

The Numerical Integration of Ordinary Differential Equations†

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Abstract. Multistep methods for initial value problems are expressed in a matrix form. The application of such methods to higher-order equations is studied with the result that new techniques for both first- and higher-order equations are found. The direct approach to higher-order equations is believed to offer speed and accuracy advantages; some numerical evidence is presented. The new technique applied to first-order equations is a slight extension of the conventional multistep method and avoids the Dahlquist [2] stability theorem, that is, these new k -step methods are of order $2k$ and yet convergent. The matrix formalism introduced provides an easy mechanism for examining the equivalence of methods as introduced by Descloux [3]. It is pointed out that the new first-order method on k -steps, Adams' method on $(2k - 1)$ -steps and Nordsieck's [7] method with $2k$ components are equivalent to each other. In fact, all methods discussed can be placed in equivalence classes so that theorems need only be proved for one member of each class. The choice between the members of a class can be made on the basis of round-off errors and amount of computation only. Arguments are given in favor of the extension of Nordsieck's method for general use because of its speed and applicability to higher order problems directly. The theorems ensuring convergence and giving the asymptotic form of the error are stated. The proofs can be found in a cited report.

1. Introduction. This paper is concerned with the integration of initial value problems for a system of ordinary differential equations of the form

$$(1.1) \quad y_i^{(p_i)} = f_i(x, y_1, \dots, y_1^{(p_1-1)}, y_2, \dots, y_s^{(p_s-1)}), \quad i = 1, 2, \dots, s,$$

where $y^{(k)} = d^k y / dx^k$. The motivation for the work was to try and integrate such equations directly rather than as a larger system of first-order equations. The study led to a matrix representation for multistep methods that is an extension of a similar representation due to Descloux [3]. This representation provides a unified approach to equations of all orders; it is sufficient and easier to study it in detail for first-order equations. The usual theorems of stability and convergence, etc. are stated for general higher-order systems in Section 5. The proofs can be found in Gear [5].

2. Multistep Methods. The equation $y' = f(x, y)$ is frequently integrated numerically by a predictor-corrector algorithm of the following form:

Let $x_n = x_0 + nh$ where h is the step size, and let y_n and y_n' be approximations to the values of $y(x_n)$ and $dy(x_n)/dx$ obtained in some manner. The values of y and y' at x_{n+1} are found by the sequence of steps: predictor formula

$$(2.1) \quad y_{n+1}^{(0)} = \sum_{j=1}^k (\alpha_j^* y_{n-j+1} + \beta_j^* h y'_{n-j+1}),$$

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where $\gamma_i = (\alpha_i^* - \alpha_i)/\beta_0$ and $\delta_i = (\beta_i^* - \beta_i)/\beta_0$. Let the column vector \mathbf{l} be the transpose of

$$[-\beta_0, 0, \dots, 0, -1, 0, \dots, 0].$$

The predictor formula (2.1) and the definition of $\mathbf{y}_{n+1}^{(0)}$ by (2.6) give

$$(2.7) \quad \mathbf{y}_{n+1}^{(0)} = B\mathbf{y}_n.$$

The corrector formula (2.2) and the definition of $\mathbf{y}_{n+1}^{(1)}$ by (2.5) give

$$(2.8) \quad \mathbf{y}_{n+1}^{(1)} = \mathbf{y}_{n+1}^{(0)} + \mathbf{l}F(\mathbf{y}_{n+1}^{(0)}),$$

where

$$F(\mathbf{v}_{n+1}) = v_{k,n+1} - hf(x_{n+1}, v_{0,n+1}),$$

and $v_{0,n+1}$ and $v_{k,n+1}$ are the zeroth and k th components of the vector \mathbf{v}_{n+1} respectively.

Further corrector iterations (2.3) and the definition of $\mathbf{y}_{n+1}^{(m)}$ by (2.5) give

$$(2.9) \quad \mathbf{y}_{n+1}^{(m+1)} = \mathbf{y}_{n+1}^{(m)} + \mathbf{l}F(\mathbf{y}_{n+1}^{(m)})$$

and

$$\mathbf{y}_{n+1} = \mathbf{y}_{n+1}^{(M)}.$$

Components of the matrix B and the vector \mathbf{l} are chosen so as to get desirable accuracy and stability properties. The most common choices make the method exact for a class of polynomials so that the error term can be expressed as a high power of the presumably small quantity h . In order to continue the discussion the following terms are defined:

Polynomial Degree. A method has polynomial degree q if it is exact for all problems whose solutions are polynomials of degree q or less.

Degree. A method has degree q' if the error after one step starting from exact values is $O(h^{q'+1})$.

Order. A method has order q'' if the error over a fixed finite interval of integration starting from exact values is $O(h^{q''})$.

q is what is commonly called the order of the predictor; that is, the degree of polynomial for which the predictor is exact, while q' is the order of the corrector provided that $q + M$ is at least q' . (The order of the error introduced by the predictor can be increased by one for each corrector iteration up to the order of the corrector.)

The well-known Dahlquist [2] stability theorem states that a k -step method cannot have order greater than $k + 2$, and even then only for weakly stable methods. Strong stability restricts the order to $k + 1$. (Instability means that the error grows unboundedly as $h \rightarrow 0$ over a fixed interval of integration.) Dahlquist has also shown that the coefficients can be chosen so as to achieve polynomial degree $2k - 1$ and degree $2k$. Assuming that a high order is desirable, it is unfortunate that such methods are necessarily unstable. Recently, effort has been made to overcome this problem by Gragg and Stetter [6], Butcher [1] and Gear [4]. However, these techniques involve one or more extra evaluations of $f(x, y)$ at points other than x_n and they only appear to be applicable for a finite number of values of k .

One necessary condition for convergence is stability. Let us examine this problem in the matrix formulation. If a method is to converge for all problems it must certainly converge for problems whose solutions are polynomials of degree q for which the method is exact. Suppose that an error has been generated by round-off in such a problem. Further, consider a problem in which $\partial f/\partial y = 0$. Let y_n^c be the correct value of $y(x_n)$ and define

$$(2.10) \quad \epsilon_n = y_n - y_n^c, \quad y_{n+1}^{(0)c} = B y_n^c,$$

$$(2.11) \quad y_{n+1}^{(m+1)c} = y_{n+1}^{(m)c} + \mathbf{l}F(y_{n+1}^{(m)c}),$$

and

$$\epsilon_n^{(m)} = y_n^{(m)} - y_n^{(m)c}.$$

Subtract (2.10) from (2.7) and (2.11) from (2.9) to get

$$\epsilon_{n+1}^{(0)} = B\epsilon_n, \quad \epsilon_{n+1}^{(m+1)} = \epsilon_{n+1}^{(m)} + \mathbf{l}(\partial F/\partial y)\epsilon_{n+1}^{(m)},$$

where $\partial F/\partial y$ is the row vector whose elements are the partial derivatives of F with respect to y . In this case, $\partial F/\partial y$ is the vector $\mathbf{e}_k^T = [0, \dots, 0, 1, 0, \dots, 0]$, a 1 in position k . Since $\epsilon_{n+1} = \epsilon_{n+1}^{(M)}$, $\epsilon_{n+1} = (I + \mathbf{l}\mathbf{e}_k^T)^M B\epsilon_n = S\epsilon_n$. Thus a necessary condition for stability is that the eigenvalues of S are inside $|z| \leq 1$ or on $|z| = 1$ and simple. Thus Dahlquist's theorem is a restriction on the degree such that S is stable.

Conventional multistep methods restrict the choice of \mathbf{l} to the form above which has one degree of freedom. It is reasonable to ask what happens if an arbitrary form of \mathbf{l} is allowed. The answer is given in the theorems stated in Section 5, namely, that stable convergent methods of order $2k$ can be found for any value of M . In fact, \mathbf{l} can be chosen to make the nonprincipal roots of S take on any set of stable values. (One root must be 1 if the method is of polynomial degree ≥ 0 , this is the principal root.) Therefore there exist modified k -step methods of order $2k$ which require only one function evaluation. An example of a 3-step method is given below. 2- and 4-step methods are given in Gear [5]. It is written in a conventional predictor-corrector form. The superscripts C_1 and C_2 refer to additional corrections of the function values due to nonzero terms in \mathbf{l} where there are zeroes in the conventional method.

$$\begin{aligned} y_{n+1}^p &= -18y_n + 9y_{n-1}^{C_1} + 10y_{n-2}^{C_2} + 9hy_n' + 18hy_{n-1}' + 3hy_{n-2}', \\ h y_{n+1}'^p &= -57y_n + 24y_{n-1}^{C_1} + 33y_{n-2}^{C_2} + 24hy_n' + 57hy_{n-1}' + 10hy_{n-2}', \\ F &= hy_{n+1}'^p - hf(x_{n+1}, y_{n+1}^p), \\ y_{n+1} &= y_{n+1}^p - (95/288)F, \\ y_{n+1}^{C_1} &= y_n + (3/160)F, \\ y_{n+1}^{C_2} &= y_{n-1}^{C_1} - (11/1440)F, \\ h y_{n+1}' &= h y_{n+1}'^p - F. \end{aligned}$$

This method is a stable, sixth-order 3-step method. It is a modification of the conventional multistep method by the addition of corrections to all saved function values at each step. It will be referred to as an " M -method" (modified multistep

method). In matrix form, this method is written as

$$\mathbf{y}_{n+1}^{(0)} = \begin{bmatrix} -18 & 9 & 10 & 9 & 18 & 3 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -57 & 24 & 33 & 24 & 57 & 10 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \mathbf{y}_n$$

and

$$\mathbf{y}_{n+1} = \mathbf{y}_{n+1}^{(0)} + \begin{bmatrix} -95/288 \\ +3/160 \\ -11/1440 \\ -1 \\ 0 \\ 0 \end{bmatrix} F.$$

The matrix $S = (I + \mathbf{1}\epsilon_k^T)B$ is of order 6 and has 5 eigenvalues equal to zero (referred to as nonprincipal eigenvalues) and one eigenvalue equal to one (referred to as the principal eigenvalue).

Because of the additional nonzero terms in $\mathbf{1}$, the definition of \mathbf{y}_n by (2.4) is no longer adequate. It can be re-expressed verbally by saying that \mathbf{y}_n is the vector of function values and derivatives given by (2.4) *as evaluated at* x_n . \mathbf{y}_n is precisely defined by (2.7) and (2.9).

3. Equivalent Methods. The modified multistep method presented in the last section can be shown to converge, but there are legitimate questions concerning its accuracy and stability for nonzero $h\partial f/\partial y$. These will be answered in this section by showing that the method is equivalent to the $(2k - 1)$ step Adams' predictor-corrector method.

It is convenient to view the algorithm in the following manner: The vector \mathbf{y}_n consists of the saved information that represents the total knowledge of the function at x_n . Using this information, the function is extrapolated to the point x_{n+1} by a method that can be chosen to be exact for any desired set of functions, for example polynomials of degree $2k - 1$. This extrapolation is specified by $\mathbf{y}_{n+1}^{(0)} = B\mathbf{y}_n$. This process alone cannot be stable because no account is taken of the differential equation. Therefore, it must be stabilized by use of the differential equation $F = hy' - hf(x, y)$. If the extrapolation is exact, then $F(\mathbf{y}_{n+1}^{(0)}) = 0$ so that any multiple of F may be added to $\mathbf{y}_{n+1}^{(0)}$ without changing it. $F(\mathbf{y}_{n+1}^{(0)})$ is the amount by which the extrapolated value fails to satisfy the differential equation locally. Hopefully, $\mathbf{1}$ can be chosen to both make the process stable and increase the degree of the method.

In this view, \mathbf{y} is a representation in some coordinate system of a member of the class of functions used in extrapolation, typically the class of polynomials of degree $2k - 1$. The class can equally well be represented with respect to another coordinate set by a linear transformation. Let Q be any nonsingular $2k \times 2k$ matrix and define

$$\mathbf{a} = Q\mathbf{y}.$$

Then the method given by (2.7) and (2.9) can be transformed into

$$(3.1) \quad \mathbf{a}_{n+1}^{(0)} = A\mathbf{a}_n \quad \text{and}$$

$$(3.2) \quad \mathbf{a}_{n+1}^{(m+1)} = \mathbf{a}_{n+1}^{(m)} + \mathbf{k}G(\mathbf{a}_{n+1}^{(m)}),$$

$$\mathbf{a}_{n+1} = \mathbf{a}_{n+1}^{(M)},$$

where $A = QBQ^{-1}$, $\mathbf{k} = Q\mathbf{l}$ and $G(\boldsymbol{\alpha}) = F(Q^{-1}\boldsymbol{\alpha})$.

Eqs. (3.1) and (3.2) give a method equivalent to (2.7) and (2.9) in the sense that equivalent methods give equivalent results from equivalent starting conditions in the absence of round-off errors. Thus the class of methods equivalent to any k -step method is given by the class of nonsingular transformations of $2k$ space. In particular, instead of the vector \mathbf{y}_n as a representation of a degree $(2k - 1)$ polynomial, the vectors

$$\mathbf{z}_n^T = \{y'_n, hy'_n, hy'_{n-1}, \dots, hy'_{n-2k+2}\}$$

and

$$\mathbf{a}_n^T = \{y_n, hy'_n, h^2y''_n/2!, h^3y'''_n/3!, \dots, h^{2k-1}y^{(2k-1)}/(2k - 1)!\}$$

can be used. When the appropriate transformation is made, methods equivalent to the k -step modified multistep method are obtained. If the particular modified multistep used has zero nonprincipal eigenvalues and degree $2k$, then the transformed methods have the same properties. In this case, the representation by the vector \mathbf{z} must lead to Adams' method where the $(2k - 1)$ th order predictor and $2k$ th order corrector is used, while the method using the vector \mathbf{a} as a representation must be Nordsieck's method, since these are the unique methods with the given properties.

The common property of each of these methods is that they save $2k$ items of information, whereas the modified method is a k -step procedure and Adams' method is a $(2k - 1)$ -step procedure. It is therefore convenient to classify methods not by the number of steps but by the number of values saved. Thus there are k -value methods for any $k > 0$ with any set of nonprincipal eigenvalues and for even k there are equivalent $k/2$ -step methods.

4. Higher-Order Equations and the Choice of Method. The question of which method to use for a given problem can now be broken into two questions. Firstly, which class of equivalent methods are most desirable. This choice determines the truncation error of the procedure so can only be answered when a specific problem is being discussed. Secondly, which member of a class is the best representative. This choice affects the round-off error and the amount of computation. Before answering the latter question we will look at the general initial value problem given in the Eqs. (1.1) since it will be claimed that the Nordsieck or N -method becomes particularly advantageous in the case of higher-order equations.

For each dependent variable y_i choose the representation $\mathbf{a}_{i,n} = \{y_{i,n}, hy'_{i,n}, \dots, h^{k_i-1}y_{i,n}^{(k_i-1)}/(k_i-1)!\}^T$, where T is the transpose operator. Extrapolate each dependent variable by suitable $k_i \times k_i$ matrices A_i to get

$$(4.1) \quad \mathbf{a}_{i,n+1}^{(0)} = A_i\mathbf{a}_{i,n}.$$

Write the differential equations as

$$F_i(\mathbf{a}_j) = h^{p_i} \{y_i^{(p_i)} - f_i(x, y_1, \dots, y_s^{(p_s-1)})\} / p_i! = 0.$$

If the extrapolation is correct, then the $F_i(\mathbf{a}_{j,n+1})$ are zero so that arbitrary multiples of F_i can be added to the predicted values of $\mathbf{a}_{i,n+1}$. Thus the corrector iteration is

$$(4.2) \quad \mathbf{a}_{i,n+1}^{(m+1)} = \mathbf{a}_{i,n+1}^{(m)} + \mathbf{l}_i F_i(\mathbf{a}_{j,n+1}^{(m)}).$$

It can be shown that A_i and \mathbf{l}_i can be picked on the basis of the order p_i of the differential equation for the i th variable only so as to get stable convergent methods.

It should also be noted that a given dependent variable need not be corrected at every step. For example, the j th variable might be corrected every S_j steps. This would be equivalent to using a step size S_j times as large for that variable, in that the function F_j need only be evaluated $1/S_j$ times as often.

Each dependent variable may be separately transformed by nonsingular matrices to get equivalent methods. One advantage of the N -form is the immediate availability of higher-order derivatives for evaluating F_i . In a multistep formulation, the derivatives must be obtained by a numerical differentiation formula, a process which can contribute to round-off errors.

Of the highest-order formulae, three types of methods might be considered as the most useful: Adams, Nordsieck, and the new modified multistep method. A fourth "extreme" that might be considered is to save $k - 1$ function values and one derivative, but it is almost uniformly worse than Adams' method from the point of view of both computation and round-off, so it will not be discussed.

Computationally, except for large values of k , the Nordsieck type method is superior. This is because the multiplications involved in forming $A\mathbf{a}$ can be avoided. In the Adams and M -methods, the matrix contains 2 nontrivial rows, whereas at first sight A contains $k(k + 1)/2$ nonzero elements. However, they form the Pascal triangle:

$$A = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ & 1 & 2 & & k - 1 \\ & & 1 & & \\ 0 & & & & \\ & & & & \\ & & & & k - 1 \\ & & & & 1 \end{bmatrix}.$$

Because of the properties of the triangular numbers the predictor step can be handled without multiplication by:

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"for i: = 0 step 1 until k - 2 do
  forj: = k - 1 step - 1 until i + 1 do
    a[j - 1]: = a[j - 1] + a[j];",

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where $a[j]$ is component j of the vector \mathbf{a} .

Restricting consideration to methods with zero nonprincipal eigenvalues since these are the most likely choices, Table 1 can be constructed. Unless k is large, the

Nordsieck method is superior. It also has computational advantages in step size changing.

If round-off error is significant, then it generally requires less effort to carry additional precision in the Nordsieck method than in any other method. In other multistep methods, each saved value may have to be carried in multiple precision. In Nordsieck, higher-order derivatives are scaled by powers of h and may be expected to decrease in significance, so that they can be saved with correspondingly less precision.

The M -method's only advantage is in starting. If function evaluation is simple, it requires less work to generate $k/2$ initial points.

For general use, this writer recommends the Nordsieck type method, particularly since in the proposed implementation, the only change required for different order equations is in the vector \mathbf{l} . (An interesting question concerns the existence of vectors \mathbf{l} which give rise to stable methods for several different order equations.)

	Multiplications	Additions
Nordsieck	$k + M - 2$	$k(k + 1)/2 + 2M - 2$
Adams	$2k + M - 2$	$2k + 2M - 3$
M -Method	$5k/2 + M - 1$	$5k/2 + 2M - 3$

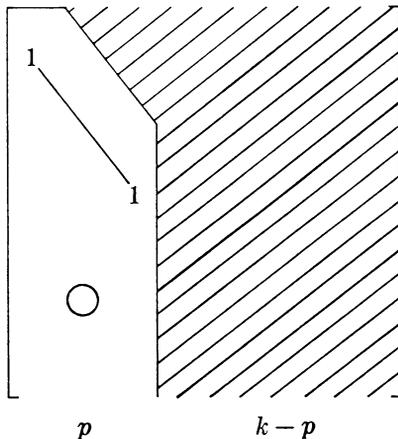
TABLE 1

Number of operations for k -value methods with M corrector iterations

5. Stability and Error. This section states the relevant theorems concerning methods in the Nordsieck formulation. By equivalence, these theorems are also valid for all other formulations. One valuable feature of this formulation is the relative simplicity of the proofs of the theorems. These proofs can be found in Gear [5].

THEOREM 1. *A k -value method of polynomial degree $k - 1$ exists. (This follows directly from the Pascal triangle matrix A .)*

THEOREM 2. *For the Pascal triangle matrix A , a vector \mathbf{l} exists such that the $k - p$ nonprincipal eigenvalues of $S = (I + \mathbf{l}\mathbf{e}_p^T)^M A$ take on any desired set of values in $|z| < 1$, that is S is stable. \mathbf{e}_p^T is the vector with a 1 in position p , so that S takes the form:*



The $p \times p$ principal minor contains the p principal roots equal to 1 for a p th order equation.

The choice of eigenvalues of S takes care of $k - p$ degrees of freedom in $\mathbf{1}$, in fact it determines exactly the last $k - p$ components. The first p can be used to improve the degree of the method.

THEOREM 3. *If the truncation error is suitably defined, the first p components of $\mathbf{1}$ can be chosen to make the degree of the method $k + p - q - 1$ where q is the largest integer such that $\partial f_i / \partial y_i^{(q)} \neq 0$. The integration of p th order equations introduces a factor of h^{-p} in the total truncation error with the result that:*

THEOREM 4. *If the matrices S_i corresponding to the i th variable ($i = 1, \dots, s$) are stable and if the degree of the method for the i th equation is d_i , then the method converges with order $t = \min_{i=1, \dots, s} (d_i - p_i + 1)$ provided that $t \geq 1$.*

Finally, for almost all values of $\mathbf{1}_i$, a truncation error $T_i(x)$ can be defined in terms of the derivatives of the solutions such that the asymptotic form of the error is $h^t e_i(x)$ where

$$e_i^{(p_i)}(x) - \sum_{j=1}^s \sum_{k=0}^{p_j-1} \frac{\partial f_i}{\partial y_j^{(k)}} e_j^{(k)}(x) = T_i(x).$$

6. Numerical Test. The two main contentions of this paper are that the Nord-sieck formulation is superior in general and that it is better to treat higher-order equations directly. The former question rests solely on programming considerations and is treated in Section 4. The latter question may depend on the equation being integrated. One lengthy computational test has been made. The differential equation for the Bessel function $J_{16}(x)$ was integrated for $x = 6(h)6138$ where h took the values $\frac{1}{16}$, $\frac{1}{8}$ and $\frac{1}{4}$ in separate runs. In the first case, it was treated as one second-order equation:

$$F = \frac{h^2}{2} y'' + \frac{h^2}{2} \frac{y'}{x} + \frac{h^2}{2} \left(1 - \frac{256}{x^2}\right) y = 0$$

or

$$F = a_2 + \frac{ha_1}{2x} + \frac{h^2}{2} \left(1 - \frac{256}{x^2}\right) a_0 = 0$$

and in the second case it was treated as the pair of first-order equations:

$$F_1 = hy' - hz \quad \text{and} \quad F_2 = hz' + \frac{hz}{x} + h \left(1 - \frac{256}{x^2}\right) y = 0,$$

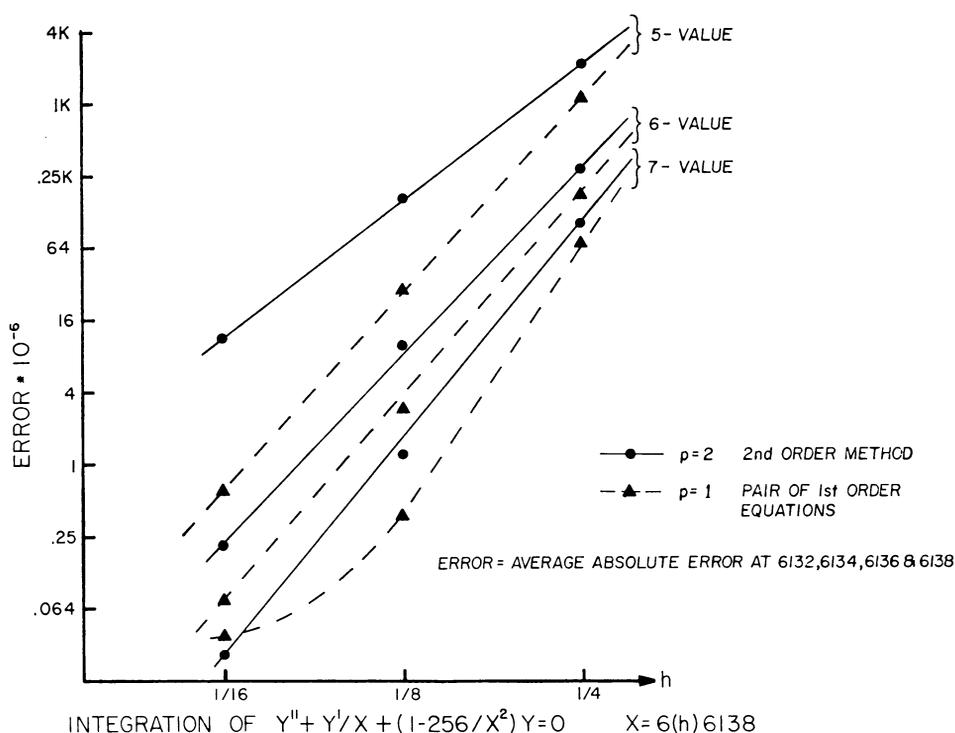
or

$$F_1 = a_{1,1} - ha_{2,0} = 0 \quad \text{and} \quad F_2 = a_{2,1} + \frac{ha_{2,0}}{x} + h \left(1 - \frac{256}{x^2}\right) a_{1,0} = 0.$$

Similar starting procedures were employed in both cases (all higher derivatives were initially set to 0, then 8 steps of $h/16$, and 4 steps each of $h/8$, $h/4$ and $h/2$ were used before a final doubling of the step size to h).

The error, computed as the average of the absolute errors at 6132, 6134, 6136, and 6138, is shown on a log-log graph in Fig. 1 for 5-, 6-, and 7-value methods with zero nonprincipal eigenvalues. These are expected to have order 5, 6 and 7 when $p = 1$ and 4, 5, and 6 when $p = 2$. The 5-value $p = 1$ method does not show this behavior and the $h = \frac{1}{16}$ point on the 7-value $p = 1$ method does not agree with the other two points. The integration was performed on a CDC 3600 in floating-point (about 10-digit precision) so rounding error should be insignificant except possibly in the latter case. The former inconsistency may be due to an unlucky choice of error measurement since it alternates in sign over the integration interval.

The conclusion that can be drawn from the graph is that there is a strong indication that the same-order method for $p = 2$ is more accurate than for $p = 1$. This is a proper comparison since a 6-value method for $p = 2$ requires that a fifth derivative of y be saved, as does a 5-value method for $p = 1$. Further, the amount of work in a $(k + 1)$ -value method for $p = 2$ is less than that in a k -value method for $p = 1$ with two equations, so, in this example at least, additional accuracy was available for less work.



7. Conclusion. There is numerical evidence to suggest that the proposed direct approach to higher order equations is superior to treating a larger first-order system. It has also been argued that the Nordsieck formulation is usually the best for any order method, although in very high-order methods for first-order equations, Adams may be superior. The new modified multistep methods may have an appli-

cation where start up time is a consideration, although these mainly serve to lay to rest the problem of getting around the Dahlquist stability result.

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