

A Class of Single-Step Methods for Systems of Nonlinear Differential Equations

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Summary. The numerical solution of a system of nonlinear differential equations of arbitrary orders is considered. General implicit single-step methods are obtained and some convergence properties studied.

1. Introduction. Consider a system of q nonlinear differential equations, which may be of different orders,

$$(1.1) \quad y_r^{(n_r)}(t) = f_r(t; \mathbf{y}(t)), \quad r = 1(1)q,$$

where

$$\mathbf{y}(t) \equiv \{y_p^{(n_p-m)}(t)\} = (y_1^{(0)}(t), \dots, y_1^{(n_1-1)}(t); \dots; y_q^{(0)}(t), \dots, y_q^{(n_q-1)}(t))$$

is a point in the real Euclidean N -space R_N ,

$$N = \sum_{r=1}^q n_r.$$

It is assumed that initial conditions, $\mathbf{y}(x)$, are given for some value, x , of the real variable t , and that approximations $\bar{\mathbf{y}}(x+h)$, to the values $\mathbf{y}(x+h)$, are to be determined for some specified step length h .

Let

$$\mu_i, \quad \alpha_{ri}^{[\nu]}, \quad \lambda_{rij}^{[\nu]}, \quad i, j = 1(1)s, \quad r = 1(1)q, \quad \nu = 1(1)n_r,$$

be a set of arbitrary bounded parameters independent of the chosen step length h . Introduce the additional fixed parameters $\mu_0 = 0$, $\mu_{s+1} = 1$, and for a given step length define abscissae

$$x_i = x + \mu_i h, \quad i = 0(1)s + 1,$$

and hence a closed interval (a, b) ,

$$a = \min_{i=0(1)s+1} \{x_i\}, \quad b = \max_{i=0(1)s+1} \{x_i\}.$$

Now let \mathbf{w} be a point in R_N ,

$$\mathbf{w} = \{w_p^{[m]}\} = (w_1^{[n_1]}, \dots, w_1^{[1]}; \dots; w_q^{[n_q]}, \dots, w_q^{[1]}),$$

where the element $w_p^{[m]}$ of \mathbf{w} corresponds to the element $y_p^{(n_p-m)}(t)$ of $\mathbf{y}(t)$. For a particular initial value problem we are concerned with a restricted set of points $\mathbf{w} \in R_N$, and this applies also to any numerical method for determining approximations, $\bar{\mathbf{y}}(x+h)$. Thus, consider a convex (finite) domain, D , of R_N . We assume that the functions $f_r(t; \mathbf{w})$ are single-valued mappings of R_{N+1} onto R_1 , which satisfy

the Lipschitz conditions,

$$(1.2) \quad |f_r(t; \mathbf{w}') - f_r(t; \mathbf{w}'')| \leq L \|\mathbf{w}' - \mathbf{w}''\|, \quad r = 1(1)q,$$

for any pair of values $\mathbf{w}', \mathbf{w}'' \in D$, and any t in (a, b) . Here L is a positive constant and $\|\mathbf{w}\|, \mathbf{w} \in D$, denotes the norm,

$$\|\mathbf{w}\| = \max_{\rho, m} |w_\rho^{[m]}|, \quad \rho = 1(1)q, \quad m = 1(1)n_\rho.$$

Then the initial-value problem has a unique solution in (a, b) [1]. It is further assumed that for some nonnegative integer, \mathbf{p} , the derivatives

$$y_r^{(n_r + \mathbf{p})}(t), \quad r = 1(1)q,$$

are continuous in (a, b) . From now on we restrict attention to problems satisfying these various conditions.

Definition (1.1). For $r = 1(1)q, \nu = 1(1)n_r$, define

$$T_r^{[\nu]}(\mu_i h) = \sum_{\tau=0}^{\nu-1} \frac{(\mu_i h)^\tau}{\tau!} y_r^{(n_r - \nu + \tau)}(x), \quad i = 1(1)s + 1,$$

$$k_{ri}(h) = f_r(x_i; \{k_{\rho i}^{[m]}(h)\}), \quad i = 1(1)s,$$

where

$$k_{ri}^{[\nu]}(h) = T_r^{[\nu]}(\mu_i h) + \frac{(\mu_i h)^\nu}{\nu!} \sum_{j=1}^s \lambda_{rij}^{[\nu]} k_{rj}(h), \quad i = 1(1)s.$$

Then an s stage single-step process which provides approximations to $\mathbf{y}(x + h)$, may be defined by

$$\bar{y}_r^{(n_r - \nu)}(x + h) = T_r^{[\nu]}(h) + \frac{h^\nu}{\nu!} \sum_{i=1}^s \alpha_{ri}^{[\nu]} k_{ri}(h), \quad r = 1(1)q, \quad \nu = 1(1)n_r.$$

This defines a class of methods. We consider subclasses defined by restraints imposed on the allowed parameter values.

This definition is a simple extension of the standard process of Runge-Kutta type [2] along the lines developed by Zurmühl [3]. There are some minor modifications which appear to lead to somewhat simpler formulae and which indicate the nature of the process. Indeed, we can define

$$(1.3) \quad \lambda_{r, s+1, j}^{[\nu]} = \alpha_{rj}^{[\nu]}, \quad r = 1(1)q, \quad \nu = 1(1)n_r, \quad j = 1(1)s.$$

In a previous article this single-step process was examined for a single linear differential equation of order n and the results obtained there suggested the present approach [4]. For explicit methods, where

$$\lambda_{rij}^{[\nu]} = 0, \quad j \geq i, \quad i, j = 1(1)s, \quad r = 1(1)q, \quad \nu = 1(1)n_r,$$

the determination of the functions $k_{ri}(h), i = 1(1)s, r = 1(1)q$, presents no particular difficulty, since we have merely to evaluate the functions $f_r(t; \mathbf{w}), r = 1(1)q$, for a sequence of known values of t and \mathbf{w} . For implicit processes, however, the functions have, in general, to be evaluated by iterative techniques.

Definition (1.2). Let

$$\Delta y_r^{(n_r-\nu)}(h) = \frac{h^{n_r-\nu}}{(n_r-\nu)!} [y_r^{(n_r-\nu)}(x+h) - T_r^{[\nu]}(h)], \quad r = 1(1)q, \quad \nu = 1(1)n_r,$$

$$\binom{\tau}{\nu} = \frac{\tau!}{\nu!(\tau-\nu)!}.$$

Consider a subclass of methods. If there exist a positive constant Y and a nonnegative integer \mathbf{p} such that for each method,

$$E_{sr}^{[\nu]}(h) \equiv \left| \Delta y_r^{(n_r-\nu)}(h) - \frac{h^{n_r}}{n_r!} \binom{n_r}{\nu} \sum_{i=1}^s \alpha_{ri}^{[\nu]} k_{ri}(h) \right| \leq Y|h|^{n_r+\mathbf{p}},$$

$$r = 1(1)q, \quad \nu = 1(1)n_r,$$

holds for all sufficiently small h , then the subclass is said to be of order \mathbf{p} . Alternatively we write

$$E_{sr}^{[\nu]}(h) = O(h^{n_r+\mathbf{p}}).$$

We state conditions which restrict the allowed values of the parameters of an s stage process and show that these conditions are sufficient for this subclass of methods to be of order \mathbf{p} . In a series of articles [5], [6], [7], Butcher has examined a single-step process of this type for a system of first-order equations. The conditions obtained here reduce to some particular results obtained by Butcher, which give implicit methods. On the other hand our present approach is more general in that a system of equations of arbitrary orders is considered and the independent variable may enter explicitly into the functional forms.

The present approach leads naturally to a discussion of convergence and error bounds. Again for a system of first-order equations, Butcher has dealt with the convergence and stability of single- and multi-step methods in a general context [8]. Our results illustrate clearly the connection between single- and multi-step methods, and the techniques used provide a useful approach to various problems of convergence and error estimation.

2. Parameter Constraints. The following elementary result is the basis of subsequent developments.

LEMMA (2.1). *If*

$$(2.1) \quad \mu_i^\tau = \binom{\nu + \tau}{\tau} \sum_{j=1}^s \mu_j^\tau \lambda_{rij}^{[\nu]},$$

$r = 1(1)q, \nu = 1(1)n_r, i = 1(1)s, \tau = 0(1)\mathbf{p} - \nu - 1$, then

$$y_r^{(n_r-\nu)}(x_i) = T_r^{[\nu]}(\mu_i h) + \frac{(\mu_i h)^\nu}{\nu!} \sum_{j=1}^s \lambda_{rij}^{[\nu]} y_r^{(n_r)}(x_j) + \psi_{ri}^{[\nu]}(h)$$

where for $\mathbf{p} > \nu$,

$$\psi_{ri}^{[\nu]}(h) = \frac{h^\mathbf{p}}{\mathbf{p}!} \left[\mu_i^\mathbf{p} y_r^{(n_r+\mathbf{p}-\nu)}(x + \theta_{ri}^{[\nu]} \mu_i h) - \binom{\mathbf{p}}{\nu} \mu_i^\nu \right. \\ \left. \times \sum_{j=1}^s \mu_j^{\mathbf{p}-\nu} \lambda_{rij}^{[\nu]} y_r^{(n_r+\mathbf{p}-\nu)}(x + \theta_{rj}^{[0]} \mu_j h) \right],$$

and for $\mathbf{p} \leq \nu$,

$$\begin{aligned} \psi_{ri}^{[\nu]}(h) &= \frac{(\mu_i h)^{\mathbf{p}}}{\mathbf{p}!} y_r^{(n_r+\mathbf{p}-\nu)}(x + \theta_{ri}^{[\nu]} \mu_i h) - \sum_{\tau=\mathbf{p}}^{\nu-1} \frac{(\mu_i h)^\tau}{\tau!} y_r^{(n_r-\nu+\tau)}(x) - \frac{(\mu_i h)^\nu}{\nu!} \\ &\quad \times \sum_{j=1}^s \lambda_{rij}^{[\nu]} y_r^{(n_r)}(x_j), \quad 0 < \theta_{ri}^{[\nu]}, \theta_{ri}^{[0]} < 1. \end{aligned}$$

Proof. Since the derivatives, $y_r^{(p)}(t)$, $r = 1(1)q$, $p = 0(1)n_r + \mathbf{p}$, are assumed continuous in (a, b) , Taylor's theorem, with Lagrange's remainder form, gives

$$y_r^{(n_r-\nu)}(x_i) = \sum_{\tau=0}^{\mathbf{p}-1} \frac{(\mu_i h)^\tau}{\tau!} y_r^{(n_r-\nu+\tau)}(x) + \frac{(\mu_i h)^{\mathbf{p}}}{\mathbf{p}!} y_r^{(n_r-\nu+\mathbf{p})}(x + \theta_{ri}^{[\nu]} \mu_i h),$$

$0 < \theta_{ri}^{[\nu]} < 1$, $i = 1(1)s$, $r = 1(1)q$, $\nu = 0(1)n_r$. The result follows on applying Eqs. (2.1) and Definition (1.1).

It is convenient to collect together some notation.

Definition (2.1). For $r = 1(1)q$, $\nu = 1(1)n_r$, $i, j = 1(1)s$, define positive elements,

$$\begin{aligned} \epsilon_{ri} &= |y_r^{(n_r)}(x_i) - k_{ri}(h)|, \quad \epsilon_i = \max_r \{\epsilon_{ri}\}, \\ \psi_i &= \max_{r,\nu} |L\psi_{ri}^{[\nu]}(h)|, \quad \psi = \max_i \{\psi_i\}, \\ z_{ij} &= \max_{r,\nu} \left| L \frac{(\mu_i h)^\nu}{\nu!} \lambda_{rij}^{[\nu]} \right|, \quad z = \max_{i,j} \{z_{ij}\}. \end{aligned}$$

The following theorem is the fundamental result of this article.

THEOREM (2.1). *If Eqs. (2.1) are satisfied then*

$$k_{ri}(h) = y_r^{(n_r)}(x_i) + O(h^{\mathbf{p}}),$$

and for $z \leq 1/2s$, $\epsilon_i \leq 2\psi$, $r = 1(1)q$, $i = 1(1)s$.

Proof. From Definition (1.1) and Eq. (1.1), we obtain, on applying the Lipschitz conditions (1.2) and Lemma (2.1),

$$\begin{aligned} |y_r^{(n_r)}(x_i) - k_{ri}(h)| &\leq \max_{\rho,m} \left| L\psi_{\rho i}^{[m]}(h) + \frac{(\mu_i h)^m}{m!} L \sum_{j=1}^s \lambda_{\rho ij}^{[m]} \{y_\rho^{(n_\rho)}(x_j) - k_{\rho j}(h)\} \right|, \\ r, \rho &= 1(1)q, \quad m = 1(1)n_\rho, \quad i = 1(1)s. \end{aligned}$$

Then Definition (2.1) gives

$$\epsilon_i \leq \psi_i + \sum_{j=1}^s z_{ij}\epsilon_j, \quad i = 1(1)s.$$

This may be regarded as a matrix inequality,

$$\begin{aligned} (\mathbf{I} - \mathbf{Z})\boldsymbol{\epsilon} &\leq \boldsymbol{\psi}, \\ \boldsymbol{\epsilon}^T &= (\epsilon_1, \dots, \epsilon_s), \quad \boldsymbol{\psi}^T = (\psi_1, \dots, \psi_s). \end{aligned}$$

Here \mathbf{I} is the identity matrix and \mathbf{Z} is the $s \times s$ square matrix with elements z_{ij} , $i, j = 1(1)s$. Since the parameters of the single-step process are assumed to be bounded and independent of h , these elements may be made arbitrarily small by a suitable choice of the step length. Thus for all sufficiently small h ,

$$(2.2) \quad 1 - \sum_{j=1}^s z_{ij} > 0, \quad i = 1(1)s,$$

and the matrix $\mathbf{I} - \mathbf{Z}$ is monotonic. In particular, the solution of the matrix equation

$$(\mathbf{I} - \mathbf{Z})\boldsymbol{\epsilon}^* = \boldsymbol{\psi}, \quad \boldsymbol{\epsilon}^{*T} = (\epsilon_1^*, \dots, \epsilon_s^*),$$

is then such that $\epsilon_i^* \geq \epsilon_i, i = 1(1)s$, [9, pp. 43–47]. Now the elements z_{ij} are positive, and so it follows from (2.2) that all the eigenvalues of \mathbf{Z} are of modulus less than unity and hence that the inverse matrix of $\mathbf{I} - \mathbf{Z}$ is given by

$$(\mathbf{I} - \mathbf{Z})^{-1} = \sum_{\tau=0}^{\infty} \mathbf{Z}^{\tau}, \quad \mathbf{Z}^0 \equiv \mathbf{I},$$

the infinite series converging [10]. This series is majorized by

$$\mathbf{I} + \left[\frac{1}{s} \sum_{\tau=1}^{\infty} (sz)^{\tau} \right] \mathbf{J}$$

where \mathbf{J} is the $s \times s$ matrix with all elements unity. For sufficiently small $h, sz < 1$ and the geometric progression may be summed. Since the elements of $\boldsymbol{\psi}$ are positive we thus obtain

$$\epsilon_i \leq \epsilon_i^* \leq \psi_i + \frac{z}{1 - sz} \sum_{j=1}^s \psi_j, \quad i = 1(1)s,$$

for sufficiently small h . For h so small that

$$z \leq \frac{1}{2s}, \quad \epsilon_i \leq 2\psi, \quad i = 1(1)s,$$

and since $\psi = O(h^p)$, this completes the proof.

The techniques used here are described by Collatz [9, pp. 109–110]. The theorem may be proved by more elementary means, but the present proof appears capable of refinement, leading to less restrictive bounds on the step length.

THEOREM (2.2). *For an s stage single-step method to be of order \mathbf{p} it is sufficient that Eqs. (2.1) and the following equations are satisfied,*

$$(2.3) \quad 1 = \binom{\nu + \tau}{\tau} \sum_{i=1}^s \mu_i^{\tau} \alpha_{ri}^{[\nu]}, \quad r = 1(1)q, \quad \nu = 1(1)n_r, \quad \tau = 0(1)\mathbf{p} - 1.$$

Proof. It has to be shown that

$$E_{sr}^{[\nu]}(h) = O(h^{n_r + \mathbf{p}}), \quad r = 1(1)q, \quad \nu = 1(1)n_r.$$

From Definition (1.2) and Taylor's theorem,

$$\begin{aligned} \Delta y_r^{(n_r - \nu)}(h) &= \sum_{\tau=0}^{\mathbf{p}-1} \binom{n_r + \tau}{n_r - \nu} \frac{h^{n_r + \tau}}{(n_r + \tau)!} y_r^{(n_r + \tau)}(x) \\ &\quad + \binom{n_r + \mathbf{p}}{n_r - \nu} \frac{h^{n_r + \mathbf{p}}}{(n_r + \mathbf{p})!} y_r^{n_r + \mathbf{p}}(x + \theta_r^{[\nu]}h), \\ &\quad 0 < \theta_r^{[\nu]} < 1, \quad r = 1(1)q, \quad \nu = 1(1)n_r. \end{aligned}$$

Taylor's theorem and Eqs. (2.3) give

$$\begin{aligned} \frac{h^{n_r}}{n_r!} \binom{n_r}{\nu} \sum_{i=1}^s \alpha_{r i}^{[\nu]} y_r^{(n_r)}(x_i) &= \sum_{\tau=0}^{p-1} \binom{n_r + \tau}{n_r - \nu} \frac{h^{n_r + \tau}}{(n_r + \tau)!} y_r^{(n_r + \tau)}(x) \\ &+ \binom{n_r + p}{n_r - \nu} \frac{h^{n_r + p}}{(n_r + p)!} \binom{\nu + p}{p} \sum_{i=1}^s \mu_i^p \alpha_{r i}^{[\nu]} y_r^{(n_r + p)}(x + \theta_{r i}^{[0]} \mu_i h), \\ 0 < \theta_{r i}^{[0]} < 1, \quad r = 1(1)q, \quad \nu = 1(1)n_r, \quad i = 1(1)s, \end{aligned}$$

and so from Definition (2.1),

$$\begin{aligned} E_{s r}^{[\nu]}(h) &\leq \frac{|h|^{n_r}}{n_r!} \binom{n_r}{\nu} \sum_{i=1}^s |\alpha_{r i}^{[\nu]}| \epsilon_{r i} + \binom{n_r + p}{n_r - \nu} \frac{|h|^{n_r + p}}{(n_r + p)!} \\ &\times \left| y_r^{(n_r + p)}(x + \theta_r^{[\nu]} h) - \binom{\nu + p}{p} \sum_{i=1}^s \mu_i^p \alpha_{r i}^{[\nu]} y_r^{(n_r + p)}(x + \theta_{r i}^{[0]} \mu_i h) \right|. \end{aligned}$$

From Theorem (2.1), $\epsilon_{r i} = O(h^p)$, and so this theorem is proved.

Since a bound was obtained for the elements, $\epsilon_{r i}$, in Theorem (2.1), this proof provides bounds for the errors $y_r^{(\nu)}(x + h) - \bar{y}_r^{(\nu)}(x + h)$, $r = 1(1)q$, $\nu = 0(1)n_r - 1$. These bounds will usually be poor estimates and in any case only apply for a restricted range of permissible values of h . By refining the Lipschitz conditions and the argument of Theorem (2.1), these bounds can be relaxed.

Theorem (2.2) provides a subclass of implicit methods. Thus the equations defining $k_{r i}(h)$, $r = 1(1)q$, $i = 1(1)s$, (Definition (1.1)) have in general to be solved iteratively. The functions $f_r(t; \mathbf{w})$, $r = 1(1)q$, may be regarded as mappings, in a complete metric space, which satisfy Lipschitz conditions, and it is a consequence that for sufficiently small h these equations have a unique solution which may be determined iteratively [11]. Define ‘iterates’,

$$\begin{aligned} k_{r i}^{[\nu, \tau]}(h) &= T_r^{[\nu]}(\mu_i h) + \frac{(\mu_i h)^\nu}{\nu!} \sum_{j=1}^s \lambda_{r i j}^{[\nu]} k_{r j}^{(\tau)}(h), \quad i = 1(1)s, \quad r = 1(1)q, \\ &\nu = 1(1)n_r, \quad \tau = 0, 1, \dots \end{aligned}$$

Then a possible iterative procedure is

$$k_{r i}^{(\tau+1)}(h) = f_r(x_i; \{k_{\rho i}^{[m, \tau]}\}), \quad i = 1(1)s, \quad r = 1(1)q, \quad \tau = 0, 1, \dots$$

Incidentally, Theorem (2.1) suggests starting values,

$$k_{r i}^{(0)}(h) = y_r^{(n_r)}(x), \quad i = 1(1)s, \quad r = 1(1)q.$$

An interesting feature of the derivation of these implicit methods is that no assumptions are required concerning the derivatives of $f_r(t; \mathbf{w})$, $r = 1(1)q$, except at the point $\mathbf{w} = \mathbf{y}$.

Equations (2.3) relate these implicit methods to quadrature methods, for

$$(2.4) \quad \int_0^1 \mu^\tau (1 - \mu)^{\nu-1} d\mu = \frac{1}{\nu} \sum_{j=1}^s \alpha_{r j}^{[\nu]} \mu_j^\tau.$$

Since $k_{r i}(h) = y_r^{(n_r)}(x_i) + O(h^p)$, we have (apart from error terms)

$$\int_0^1 y_r^{(n_r)}(x + \mu h) (1 - \mu)^{\nu-1} d\mu = \frac{1}{\nu} \sum_{j=1}^s \alpha_{r j}^{[\nu]} y_r^{(n_r)}(x_j) = \frac{1}{\nu} \sum_{j=1}^s \alpha_{r j}^{[\nu]} k_{r j}(h)$$

and integration by parts gives

$$\Delta y_r^{(n_r-\nu)}(h) = \frac{h^{n_r}}{n_r!} \binom{n_r}{\nu} \sum_{j=1}^s \alpha_{rj}^{[\nu]} y_r^{(n_r)}(x_j) .$$

Exact results are thus obtained if the solutions $y_r^{(0)}(x + \mu h)$, $r = 1(1)q$, are polynomials in μ of degree less than \mathbf{p} . For then the error terms vanish (Lemma (2.1)).

In a previous article [4] the solution of equations of the type (2.1), (2.3), was considered. It was pointed out that, by selecting distinct abscissae, μ_i , $i = 1(1)s$, the other parameters can be determined by solving sets of matrix equations, with the same matrix of coefficients, to give methods of order at least $\mathbf{p} = s$. It is convenient to only consider parameters independent of r . As described in [4], Theorem (2.1) and Lemma (2.1) provide ways to automatically estimate the error. Thus it seems possible to fully automate a procedure for solving an arbitrary system of nonlinear differential equations.

By choosing as abscissae the zeros of the Legendre polynomial $P_s(2\mu - 1)$, Eqs. (2.4) and hence (2.3), can be satisfied for $\mathbf{p} = 2s + 1 - n$, $n = \max \{n_r\}$, and thus the maximum attainable order of these implicit processes is $\mathbf{p}_{\max} \leq 2s + 1 - n$, $s \geq n$, [4]. It seems likely that the maximum order can be attained and this can certainly be achieved when $s \leq n$. Indeed, Butcher has shown that this is so generally for a system of first-order equations [7]. It appears that we can do rather better than this if we only wish to compute some of the values $\bar{y}_r^{(\nu)}(x + h)$. Thus if we have only to determine the values $\bar{y}_r^{(0)}(x + h)$, $r = 1(1)q$, Eqs. (2.4) need only be satisfied for $\nu = n_r$. Assume that $n_r = n$, $r = 1(1)q$. Then by taking as abscissae the zeros of the orthogonal polynomial of degree s , associated with the weight function $(1 - \mu)^{n-1}$ and the interval $(0, 1)$, we have $\mathbf{p}_{\max} \leq 2s$.

For methods of maximum order Eqs. (2.1) are not generally satisfied with $\mathbf{p} = \mathbf{p}_{\max}$. Indeed, $\mathbf{p} \leq s + 1$ and a more detailed analysis is required.

3. A Convergence Problem. A rather unusual type of convergence (for single-step methods) is examined here. A single step of fixed length h is considered and conditions obtained such that

$$\lim_{s \rightarrow \infty} E_{sr}^{[\nu]}(h) = 0, \quad r = 1(1)q, \quad \nu = 1(1)n_r .$$

It is not clear, however, whether these conditions can be met.

Definition (3.1). For $r = 1(1)q$, $\nu = 1(1)n_r$, $i, j = 1(1)s$, define for all s ,

$$\begin{aligned} \mu &= \max_i |\mu_i|, & \bar{\mu} &= \max_s \{\mu\}, \\ \alpha &= \max_{r,\nu,i} |\alpha_{ri}^{[\nu]}|, & \lambda &= \max_{r,\nu,i,j} |\lambda_{rij}^{[\nu]}|, \end{aligned}$$

where μ, α, λ , depend on s .

Consider implicit methods of the type derived in Section 2. Let c be a fixed positive constant. We assume that there exists a sequence of methods of increasing order \mathbf{p} , $s \leq \mathbf{cp}$, such that

- (i) $\bar{\mu}$ is bounded,
- (ii) there exist constants, $\alpha^* \geq 1, \bar{\lambda}$, so that for all s , $\alpha \leq (\alpha^*)^s, \lambda \leq \bar{\lambda}/s$.

We further assume that

- (iii) for some constant $\omega, \omega \geq 1$, and all \mathbf{p} ,

$$|y_r^{(p)}(t)| \leq \omega^p, \quad r = 1(1)q, \quad t \in (a, b).$$

The interval (a, b) depends on the step length h and is finite, so that this bound is not severe. Indeed, the only bound that is difficult to satisfy is that on λ . For Eqs. (2.1), with $\tau = 0$, give $\lambda \geq 1/s$. As previously remarked, we can readily obtain sequences of methods of increasing order $\mathbf{p} \leq s$ ($0 < c \leq 1$).

THEOREM (3.1). *Assume that there exists a sequence of methods of increasing order \mathbf{p} , $s \leq \mathbf{c}\mathbf{p}$, such that (i), (ii) are satisfied. For a step length h such that*

$$1 \geq 2L\bar{\lambda}\bar{\mu}|h|e^{\bar{\mu}|h|},$$

and such that the bounds (iii) are satisfied,

$$\lim_{s \rightarrow \infty} E_{sr}^{[\nu]}(h) = 0, \quad r = 1(1)q, \quad \nu = 1(1)n_r.$$

Proof. From Definition (2.1) the bound on h gives $z \leq 1/2s$, so that the analysis of Theorem (2.1) applies and $\epsilon_i \leq 2\psi$, $i = 1(1)s$. Thus from the proof of Theorem (2.2) and Lemma (2.1),

$$E_{sr}^{[\nu]} \leq \omega_{r\mathbf{p}} = \frac{\mathbf{p}|h|^{n_r+\mathbf{p}} \omega^{n+\mathbf{p}}}{(\mathbf{p} - n)!} [1 + c(\bar{\alpha}\bar{\mu})^{\mathbf{p}}\{1 + 2L(1 + \bar{\lambda})\}]$$

for $\mathbf{p} > n$, $n = \max \{n_r\}$, $\bar{\alpha} = (\alpha^*)^c$. For all sufficiently large p ,

$$\omega_{r,p+1} < d\omega_{rp}, \quad d < 1,$$

and the required result follows.

Here the bound on λ depends on that for z and, although the results of Theorem (2.1) can be sharpened, the dependence on s seems essential. It seems unlikely that such sequences of methods can be obtained. We have *not* shown that *other* sequences of methods do not converge.

4. Stability and Convergence. Here we treat the problem of stability and the related (conventional) convergence problem. Consider a fixed step length, H . We wish to determine approximations, $\bar{y}_r^{(\nu)}(x' + H)$, to the values $y_r^{(\nu)}(x' + H)$, $r = 1(1)q$, $\nu = 0(1)n_r - 1$, by applying a particular single-step method to a sequence of subintervals of $(0, H)$. Thus, the errors at $x' + H$ will be due to the *accumulation* of truncation errors from step to step.

Definition (4.1). *Define abscissae,*

$$\begin{aligned} x_{\rho i} &= x_{\rho 0} + \mu_i h, & i &= 0(1)s + 1, & \rho &= 0(1)M - 1, \\ x_{00} &= x', & x_{\rho, s+1} &= x_{\rho+1, 0}, & x_{M0} &= x' + H, & Mh &= H. \end{aligned}$$

Further define, for $r = 1(1)q$, 'initial value approximations',

$$\begin{aligned} \bar{y}_r^{(\nu)}(x_{\rho 0}) &= y_r^{(\nu)}(x_{\rho 0}) - \eta_{r\rho}^{[\nu]}, & \rho &= 0(1)M, & \nu &= 0(1)n_r - 1, \\ \bar{T}_r^{[\nu]}(\mu_i h, \rho) &= \sum_{\tau=0}^{\nu-1} \frac{(\mu_i h)^\tau}{\tau!} \bar{y}_r^{(n_r-\nu+\tau)}(x_{\rho 0}), & \rho &= 0(1)M - 1, & \nu &= 1(1)n_r. \end{aligned}$$

Let $\eta_\rho = \max_{r,\nu} |\eta_{r\rho}^{[\nu]}|$, $\rho = 0(1)M$.

We consider a selected method of order \mathbf{p} of the type described in Section 2. To derive these methods we have assumed that the derivatives,

$$y_r^{(n_r + \mathbf{p})}(t), \quad r = 1(1)q,$$

are continuous in a closed interval (a, b) defined with respect to the step length h and the abscissae $\mu_i, i = 1(1)s$. We thus require that there exists a constant γ such that

$$|y_r^{(p)}(t)| \leq \gamma, \quad r = 1(1)q, \quad p = 0(1)n_r + \mathbf{p},$$

for $t \in (a, b)$ for a sequence of intervals (a, b) corresponding to the selected $x_{\rho 0}$.

LEMMA (4.1). *If A, B , are positive constants independent of ρ , such that for some positive integer M*

$$\eta_{\rho+1} \leq A/M + (1 + B/M)\eta_{\rho}, \quad \rho = 0(1)M - 1,$$

then

$$\eta_M \leq [A/B + \eta_0]e^B.$$

Proof. For any value of $\rho, \rho = 0(1)M - 1$,

$$(4.1) \quad \eta_{\rho+1} \leq \frac{A}{M} \sum_{\tau=0}^{\rho} \left(1 + \frac{B}{M}\right)^{\tau} + \left(1 + \frac{B}{M}\right)^{\rho+1} \eta_0.$$

For, this relation holds for $\rho = 0$. Assume it holds for some value of $\rho, 0 \leq \rho < M - 1$. Then

$$\eta_{\rho+2} \leq A/M + (1 + B/M)\eta_{\rho+1},$$

and inserting (4.1) we obtain

$$\eta_{\rho+2} \leq \frac{A}{M} \sum_{\tau=0}^{\rho+1} \left(1 + \frac{B}{M}\right)^{\tau} + \left(1 + \frac{B}{M}\right)^{\rho+2} \eta_0.$$

This completes an inductive proof of (4.1). Thus putting $\rho = M - 1$ in (4.1) and summing the geometric progression we obtain

$$\eta_M \leq [A/B + \eta_0](1 + B/M)^M.$$

Now $e^{B/M} \geq 1 + B/M$, completing the proof.

THEOREM (4.1). *If, for the method selected, $z \leq 1/2s$, and if for each step the initial values used, $\bar{y}_r^{(\nu)}(x_{\rho 0})$, are the approximations obtained from the previous step,*

$$\bar{y}_r^{(\nu)}(x_{\rho-1,0} + h), \quad r = 1(1)q, \quad \nu = 0(1)n_r - 1, \quad \rho = 1(1)M - 1,$$

then for $|h| \leq 1, \mathbf{p} > n, n = \max \{n_r\}$,

$$|y_r^{(\nu)}(x' + H) - \bar{y}_r^{(\nu)}(x' + H)| \leq [A/B + \eta_0]e^B,$$

$$A = (|h|^{\mathbf{p}}/(\mathbf{p} - n)!)|H|\gamma[1 + 3s\alpha\mu^{\mathbf{p}} + 2s^2\alpha\lambda\mu^{\mathbf{p}}], \quad B = |H|(e^{|h|} + 2Ls\alpha e^{\mu|h|}).$$

Proof. For some value of ρ let $x = x_{\rho 0}$. To step from x to $x + h$ we apply a single-step method as given in Definition (1.1), but with $\bar{T}_r^{[\nu]}(\mu_i h, \rho)$ replacing $T_r^{[\nu]}(\mu_i h)$, $i = 1(1)s + 1, r = 1(1)q, \nu = 1(1)n_r$. From Lemma (2.1) we have

$$\begin{aligned} y_r^{(n_r - \nu)}(x_{\rho i}) &= \bar{T}_r^{[\nu]}(\mu_i h, \rho) + \frac{(\mu_i h)^{\nu}}{\nu!} \sum_{j=1}^s \lambda_{r ij}^{[\nu]} y_r^{(n_r)}(x_{\rho j}) \\ &\quad + \psi_{ri}^{[\nu]}(h, \rho) + \sum_{\tau=0}^{\nu-1} \frac{(\mu_i h)^{\tau}}{\tau!} \eta_{r\rho}^{[n_r - \nu + \tau]} \end{aligned}$$

$i = 1(1)s, r = 1(1)q, \nu = 1(1)n_r$. For $z \leq 1/2s$, Theorem (2.1) carries over, and using Definition (3.1)

$$\epsilon_{ri} \leq \epsilon_i \leq 2\psi + 2e^{\mu|h|}L\eta_\rho,$$

and from Lemma (2.1) we obtain for $\mathbf{p} > n$,

$$(4.2) \quad \epsilon_{ri} \leq \epsilon_i \leq |h|^{\mathbf{p}} \frac{2\gamma\mu^{\mathbf{p}}}{(\mathbf{p} - n)!} (1 + s\lambda) + 2e^{\mu|h|}L\eta_\rho.$$

We have

$$\begin{aligned} \eta_{r,\rho+1}^{[n_r-\nu]} &= y_r^{(n_r-\nu)}(x+h) - \bar{y}_r^{(n_r-\nu)}(x+h) \\ &= y_r^{(n_r-\nu)}(x+h) - \frac{h^\nu}{\nu!} \sum_{i=1}^s \alpha_{ri}^{[\nu]} y_r^{(n_r)}(x_{\rho i}) - T_r^{[\nu]}(h) \\ &\quad + \sum_{\tau=0}^{\nu-1} \frac{h^\tau}{\tau!} \eta_{r\rho}^{[n_r-\nu+\tau]} + \frac{h^\nu}{\nu!} \sum_{i=1}^s \alpha_{ri}^{[\nu]} \{y_r^{(n_r)}(x_{\rho i}) - k_{ri}(h)\}. \end{aligned}$$

Proceeding as in the proof of Theorem (2.2) we obtain

$$(4.3) \quad \begin{aligned} \eta_{r,\rho+1}^{[n_r-\nu]} &= \frac{h^{\nu+\mathbf{p}}}{(\nu + \mathbf{p})!} \left[y_r^{(n_r+\mathbf{p})}(x + \theta_r^{[\nu]}h) - \binom{\nu + \mathbf{p}}{\mathbf{p}} \sum_{i=1}^s \alpha_{ri}^{[\nu]} \mu_i^{\mathbf{p}} y_r^{(n_r+\mathbf{p})}(x + \theta_{ri}^{[0]} \mu_i h) \right] \\ &\quad + \sum_{\tau=0}^{\nu-1} \frac{h^\tau}{\tau!} \eta_{r\rho}^{[n_r-\nu+\tau]} + \frac{h^\nu}{\nu!} \sum_{i=1}^s \alpha_{ri}^{[\nu]} \{y_r^{(n_r)}(x_{\rho i}) - k_{ri}(h)\}. \end{aligned}$$

Since this relation holds for $r = 1(1)q, \nu = 1(1)n_r$, we have for $|h| \leq 1$,

$$\eta_{\rho+1} \leq |h|^{\mathbf{p}+1} \frac{\gamma}{\mathbf{p}!} (1 + s\alpha\mu^{\mathbf{p}}) + \eta_\rho(1 + |h|e^{|h|}) + |h|\alpha \sum_{i=1}^s \epsilon_i.$$

Thus, for $\mathbf{p} > n, |h| \leq 1, \rho = 0(1)M - 1$,

$$\eta_{\rho+1} \leq \frac{|h|^{\mathbf{p}+1}\gamma}{(\mathbf{p} - n)!} [1 + 3s\alpha\mu^{\mathbf{p}} + 2s^2\alpha\lambda\mu^{\mathbf{p}}] + \eta_\rho[1 + |h|(e^{|h|} + 2Ls\alpha e^{\mu|h|})].$$

Since $M|h| = |H|$ Lemma (4.1) can be applied to complete the proof.

The result can be easily extended and refined. Thus the restrictions $\mathbf{p} > n, |h| \leq 1$, are not necessary. Different step lengths $h_\rho, \rho = 0(1)M - 1$, can be considered and methods of differing orders applied. The essential restriction is $z \leq 1/2s$, and for sufficiently large M this can always be achieved.

COROLLARY.

$$\lim_{M \rightarrow \infty} \eta_M \leq \lim_{M \rightarrow \infty} \left[\frac{A}{B} + \eta_0 \right] e^B, \quad M|h| = |H|.$$

Thus, if $\eta_0 = 0$ (exact initial conditions), the step-by-step procedure converges to the exact result as M increases. Again the restrictions are unnecessary, though for differing step lengths we require

$$\lim_{M \rightarrow \infty} h_\rho = 0, \quad \rho = 0(1)M - 1.$$

The theorem provides bounds on the errors at $x' + H$ and can thus be interpreted as a stability criterion for fixed M . It does not provide a bound for $z > 1/2s$.

5. Multi-Step and Mixed Methods. Theorem (2.1) provides a connection with multi-step methods and various methods of mixed type. We can use intervals $(x, x + h)$ which contain points already integrated or we can use some negative values for the parameters $\mu_i, i = 1(1)s$. The theorem then provides approximations to the functions $k_{ri}(h), r = 1(1)q$, at these points.

As a simple example we consider a three-stage method of order $\mathbf{p} = 3$, applicable to an arbitrary system of differential equations of the form (1.1). We use the notation of Section 4 and consider stepping from x' to $x' + H$ using M equal subdivisions of length h . It is assumed that some special starting method has already given adequate approximations $\bar{y}(x + h)$.

To step from $x_{\rho,0}$ to $x_{\rho+1,0}, \rho = 1(1)M - 1$, we take

$$\mu_1 = -1, \quad \mu_2 = 0, \quad \mu_3 = 1.$$

Then a particular choice of parameters, which satisfies Eqs. (2.1), (2.3), with $\mathbf{p} = 3$ is

$$\alpha_{r1}^{[\nu]} = \frac{-\nu}{2(\nu + 1)(\nu + 2)}, \quad \alpha_{r2}^{[\nu]} = \frac{2\nu(\nu + 3)}{2(\nu + 1)(\nu + 2)}, \quad \alpha_{r3}^{[\nu]} = \frac{\nu + 4}{2(\nu + 1)(\nu + 2)},$$

$$\lambda_{ri1}^{[\nu]} = \frac{2 - i}{\nu + 1}, \quad \lambda_{ri2}^{[\nu]} = \frac{\nu + i - 1}{\nu + 1}, \quad \lambda_{ri3}^{[\nu]} = 0,$$

for $r = 1(1)q, \nu = 1(1)n_r, i = 1, 2, 3$. Definition (1.1) now gives a method for stepping ahead. We insert the additional parameter, ρ , to refer to the current step, and obtain,

$$\bar{T}_r^{[\nu]}(\mu_i h, \rho) = \sum_{\tau=0}^{\nu-1} \frac{(\mu_i h)^\tau}{\tau!} \bar{y}_r^{(n_r-\nu+\tau)}(x_{\rho 0}), \quad i = 1(1)s + 1,$$

$$k_{ri}^{[\nu]}(h, \rho) = \bar{T}_r^{[\nu]}(\mu_i h, \rho) + \frac{(\mu_i h)^\nu}{(\nu + 1)!} [(2 - i)k_{ri}(h, \rho) + (\nu + i - 1)k_{r2}(h, \rho)],$$

$$k_{ri}(h, \rho) = f_r(x_{\rho i}; k_1^{[n_1]}(h, \rho), \dots, k_1^{[1]}(h, \rho); \dots; k_{q_i}^{[n_{q_i}]}(h, \rho), \dots, k_{q_i}^{[1]}(h, \rho)),$$

$$r = 1(1)q, \quad \nu = 1(1)n_r, \quad i = 1, 2, 3$$

We now have

$$\bar{y}^{(n_r-\nu)}(x_{\rho+1,0}) = \bar{T}_r^{[\nu]}(h, \rho) + \frac{h^\nu}{2(\nu + 2)!} [-\nu k_{r1}(h, \rho) + 2\nu(\nu + 3)k_{r2}(h, \rho) + (\nu + 4)k_{r3}(h, \rho)],$$

$$y_r^{(n_r-\nu)}(x_{\rho+1,0}) - \bar{y}_r^{(n_r-\nu)}(x_{\rho+1,0}) = O(h^{n_r+3-\nu}).$$

Theorem (2.1) gives

$$k_{ri}(h, \rho) = k_{r, i+1}(h, \rho - 1) + O(h^3), \quad i = 1, 2,$$

and we thus have excellent starting values for an iterative determination of the functions $k_{ri}(h, \rho)$. The analysis of Section 4 still applies. If we proceed in this fashion we have a method of predictor-corrector type. On the other hand, we can accept these estimates as adequate and immediately obtain $k_{r3}(\rho, h)$ which is defined explicitly. The analysis of Section 4 does not apply and we have a method of linear multi-step type. We can, of course, use the method also to obtain the starting

values. But now the functions $k_{r,i}(h, 1)$ must be determined iteratively.

An alternative procedure is to step from $x_{\rho-1,0}$ to $x_{\rho+1,0}$, $\rho = 1(1)M - 1$, steps of length $2h$, with $\mu_1 = 0$, $\mu_2 = \frac{1}{2}$, $\mu_3 = 1$. Higher-order methods can likewise be obtained.

6. The Definition of Order. Definition (1.2) implies that the Taylor series expansions of $y_r^{(\nu)}(x + h)$, $\bar{y}_r^{(\nu)}(x + h)$, agree up to, but not including, terms of $O(h^{nr+p-\nu})$, $r = 1(1)q$, $\nu = 0(1)n_r - 1$. This definition leads to Eqs. (2.1), (2.3), which give implicit methods of arbitrary order \mathbf{p} . We observe that (2.1) may be solved for all ν , in terms of a solution for $\nu = 1$, by the conditions

$$(6.1) \quad \begin{aligned} \lambda_{r,ij}^{[\nu+1]} &= (\nu + 1)[1 - \mu_j/\mu_i]^\nu \lambda_{r,ij}^{[1]}, & \mu_i \neq 0, \\ &= 0, & \mu_i = 0, \end{aligned}$$

$$i, j = 1(1)s, r = 1(1)q, \nu = 1(1)n_r - 1.$$

It may appear more natural to define order by the requirement,

$$E_{sr}^{[\nu]}(h) = O(h^{nr+p-\nu}), \quad r = 1(1)q, \quad \nu = 1(1)n_r,$$

whence the expansions of $y_r^{(\nu)}(x + h)$, $\bar{y}_r^{(\nu)}(x + h)$, agree up to, but excluding, terms of $O(h^p)$. For then, using (1.3), the resulting parameter constraints can be written as a *single* set of equations,

$$\begin{aligned} \mu_i^\tau &= \binom{\nu + \tau}{\tau} \sum_{j=1}^s \lambda_{r,ij}^{[\nu]} \mu_j^\tau, & i = 1(1)s + 1, & \quad r = 1(1)q, \\ & & \nu = 1(1)n_r, & \quad \tau = 0(1)\mathbf{p} - \nu - 1. \end{aligned}$$

The solution (6.1) can now be extended to cover the case $i = s + 1$.

However, the additional constraints in (2.3) give more accurate values for the lower-order derivatives. In either case Theorem (2.1) holds and we further have,

$$k_{r,i}^{[\nu]}(h) = y_r^{(n_r-\nu)}(x_i) + O(h^p), \quad \nu = 1(1)n_r,$$

an extra aid for error estimation.

7. Systems of First-Order Equations. It is sometimes stated that it is adequate to treat an equation of order n as a system of n first-order equations. We show here that this results in a decrease of *local* accuracy and an increase in computation. The final accuracy, after a number of steps, appears to be unimpaired. Consider the single equation

$$(7.1) \quad y^{(n)}(t) = f(t; y^{(0)}(t), \dots, y^{(n-1)}(t)),$$

which may be replaced by the system,

$$(7.2) \quad \begin{aligned} y_n^{(1)}(t) &= f_n(t; y_1(t), \dots, y_n(t)), \\ y_r^{(1)}(t) &= f_r(y_{r+1}(t)) = y_{r+1}(t), & r = 1(1)n - 1. \end{aligned}$$

Equations (2.1), (2.3), provide an s stage method of order \mathbf{p} for both (7.1) and (7.2). Additional work is required to obtain the parameters for (7.1) but this can be reduced by using (6.1). Consider applying the method for a single step. To solve

(7.1) we need to evaluate s functions $k_i(h)$, $i = 1(1)s$. To solve (7.2) we have in general to evaluate $k_{ri}(h)$, $r = 1(1)n$, $i = 1(1)s$. If, however, we make use of the particular properties of the system, these functions can all be expressed in terms of $k_{ni}(h)$, $i = 1(1)s$. Nevertheless, the organization required is appreciable, and the resulting s equations do not in general have as simple a structure. When we solve (7.1) we are in effect solving the system (7.2) using a special sequence of *different* methods, which give an *over-all* simple structure.

Furthermore, this special sequence uses all the available initial terms of the Taylor series expansion. Thus solving (7.1) gives

$$y^{(\nu)}(x + h) - \bar{y}^{(\nu)}(x + h) = O(h^{n+p-\nu}), \quad \nu = 0(1)n - 1,$$

whereas the solution of (7.2) gives

$$y_{\nu+1}(x + h) - \bar{y}_{\nu+1}(x + h) = y^{(\nu)}(x + h) - \bar{y}^{(\nu)}(x + h) = O(h^{p+1}).$$

That is, the local accuracy is better, for ν small, if the equation is treated intact.

We now consider applying our method to a sequence of intervals as in Section 4. Although the proof of Theorem (4.1) is crude, the result indicates that the order of the global accuracy does not depend on which way the equation is treated. We examine this a little more closely. From (4.2), (4.3), and the result of the theorem we obtain

$$(7.3) \quad |\eta_{r,\rho+1}^{[n_r-\nu]}| \leq \phi |h|^{p+\nu} + \sum_{\tau=0}^{\nu-1} \frac{|h|^\tau}{\tau!} |\eta_{r\rho}^{[n_r-\nu+\tau]}|,$$

and we assume that

$$|\eta_{r0}^{[n_r-\nu]}| \leq \Gamma |h|^{p+\nu}, \quad r = 1(1)q, \quad \nu = 1(1)n_r, \quad \rho = 0(1)M - 1.$$

Here ϕ , Γ , are constants independent of ν , ρ . Repeated application of (7.3) gives

$$|\eta_{r\rho}^{[n_r-\nu]}| \leq |h|^{p+\nu} (\rho + \nu)^{\rho-1} [(\rho + \nu)\phi + \Gamma],$$

and this can be established by induction. If we now take $\rho = M$, we have since $Mh = H$,

$$|\eta_{rM}^{[n_r-\nu]}| = O(h^p).$$

This is essentially the same result as that of Theorem (4.1). Thus *if* the number of steps is $O(|h|^{-1})$, it is immaterial which way the equation is solved, at least from the viewpoint of final accuracy achieved [12].

The remarks of this and the previous section require modification if methods of maximum order are considered.

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