$$M = (\mu\delta)^{-1}\left\{F - \frac{1}{3}\nabla F\right\}. \tag{16}$$

The difference correction is extremely small and will be denoted by $\gamma$. The quantities involved in the computations are suitably arranged in two or three tables: a *main table*

[8] See formula (6), first line.

recording the quantities $x$, $y$, $(M + \gamma)$, $\gamma$, $M$, and $F$, a *difference table* giving the differences of $F$, and—for non-linear equations (1)—an iteration table. As to the difference correction the integration will be divided in three parts: the start, the marching process, and the aftercorrection.

II) *THE MARCHING PROCESS.* At first we will assume that the integration has been performed up to the point $n$ with $x = x_0 + nh$. In order to carry out the next step of the integration, we will then write eq. (15) under the form

$$\begin{cases} M_{n+1} = M_{n-1} + 2F_n - \frac{2}{3}\nabla F_n , & (17') \\ \gamma_{n+1} = -\frac{1}{180}\mu\,\delta^3 F_{n+1} + \frac{31}{15120}\mu\,\delta^5 F_{n+1} - \frac{557}{907200}\mu\,\delta^7 F_{n+1} + \cdots , & (17'') \\ h^{-1}y_{n+1} - \frac{1}{3}F_{n+1} = (M + \gamma)_{n+1} . & (17''') \end{cases}$$

First the new main term $M_{n+1}$ is computed from the quantities in the previous part of the main table according to eq. (17′), which is obtained by letting $2\mu\delta$ work on both members of (16). Then we will extrapolate[9] the CD occurring in the difference correction $\gamma_{n+1}$ by means of the known BD in the backward line $n$ by using formulas (7):

$$\begin{aligned} 2\mu\,\delta^3 F_{n+1} &= 2\nabla^3 F_n + 5\nabla^4 F_n + 9\nabla^5 F_n + 14\nabla^6 F_n + \cdots , \\ 2\mu\,\delta^5 F_{n+1} &= 2\nabla^5 F_n + 7\nabla^6 F_n + 16\nabla^7 F_n + 30\nabla^8 F_n + \cdots , \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \end{aligned} \qquad (18)$$

Finally we will determine the values of $y_{n+1}$ and $F_{n+1}$ by solving the algebraic equation[10] (17‴). For linear equations (1) the solution is obvious, and for non-linear equations we will recommend the use of an iteration process, which will be discussed later (VI). The quantities $y_{n+1}$ and $F_{n+1}$ are written down on their places in the main table, a new backward line $(n + 1)$ is calculated in the difference scheme for $F$, and then the process can be repeated for the point $(n + 2)$ with $x = x_0 + (n + 2)h$, etc. This integration process is quite straightforward, and it gives a preliminary solution $y$ with a high accuracy, due to the smallness of the difference correction.

III) *THE AFTERCORRECTION.* The preliminary solution obtained in the marching process has an accuracy which is determined by the "mixed" CD-BD character of the integration formulas (17) and (18). However, when the marching process has been finished for the whole range of integration under consideration (including some additional points), it is possible to improve the accuracy of $y$ by utilizing the actual values

[9] A necessary condition for the usefulness of such extrapolation is, of course, that the higher differences of $F$ converge rapidly against zero; this can be obtained by choosing the interval $h$ sufficiently small. In general we will calculate the differences of $F$ only up to the order where the irregularities, due to the effect of rounding-off errors, become to be of about the same magnitude as the differences themselves.

[10] In agreement with Hartree (1949, p. 235) the term "algebraic" is here meant only as an antithesis to the term "differential."

of the CD found on later stages of the calculation. For this purpose we will introduce the correction

$$\begin{aligned}\mathrm{corr}_n &= \gamma_n\text{, actual} - \gamma_n\text{, extrapolated} \\ &= -\frac{1}{180}\{\mu\,\delta^3 F_{n,\mathrm{act}} - \mu\,\delta^3 F_{n,\mathrm{ext}}\} + \frac{31}{15120}\{\mu\,\delta^5 F_{n,\mathrm{act}} - \mu\,\delta^5 F_{n,\mathrm{ext}}\} - .\end{aligned} \tag{19}$$

We note that, in the main table, the quantities $y$ and $M$ are usually recorded with the same number of significant figures, whereas it is often sufficient to record $F$ with at least one figure less[11] than $M$. The correction (19) will, in general, influence the value of $y$, but the idea of our method is now that the interval $h$ should be chosen so small, that the change in $y$ should *not* influence the recorded figures of $F$. In this case the columns for $F$ and $M$ in the main table will be unchanged by the aftercorrection, and, according to (17‴), the final solution can be computed from the simple formula

$$y_{n,\mathrm{final}} = y_{n,\mathrm{preliminary}} + h\,\mathrm{corr}_n\,. \tag{20}$$

In this way it is possible to carry out the transition from a mixed CD-BD-result into a pure CD-result by a single iteration of a very simple type (compare §3).

During the marching process it is suitable to check the extrapolations (18), e.g. in every fifth point, by comparing the extrapolated value of $2\mu\delta^3 F_n$ in the point $n$ with the actual value, found when the integration has reached the point $(n + 2)$. If the value of $h$ seems to begin to become too large, it is then necessary to change the length of the interval by some of the well-known processes of subtabulation.

IV) *THE START.* Even the start will here be treated by means of our basic formula (15) by using an auxiliary formula[12] and a method of successive approximations. Letting the operator $\Delta = \mu\delta + \delta^2/2$ work on both members of (15) and using (4), we get

$$\Delta M = F + \frac{1}{6}\mu^{-1}\,\delta F = F + \frac{1}{6}\left(1 + \frac{\delta^2}{4}\right)^{-1}\mu\,\delta F, \tag{21}$$

which for $x = x_0$ gives the expansions

$$\begin{aligned}M_1 - M_0 &= F_0 + \frac{1}{6}\mu\,\delta F_0 - \frac{1}{24}\mu\,\delta^3 F_0 + \frac{1}{96}\mu\,\delta^5 F_0 - + \cdots \\ &= F_0 + \frac{1}{6}hF_0' + \frac{5}{2}\gamma_0 + \frac{1}{21}\delta^2\gamma_0 + \cdots\,,\end{aligned} \tag{22}$$

where the latter is derived from the former by using (5) and (17″); the second form is the best for our purpose. The integration will now be started from the initial condition $y = y_0$ for $x = x_0$ and by using the formulas

$$\begin{aligned}M_0 &= h^{-1}y_0 - \frac{1}{3}F_0 - \gamma_0\,, \\ M_1 &= h^{-1}y_0 + \frac{2}{3}F_0 + \frac{h}{6}F_0' + \frac{3}{2}\gamma_0 + \frac{1}{21}\delta^2\gamma_0 + \cdots\,.\end{aligned} \tag{23}$$

[11]Compare footnote 9.

[12]Compare Richardson and Gaunt (1927).

In a zero-order approximation, the quantity $\gamma$ is entirely neglected: $\gamma \equiv 0$. The quantities $M_0$ and $M_1$ found from (23) are written down on their places in the main table, and then the quantities $y_1$ , $F_1$ , $M_2$ , $y_2$ , $F_2$ , $M_3$ , $\cdots$ etc. are computed successively by using (17′) and (17‴). In this way some approximate values of $y$ and $F$, forwards and backwards[13] from the starting point, are determined.

Now the difference scheme for $F$ provides a first-order approximation of $\gamma$ in the neighbourhood of the starting point. Using these values of $\gamma$, we can then repeat the start until two consecutive approximations of $\gamma$ agree within the significant figures; the integration can then be continued as a marching process (II). Due to the extreme smallness of the difference correction, the first order approximation of $\gamma$ shows a sufficient accuracy in most problems.

In problems where the functions involved in eq. (1) are specified only in one direction from the starting point, it may be necessary to extrapolate the CD in the range of $x = x_0$ by means of *forward* differences, using a particularly small interval.

The method of successive approximations described here can easily be extended to the whole range of integration,[14] but, if the computations have to be carried out only by the aid of desk machines, it is certainly suitable to confine the method to the start.

V) *THE AUTOMATIC ELIMINATION OF OSCILLATING ERRORS.* A particular phenomenon in the first approximation of the start will here be briefly mentioned. Due to the neglection of $\gamma_0$ in (23), the approximate values of $M_0$ and $M_1$ are affected with small errors of about the magnitude $-\gamma_0$ and $+1.5\gamma_0$ . This implies that there is also an *oscillating error* in the first difference scheme for $F$, which is propagated to the higher differences with a steadily increasing magnitude, and the difference scheme can therefore have a rather irregular appearance.[15]

At first sight it seems impossible to determine $\gamma$ with a sufficient accuracy from a difference scheme which is disturbed by an oscillating error. However, it is easily proved that an error of the type $(-1)^n f_n$ , where $f$ is a polynomial in $x$ of the degree $p$, can be entirely eliminated by the operator $\mu^{p+1}$:

$$\mu^{p+1}\{(-1)^n f_n\} \equiv 0. \tag{24}$$

The operator $\mu$ can be introduced in any difference formula by the repeated use of the unity operator $1 = \mu^2(1 + \delta^2/4)^{-1}$, and we note that the application of the refinement process

$$F_{\text{refined}} = \mu^2 F - \frac{1}{4}\mu^2\,\delta^2 F + \frac{1}{16}\mu^2\,\delta^4 F - \frac{1}{64}\mu^2\,\delta^6 F + -\cdots . \tag{25}$$

will every time diminish the degree of the oscillating error by two.

In our case, i.e. the first approximation of the start, the magnitude of the error is very slowly varying, and we can therefore conclude that, due to the appearance of the mean-value operator $\mu$ in (17″), the oscillating error will automatically be almost entirely eliminated in forming the difference correction $\gamma$. In the second approximation the phenomenon has therefore disappeared. A numerical example may be found in Table II.

[13]When working backwards, we obtain the formulas needed by substituting $-h$ instead of $h$ in (15); we note that there are different values of $M_0$ for the two directions.

[14]Compare the treatments of linear equations (1) by Hausmann and Schwarzschild (1947) and by Fox and Goodwin (1949).

[15]The existence of oscillating errors has been reported also by other authors (e.g. Fox and Goodwin 1949) in connection with other methods.

VI) *THE SOLUTION OF THE ALGEBRAIC EQUATION.* The straightforwardness of our integration method based on (15) is essentially depending on the fact that we have introduced a certain algebraic[16] equation, by means of which the largest unknown central term $F$ is determined for each step of integration. A similar idea has previously been used by Noumerov in treating second order equations. The eq. (17‴) may be written in the form

$$y = N + cF(x, y), \tag{26}$$

where $N = h(M + \gamma)$ and $c = h/3$. For linear equations (1) the solution of (26) is obvious, and we will therefore confine the following discussion to the non-linear case.

A well-known analytical solution of (26) is given by Laplace's formula, but, from the practical point of view, we will here instead recommend the use of an iteration process. Let us first consider the marching process (II), and let us assume that the integration has been performed up to the point $n$. According to (6) a zero-order approximation $F_{n+1}^{(0)}$ of $F_{n+1}$ can then be found by extrapolation:

$$F_{n+1}^{(0)} = F_n + \nabla F_n + \nabla^2 F_n + \cdots + \nabla^p F_n \,. \tag{27}$$

By putting this value of $F_{n+1}$ into the right-hand member of (26), a first-order approximation of $y_{n+1}$ is obtained; then a new value of $F_{n+1}$ is calculated etc., until two consecutive approximations of $y_{n+1}$ agree within the significant figures. The solution is illustrated by

$$y^{(1)} = N + cF^{(0)}; \qquad y^{(2)} = N + cF^{(1)}; \qquad y^{(3)} = N + cF^{(2)}; \cdots \tag{28}$$

where the upper index gives the order of approximation. This iteration process is of the first order,[17] and the condition for convergency is $| cF_y | < 1$. Since the zero-order approximation of $F$ is in general rather accurate,[18] the solution is rapidly obtained. A numerical example may be found in Table IV. A check on the calculations in the difference scheme is provided by the relation

$$\nabla^{p+1} F_{n+1} = F_{n+1} - F_{n+1}^{(0)} \,. \tag{29}$$

Let us then consider the start (IV). From the practical point of view we will here recommend the use of a second order process of a simple type. Since the process (28) is of the first order, the differences $y^{(2)} - y^{(1)}$, $y^{(3)} - y^{(2)}$, $\cdots$ etc. form approximately a geometric series[19] with the quotient $q = cF_y$. Summing this series, we get

$$\begin{aligned} y^* &= y^{(1)} + \{y^{(2)} - y^{(1)}\} + \{y^{(3)} - y^{(2)}\} + \cdots \approx y^{(1)} + \frac{y^{(2)} - y^{(1)}}{1 - q} \\ &\approx y^{(1)} - \frac{\{y^{(1)} - y^{(2)}\}^2}{y^{(1)} - 2y^{(2)} + y^{(3)}}, \end{aligned} \tag{30}$$

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[16] Compare footnote 10.

[17] Iteration processes of this type were first classified by Schröder (1870); see also Hartree (1949). A formula due to Theremin (1855) corresponds to a process of order $\infty$.

[18] This fact forms the basis of all the classical BD-methods.

[19] This is easily proved by putting $y = y^{(n)} + \eta^{(n)}$, and expanding $F(x,y)$ into a power series in $\eta^{(n)}$.

where the middle step for $q = cF_y^{(1)}$ corresponds to the Newton-Raphson formula.[20] We will instead use the formula given in the last step. The value $y^*$ of $y$ found in this way can be checked by a new iteration $y^{**} = N + cF^*$. If a still higher accuracy is required, the whole process can be repeated by introducing the values of $y^*$, $y^{**}$, and $y^{***} = N + cF^{**}$ in (30). This manner of proceeding corresponds to a well-known iteration process of the second order.[21]

Putting (28) into (30), we get the final formula

$$y \approx y^{(1)} - c\frac{\{F^{(1)} - F^{(0)}\}^2}{F^{(0)} - 2F^{(1)} + F^{(2)}}, \tag{31}$$

which seems to be the best for our purpose. In using this formula, $F^{(0)}$ is determined from the few terms available in (27), and then the final result can be obtained by means of only *two* computations of the function $F = F(x, y)$; for a numerical example, see Table V.

The results obtained in this section show that the rather laborious iterations of the whole difference scheme for each step of integration, characteristic for the classical CD-methods and for many of the BD-methods (§3), have here been reduced to the after-correction (20) and to the simple iteration processes described above for solving the algebraic equation (26). For linear equations (1) the simplifications are still more considerable.

VII) *CHECK OF THE SOLUTION.* In all step-by-step methods based on the use of recurrence relations, it is necessary to have an accurate check on each stage of the calculation, since a mistake somewhere will vitiate the whole subsequent work. The most important check is here provided by the difference scheme for $F$, since a small error in the solution will give rise to a large irregularity in the higher differences of $F$; in this connection even eq. (29) may be of value. By letting the operator $2\mu\delta$ work on both members of (15), we get

$$y_{n+1} - y_{n-1} = \frac{h}{3}(F_{n+1} + 4F_n + F_{n-1}) + 2h\mu\,\delta\gamma_n\,, \tag{32}$$

which relation may also be used for check purpose. A more independent check is provided by the differential equation itself in the form (8).

VIII) *NUMERICAL EXAMPLE.* In order to illustrate how our integration method works in a practical case, we will here give some results from a treatment of the non-linear equation

$$\frac{dy}{dx} = x - y^2 \tag{33}$$

with the initial condition $y = 0.72\ 901\ 1133\ \cdots$ for $x = 0$. The exact solution is here the logarithmic derivative of the Airy integral

$$y = \frac{d}{dx}\log \mathrm{Ai}(x), \tag{34}$$

which has been carefully tabulated by Miller (1946). The start of the integration is illustrated in Table I, the elimination of oscillating errors in Table II, the marching

[20]Compare Collatz and Zurmühl (1942a).

[21]Aitken (1925), Samuelson (1945), and Hartree (1949).

process in Table III, and the solution of the algebraic equation in Tables IV and V. The calculation was carried out with nine figures with a speed of 12-15 points an hour by the aid of ordinary table machines (Facit ESA and Hamann-Selecta). It was found that, except for rounding-off errors in the 8th decimal, even the preliminary solution was in agreement with the values in Miller's table.

*Table I.* Start integration for the equation $y' = x - y^2$ by means of successive approximations. The computations are arranged as in Table III, and we will here give only the solution $y$ in the different approximations in comparison to Miller's values.

| $x$ | $y_{\text{Miller}}$ | $y^{(1)}$ | $h\cdot\gamma^{(1)}$ | $y^{(2)}$ | $h\cdot\gamma^{(2)}$ |
|---|---|---|---|---|---|
| −0.5 | −.42 898 806 | −.42 898 723 | $\times 10^{-8}$ | | $\times 10^{-8}$ |
| −0.4 | −.49 541 771 | −.49 541 759 | | | |
| −0.3 | −.55 823 486 | −.55 823 422 | $39_8$ | −.55 823 485 | $39_3$ |
| −0.2 | −.61 787 457 | −.61 787 457 | $31_6$ | −.61 787 458 | $31_5$ |
| −0.1 | −.67 469 872 | −.67 469 819 | $25_4$ | −.67 469 873 | $25_4$ |
| −0. | −.72 901 113 | −.72 901 113 | $20_6$ | −.72 901 113 | $20_6$ |
| +0. | −.72 901 113 | −.72 901 113 | $-20_6$ | −.72 901 113 | $-20_6$ |
| 0.1 | −.78 106 918 | −.78 106 869 | $-16_8$ | −.78 106 919 | $-16_8$ |
| 0.2 | −.83 109 270 | −.83 109 265 | $-13_9$ | −.83 109 269 | $-13_9$ |
| 0.3 | −.87 927 067 | −.87 927 016 | $-11_5$ | −.87 927 068 | $-11_6$ |
| 0.4 | −.92 576 688 | −.92 576 675 | | | |
| 0.5 | −.97 072 392 | −.97 072 337 | | | |

There is an error of ±1 in the 6th decimal in the first approximation $y^{(1)}$ and a corresponding error in the 8th decimal in the second approximation $y^{(2)}$. The marching process can be based on $y^{(2)}$.

*Table II.* Calculation of $\gamma$ in the start. The table shows the elimination of the oscillating errors in the first approximation by the mean-value formation, cf. formula (17″). The difference scheme for $F$ is rather irregular in the first approximation, but still it gives almost the same values of $2\mu\delta^3F$ and $2\mu\delta^5F$ as the second approximation. The unity = $10^{-8}$.

| | First approximation | | | | Second approximation | | | |
|---|---|---|---|---|---|---|---|---|
| $x$ | $\delta^3F$ | $\delta^5F$ | $2\mu\delta^3F$ | $2\mu\delta^5F$ | $\delta^3F$ | $\delta^5F$ | $2\mu\delta^3F$ | $2\mu\delta^5F$ |
| | 82 163 | | | | 82 212 | | | |
| −.3 | | | 147 319 | | | | 147 092 | |
| | 65 156 | 3 271 | | | 64 880 | 4 222 | | |
| −.2 | | | 116 576 | 7 531 | | | 116 586 | 7 337 |
| | 51 420 | 4 260 | | | 51 706 | 3 115 | | |
| −.1 | | | 93 364 | 5 376 | | | 93 353 | 5 415 |
| | 41 944 | 1 116 | | | 41 647 | 2 300 | | |
| 0. | | | 75 528 | 4 024 | | | 75 535 | 3 993 |
| | 33 584 | 2 908 | | | 33 888 | 1 693 | | |
| .1 | | | 61 716 | 2 955 | | | 61 710 | 2 974 |
| | 28 132 | 47 | | | 27 822 | 1 281 | | |
| .2 | | | 50 859 | 2 260 | | | 50 859 | 2 254 |
| | 22 727 | 2 213 | | | 23 037 | 973 | | |
| .3 | | | 42 262 | | | | 42 262 | |
| | 19 535 | | | | 19 225 | | | |

*Table III.* A part of the main table for the marching process in the numerical integration of $y' = x - y^2$.

| $x$ | $y$ | $M + \gamma$ | $\gamma$ | $M$ | $F$ | $-\frac{1}{2}\nabla F$ |
|---|---|---|---|---|---|---|
| − .3 | −.55 823 4850 | 5.78 622 388 | 393 | 5.78 621 995 | −.61 162 615 | |
| | | | | | | 995 238 |
| −.2 | −.61 787 4584 | 6.37 266 884 | 315 | 6.37 266 569 | −.58 176 900 | |
| | | | | | | 885 021 |
| −.1 | −.67 469 8729 | 6.93 206 008 | 254 | 6.93 205 754 | −.55 521 838 | |
| | | | | | | 792 038 |
| −0. | −.72 901 1133 | 7.46 726 374 | 206 | 7.46 726 168 | −.53 145 723 | |
| +0. | −.72 901 1133 | −7.11 295 892 | −206 | −7.11 295 686 | −.53 145 723 | |
| | | | | | | −712 939 |
| .1 | −.78 106 9189 | −7.64 066 886 | −168 | −7.64 066 718 | −.51 006 908 | |
| | | | | | | −645 134 |
| .2 | −.83 109 2686 | −8.14 735 518 | −139 | −8.14 735 379 | −.49 071 505 | |
| | | | | | | −586 604 |
| .3 | −.87 927 0676 | −8.63 500 112 | −115 | −8.63 499 997 | −.47 311 692 | |
| | | | | | | −535 754 |
| .4 | −.92 576 6881 | −9.10 532 070 | −98 | −9.10 531 972 | −.45 704 432 | |
| | | | | | | −491 311 |
| .5 | −.97 072 3954 | −9.55 980 454 | −86 | −9.55 980 368 | −.44 230 500 | |
| | | | | | | −452 254 |
| .6 | −1.01 426 6910 | −9.99 975 664 | −71 | −9.99 975 593 | −.42 873 737 | |
| | | | | | | −417 755 |
| .7 | −1.05 650 5902 | −10.42 632 411 | −61 | −10.42 632 350 | −.41 620 472 | |
| | | | | | | −387 135 |
| .8 | −1.09 753 8455 | −10.84 052 100 | −53 | −10.84 052 047 | −.40 459 066 | |
| | | | | | | −359 839 |
| .9 | −1.13 745 1315 | −11.24 324 799 | −46 | −11.24 324 753 | −.39 379 549 | |
| | | | | | | −335 403 |
| 1.0 | −1.17 632 1976 | −11.63 530 863 | −39 | −11.63 530 824 | −.38 373 339 | |
| ..... | | | | | | |

A comparison with Miller's table shows that there is an error of ±1 in the 8th decimal in the preliminary solution; the aftercorrection is so small that it changes only the rounding-off.

*Table IV.* Solution of the algebraic equation (26) in the marching process according to the iteration process (28). $r$ gives the order of approximation.

$x = 1.0 \quad h = 0.1 \quad N = -1.16\ 353\ 0863$

| $r$ | $y^{(r)}$ | $F(r)$ |
|---|---|---|
| 0 | | −.38 373 343 |
| 1 | −1.17 632 1977 | −.38 373 340 |
| 2 | −1.17 632 1976 | −.38 373 339 |

*Table V.* Solution of the algebraic equation (26) in the start by using formula (28) and (31), respectively. First approximation.

$x = 0.1 \quad h = 0.1 \quad N = -0.76\ 406\ 6409$

| $r$ | $y^{(r)}$ | $F^{(r)}$ | Order | $y^{(r)}$ | $F^{(r)}$ |
|---|---|---|---|---|---|
| 0 | | −.53 145 723 | | | |
| 1 | −.78 178 1650 | −.51 118 255 | | | |
| 2 | −.78 110 5827 | −.51 012 631 | * | −.78 106 8685 | −.51 006 829 |
| 3 | −.78 107 0619 | −.51 007 131 | ** | −.78 106 8685 | |
| 4 | −.78 106 8786 | −.51 006 845 | | | |
| 5 | −.78 106 8691 | −.51 006 830 | | | |
| 6 | −.78 106 8686 | −.51 006 829 | | | |
| 7 | −.78 106 8685 | | | | |

This example shows that the use of (31) can spare a considerable amount of work in the start integration

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[22] *Note added in proof:* A similar approach for integrating the second order equation $y'' = F(x, y)$ has recently been published in P. O. Löwdin and A. Sjölander, Arkiv för Fysik **3**, 155 (1951) and in P. O. Löwdin, Report from the NAS-ONR Conference on Quantum-mechanical Methods in Valence Theory, Shelter Island 1951. Related methods for integrating the equations $y'' = F(x, y, y')$ and $y''' = F(x, y, y', y'')$ have also been developed by the author and will be published elsewhere.

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