A CLASS OF TWO-STAGE IMPLICIT HYBRID METHODS FOR ORDINARY EQUATIONS*

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Abstract

A k-step, $(k+2)$th order two-stage implicit hybrid method which has all the advantages of Enright's method but not its principal disadvantages is proposed. A "simple" approach to estimate the local truncation error is developed. Preliminary numerical results indicate that the hybrid method compares favorably with Enright's method.

1. Introduction

In this paper we shall propose a class of two-stage implicit hybrid multistep methods. The main reason is that they are able to replace the existing second derivative multistep methods which are suitable for the approximate numerical integration of stiff systems of first order ordinary differential equations and to overcome the main shortcoming of the latter. To show this, first of all we discuss a second derivative multistep method of the following type:

$$\sum_{j=0}^{k}\alpha_j y_{n+j}=h\sum_{j=0}^{k}\beta_j y'_{n+j}+h^2\sum_{j=0}^{k}\gamma_j y''_{n+j},\quad k=1,\ 2,\ \cdots \tag{1.1}$$

for the numerical integration of the stiff systems

$$y'=f(y),\quad t\in[0,\ T] \tag{1.2}$$

with the initial conditions

$$y(0)=y_0, \tag{1.3}$$

where the α_j, β_j and γ_j are constants normalized by making $\alpha_k=1$, y_{n+j} is the approximate numerical solution obtained at t_{n+j}.

Note that y is a vector, although sometimes we consider only the scalar case. Suppose for the moment that $y(t)$ has a convergent Taylor series expansion at the point $t=t_n$. Consider the expansion

$$\begin{aligned}L[y(t_n);\ h]&=\sum_{j=0}^{k}\alpha_j y(t_n+jh)-\sum_{j=0}^{k}\beta_j y'(t_n+jh)-h^2\sum_{j=0}^{k}\gamma_j y''(t_n+jh)\\&=C_0y(t_n)+C_1hy'(t_n)+\cdots+C_ph^py^{(p)}(t_n)+\cdots,\end{aligned}$$

where $h=t_{j+1}-t_j$, $j=0,\ 1,\ 2,\ \cdots$, is the step length and

$$\begin{cases}C_0=\sum_{j=0}^{k}\alpha_j,\\C_1=\sum_{j=0}^{k}(j\alpha_j-\beta_j),\end{cases} \tag{1.4}$$

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$$C_i=\sum_{j=0}^{k}\left(j^i\frac{\alpha_j}{i!}-j^{(i-1)}\frac{\beta_j}{(i-1)!}-j^{(i-2)}\frac{\gamma_j}{(i-2)!}\right),\ \text{for } i=2,3\cdots.$$

Definition 1. *If $C_0=C_1=\cdots=C_p=0$ but $C_{p+1}\neq 0$, then* (1.1) *is said to have order p. Thereafter the expression* (1.4) *is said to be the order condition of the method* (1.1).

If (1.1) is of order p, and we solve (1.1) for y_{n+k} with exact y_n, y_{n+1}, $\cdots$, y_{n+k-1}, i. e. with $y_{n+i}=y(t_{n+i})$ for $i=0(1)(k-1)$, where $y(t)$ is the solution of (1.2), then we have

$$y_{n+k}=y(t_{n+k})+O(h^{p+1}). \tag{1.5}$$

A count of the available coefficients shows that order $(3k+1)$ is attainable for the method (1.1) if it is implicit. However, the coefficients α_j, $j=0(1)k$, must satisfy the usual zero-stable condition, and this may prevent the above orders from being attained for some k. At present the maximum order for the zero-stable k-step method (1.1) $(k=1, 2, \cdots)$ is still unknown.

Some particular cases of (1.1) have been discussed. For example the fourth order method

$$y_{n+1}=y_n+\frac{1}{2}h(y'_n+y'_{n+1})+\frac{1}{12}h^2(y''_n-y''_{n+1}) \tag{1.6}$$

has been considered by Obrechkoff [2] and in connection with stiff systems by Ehle[3], Thompson [4] and others. This method is A-stable but not stable at infinity. Liniger and Willoughby [5] have considered the two-parameter method

$$y_{n+1}=y_n+\frac{h}{2}[(1-a)y'_n+(1+a)y'_{n+1}]+\frac{h^2}{4}[(b-a)y''_n-(b+a)y''_{n+1}]. \tag{1.7}$$

If a and b satisfy $0\leqslant a\leqslant 1/3$ and $b=1/3$ respectively, then this method is A-stable and is of order three at least. In particular, if $a=b=1/3$ then the obtained third order method is A-stable and stable at infinity.

Enright[6] attempted to derive for (1.1) stiffly stable methods satisfying the following three principal requirements:

(1) stability at infinity;

(2) a reasonable stability property in the neighborhood of the origin;

(3) an order as high as possible.

He obtained a k-step, $(k+2)$th order method of the following type:

$$y_{n+k}=y_{n+k-1}+h\sum_{j=0}^{k}\beta_j y'_{n+j}+h^2\gamma_k y''_{n+k},\quad k\leqslant 7. \tag{1.8}$$

Note that for $k=1$ the method corresponds to (1.7) with $a=b=1/3$.

The coefficients and plots of the stability regions for (1.8) for $k\leqslant 7$ are given in [6]. Thereafter (1.8) is called Enright's method.

The iteration scheme adopted to solve the implicit set of equations (1.8) is a modified Newton-Raphson technique:

$$W_{n+k}(y^{(l+1)}_{n+k}-y^{(l)}_{n+k})=-y^{(l)}_{n+k}+h\beta_k f(y^{(l)}_{n+k})+h^2\gamma_k\left(\frac{\partial f}{\partial y}\right)f(y^{(l)}_{n+k})$$
$$+y_{n+k-1}+h\sum_{j=0}^{k-1}\beta_j f_{n+j}, \tag{1.9}$$

where $W_{n+k}=\left(1-h\beta_k\left(\frac{\partial f}{\partial y}\right)-h^2\gamma_k\left(\frac{\partial f}{\partial y}\right)^2\right)$. In fact, for non-linear stiff systems the iteration schen e (1.9) neglects the terms involving $\left(\frac{\partial^2 f}{\partial y^2}\cdot f\right)$ in W_{n+k}.

According to the results and conclusions in [7], Enright's method is reliable and efficient for general stiff systems. Comparing the results of Enright's method with that of Gear's[7] we notice that Enright's method is less competitive for "highly" non-linear stiff systems. This is because the iteration scheme used neglects the term $\left(\frac{\partial^2 f}{\partial y^2}\cdot f\right)$, and as the one-step-two-half-step error estimator is used, one has to solve the non-linear equations three times per step. Here the term $\left(\frac{\partial^2 f}{\partial y^2}\cdot f\right)$ arising in the iteration scheme can be attributed to the second derivative y'' in Enright's method. As a result, Enright's method requires that Jacobian $\left(\frac{\partial f}{\partial y}\right)$ be exact. If the Jacobian were not exact, the order of Enright's method would have to be reduced.

From the discussion on Enright's method we can see that people are not very much interested in high-derivative methods although they are possessed of good stability properties and higher order accuracy.

In Sect. 2 we derive a two-stage implicit hybrid multistep method such that it has the advantages of the second derivative method but not its principal disadvantages. In Sect. 3 we obtain a k-step, $(k+2)$th order two-stage implicit hybrid method which has the stability properties of Enright's method for the linear system $y'=Ay$ but not its principal disadvantages. Sect. 4 some numerical results are presented and it is shown that the hybrid method compares favorably with Enright's method.

2. The Two-stage Implicit Hybrid Method

In this section, we are concerned with the two-stage implicit hybrid method having the general form[8]

$$\sum_{j=0}^{k}\bar{\alpha}_j y_{n+j}=h\sum_{j=0}^{k}\bar{\beta}_j f_{n+j}+h\beta_\nu f_{n+\nu},\quad \nu\neq j,\ j=0(1)k, \tag{2.1a}$$

$$y_{n+\nu}+\sum_{j=0}^{k}\hat{\alpha}_j y_{n+j}=h\sum_{j=0}^{k}\hat{\beta}_j f_{n+j} \tag{2.1b}$$

or

$$\sum_{j=0}^{k}\bar{\alpha}_j y_{n+j}=h\sum_{j=0}^{k}\bar{\beta}_j f_{n+j}+h\beta_\nu f\left(t_{n+\nu},\ -\sum_{j=0}^{k}\hat{\alpha}_j y_{n+j}+h\sum_{j=0}^{k}\hat{\beta}_j f_{n+j}\right), \tag{2.1$'$}$$

where $\bar{\alpha}_j$, $\hat{\alpha}_j$, $\bar{\beta}_j$, $\hat{\beta}_j$ and β_ν are constants normalized by making

$$\bar{\alpha}_k=1,\ f_{n+j}\equiv f(t_{n+j},\ y_{n+j})\quad\text{and}\quad f_{n+\nu}\equiv f(t_{n+\nu},\ y_{n+\nu}).$$

Thereafter (2.1a) is said to be a principal formula, and (2.1b) an auxiliary formula.

In fact, the implicit hybrid method (2.1) is special class of composite multistep methods using "non-step" point. Following the order condition (1.4) we can obtain the order conditions of (2.1a) and (2.1b) respectively

$$\begin{cases}\bar{C}_0\equiv\sum_{j=0}^{k}\bar{\alpha}_j,\\ \bar{C}_i\equiv\sum_{j=0}^{k}\left(j^i\frac{\bar{\alpha}_j}{i!}-j^{(i-1)}\frac{\bar{\beta}_j}{(i-1)!}-\frac{\nu^{(i-1)}}{(i-1)!}\beta_\nu\right),\quad i=1,\ 2,\ \cdots\end{cases} \tag{2.2a}$$

and

$$\begin{cases} \hat{C}_0 \equiv 1+\sum_{j=0}^{k} \hat{a}_j, \\ \hat{C}_i \equiv \frac{1}{i!}\left(\nu^i+\sum_{j=0}^{k} j^i \hat{a}_j\right)-\frac{1}{(i-1)!}\sum_{j=0}^{k} j^{(i-1)}\hat{\beta}_j, \quad i=1,\ 2,\ \cdots. \end{cases} \tag{2.2b}$$

Definition 2. *If* $\bar{C}_0=\bar{C}_1=\cdots=\bar{C}_q=0$ *but* $\bar{C}_{q+1}\neq 0$, *then* (2.1a) *is said to have order* q.

Definition 3. *If* $\hat{C}_0=\hat{C}_1=\cdots=\hat{C}_r=0$ *but* $\hat{C}_{r+1}\neq 0$, *then* (2.1b) *is said to have order* r.

If the principal formula (2.1a) is of order q and the auxiliary formula (2.1b) is of order r, from (1.5) it is easy to prove that the implicit hybrid formula (2.1) is of order

$$p=\min\{q,\ r+1\}. \tag{2.3}$$

Obviously there are $(2k+3)$ parameters in (2.1b). We can make (2.1a), (2.1b) of order $q=2k+2$ and $r=2k+1$ respectively. The investigations in [9] and [10] show that the principal formula (2.1a) of order $q=(2k+2)$ is zero-stable if and only if $k\leqslant 6$. It follows that the zero-stable implicit hybrid method (2.1) can achieve the order $p=k+2$.

Now we discuss the relations between the two-stage implicit hybrid method (2.1) and the second derivative multistep method (1.1).

Consider the application of (2.1) to the linear system $y'=Ay$, where A is a constant matrix. We obtain

$$\sum_{j=0}^{k} \bar{a}_j y_{n+j}=h\sum_{j=0}^{k}(\bar{\beta}_j-\beta_\nu\hat{a}_j)Ay_{n+j}+h^2\sum_{j=0}^{k}\beta_\nu\hat{\beta}_j A^2 y_{n+j}. \tag{2.4}$$

Obviously, (2.4) is a second derivative multistep method for the linear system $y'=Ay$.

Let

$$\begin{cases} \alpha_j\equiv\bar{a}_j, \\ \beta_j\equiv(\bar{\beta}_j-\beta_\nu\hat{a}_j), \\ \gamma_j\equiv\beta_\nu\hat{\beta}_j \end{cases} \tag{2.5}$$

in (1.1), we have the following results:

Theorem 1. *Let the two-stage implicit hybrid method* (2.1) *be zero-stable and have order* p. *Then* (i) (1.1) *derived from* (2.5) *is zero-stable and has at least order* p; (ii) (1.1) *has the stability properties of* (2.1) *for the test equation* $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$.

Proof. Obviously, we only have to prove that (1.1) has at least order p.

According to definition 1 the method (1.1) has at least order p only if $C_i=0$, $i=0(1)p$. From (2.5) we obtain

$$C_0=\sum_{j=0}^{k}\alpha_j=\sum_{j=0}^{k}\bar{a}_j=0,$$

$$C_1=\sum_{j=0}^{k}(j\alpha_j-\beta_j)=\sum_{j=0}^{k}(j\bar{a}_j-(\bar{\beta}_j-\beta_\nu\hat{a}_j))$$

$$=\left\{\sum_{j=0}^{k}(j\bar{a}_j-\bar{\beta}_j)-\beta_\nu\right\}+\beta_\nu\left(1+\sum_{j=0}^{k}\hat{a}_j\right)=\bar{C}_1+\beta_\nu\hat{C}_0=0,$$

$$\begin{aligned}C_i&=\sum_{j=0}^{k}\left(j^i\frac{\alpha_j}{i!}-j^{(i-1)}\frac{\beta_j}{(i-1)!}-j^{(i-2)}\frac{\gamma_j}{(i-2)!}\right)\\&=\left\{\sum_{j=0}^{k}\left(j^i\frac{\bar{\alpha}_j}{i!}-j^{(i-1)}\frac{\bar{\beta}_j}{(i-1)!}\right)-\frac{\nu^{i-1}}{(i-1)!}\beta_\nu\right\}\\&\quad+\beta_\nu\left\{\frac{1}{(i-1)!}\left(\nu^{i-1}+\sum_{j=0}^{k}j^{i-1}\hat{\alpha}_j\right)-\frac{1}{(i-2)!}\sum_{j=0}^{k}j^{i-2}\hat{\beta}_j\right\}\\&=\bar{C}_i+\beta_\nu\hat{C}_{i-1}=0,\qquad i=2,\ 3,\ \cdots,\ p.\end{aligned}$$

Theorem 2. *Let the zero-stable* (1.1) *and* (2.1b) *have respectively orders* q *and* r. *Then* (i) *the hybrid method* (2.1) *derived from* (2.5) *is zero-stable and has order* $p=\min(q, r+1)$; (ii) (2.1) *has the stability properties of* (1.1) *for the test equation* $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$.

The proof is analogous to that of Theorem 1.

From the above discussions it is easy to see that the main advantage of (2.1) is that it has all good properties of (1.1) while the term containing the second derivative y'' does not arise, therefore it does not require Jacobian $\left(\frac{\partial f}{\partial y}\right)$ to be exact, and the term $\left(\frac{\partial^2 f}{\partial y^2}\cdot f\right)$ disappear naturally in the iteration scheme based on a modified Newton-Raphson technique. It appears that the two-stage implicit hybrid method (2.1) is superior to the second derivative multistep method (1.1) in handling "highly" nonlinear stiff systems and therefore worth further studying.

Before discussing the choice of coefficients we shall mention some particular cases of (2.1) that correspond to the method (1.6) and (1.7).

(i) The fourth order one-step hybrid method

$$\begin{cases}y_{n+1}=y_n+\frac{1}{6}h(f_n+f_{n+1})+\frac{2}{3}hf_{n+\frac{1}{2}},\\ y_{n+\frac{1}{2}}=\frac{1}{2}(y_n+y_{n+1})+\frac{1}{8}h(f_n-f_{n+1})\end{cases}\tag{2.6}$$

corresponds to (1.6) for the test equation $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$.

(ii) The two-parameter method

$$\begin{cases}y_{n+1}=y_n+h\left(\frac{1}{2}-\frac{1}{6\nu}\right)f_n+h\left(\frac{1}{2}+\frac{1}{6(\nu-1)}\right)f_{n+1}-\frac{h}{6\nu(\nu-1)}f_{n+\nu},\\ y_{n+\nu}=(\nu-1)^2(1+2\alpha\nu)y_n-\nu[2\alpha(\nu-1)^2+(\nu-2)]y_{n+1}\\ \qquad+\alpha\nu(\nu-1)^2hf_n+\nu(\nu-1)[1+\alpha(\nu-1)]hf_{n+1}.\end{cases}\tag{2.7}$$

If α and ν satisfy $-1/2\leqslant\alpha(\nu-1)\leqslant 0$, then (2.7) has at least order 3, and for the test equation $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$, it corresponds to (1.7) with $0\leqslant a\leqslant 1/3$ and $b=1/3$; if $\alpha=0$ then this method has order 3, and for test equation $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$, it corresponds to (1.7) with $a=b=1/3$.

3. Homologue of Enright's Method and Error Estimate

For two-stage implicit hybrid method (2.1) our purpose is to derive stiffly stable formulas corresponding to those of Enright's method. Therefore these formulas should also satisfy the three principal requirements described in the first section. According to Theorem 2 they can be written as

$$y_{n+k}=y_{n+k-1}+h\sum_{j=0}^{k}\bar{\beta}_j^{(k)}(\nu)f_{n+j}+h\beta_\nu^{(k)}f_{n+\nu},\quad \nu\neq j,\ j=0(1)k, \tag{3.1a}$$

$$y_{n+\nu}=-\sum_{j=0}^{k}\hat{\alpha}_j^{(k)}(\nu)y_{n+j}+h\hat{\beta}_k^{(k)}(\nu)f_{n+k},\quad k\leqslant 7. \tag{3.1b}$$

If the auxiliary formula (3.1b) is of order $(k+1)$, then the two-stage hybrid method (3.1) derived from (2.5) has order $(k+2)$ and the stability properties of Enright's method for the test equation $y'=\lambda y$, $\mathrm{Re}(\lambda)<0$. Therefore we need only to construct the $(k+1)$th order auxiliary formula (3.1b).

In [1] we have derived the k-step $(k+1)$th order auxiliary formula (3.1b). Its coefficients read respectively

$$\begin{cases}\hat{\alpha}_j^{(k)}(\nu)=\hat{\alpha}_j^*(k)\,(\nu-k)\prod\limits_{\substack{l=0\\ l\neq j}}^{k-1}(\nu-l), & j=0(1)(k-1),\\ \hat{\alpha}_k^{(k)}(\nu)=\dfrac{(\hat{a}_k\nu+\hat{b}_k)}{k!}\prod\limits_{l=0}^{k-1}(\nu-l),\\ \hat{\beta}_k^{(k)}(\nu)=\dfrac{1}{k!}\prod\limits_{l=0}^{k}(\nu-l),\end{cases} \tag{3.2}$$

where

$$\begin{cases}\hat{\alpha}_j^*(k)=-\dfrac{1}{(j-k)^2}\prod\limits_{\substack{l=0\\ l\neq j}}^{k-1}(j-l)^{-1},\\ \hat{a}_k=\sum\limits_{j=0}^{k-1}(k-j)^{-1},\quad \hat{b}_k=-(1+k\hat{a}_k).\end{cases} \tag{3.3}$$

In addition these coefficients satisfy the following recurrence formulas

$$\begin{cases}\hat{\alpha}_0^*(k)=\dfrac{(-1)^k}{k\cdot(k!)}, & k=1(1)7,\\ \hat{\alpha}_j^*(k+1)=\dfrac{1}{j}\,\hat{\alpha}_{j-1}^*(k), & j=1(1)k,\ k=1(1)6,\\ \hat{a}_1=1,\ \hat{b}_1=-2,\\ \hat{a}_{k+1}=\hat{a}_k+\dfrac{1}{(k+1)}, & k=1(1)6,\\ \hat{b}_{k+1}=-[1+(k+1)\hat{a}_{k+1}]=\hat{b}_k-(1+\hat{a}_k).\end{cases} \tag{3.4}$$

The local truncation error of (3.1) reads

$$e_H=\left\{\left[C_{k+3}-\frac{(\nu-k)\gamma_k}{(k+1)(k+2)}\right]y^{(k+3)}(t_n)+\frac{(\nu-k)\gamma_k}{(k+1)(k+2)}\frac{\partial f}{\partial y}y^{(k+2)}(t_n)\right\}h^{k+3}, \tag{3.5}$$

where C_{k+3} (see Table 5) denotes the error constant of Enright's method (1.8).

From (3.5) it is easy to see that if the principal formula (3.1a) is of order $(k+3)$ then

$$\bar{C}_{k+3}\equiv C_{k+3}-\frac{(\nu-k)\gamma_k}{(k+1)(k+2)}=0,$$

namely

$$\nu=\nu^*\equiv k+C_{k+3}(k+1)(k+2)/\gamma_k, \tag{3.6}$$

where $\bar{C}_{k+3}$ denotes the error constant of the principal formula (3.1a).

The second problem is that of estimating the local truncation error of (3.1). In fact what we shall do is to find a more accurate y_{n+k} as the solution given by the k-step $(k+3)$th order implicit hybrid method and use $\|y_{n+k}-\bar{y}_{n+k}\|_\infty$ as an estimate of the error in the solution $\tilde{y}_{n+k}$ of (3.1). The method which is quite similar to (3.1) can be written in the form

$$\begin{cases} \text{the principal formula (3.1a) with } \nu=\nu^*, & (3.7a) \\ y_{n+\nu^*}+\sum_{j=0}^{k}\tilde{\alpha}_j^{(k)}(\nu^*)y_{n+j}=h\tilde{\beta}_{k-1}^{(k)}(\nu^*)f_{n+k-1}+h\tilde{\beta}_k^{(k)}(\nu^*)f_{n+k}. & (3.7b) \end{cases}$$

What remains to be done is to construct the k-step $(k+2)$th order auxiliary formula (3.7b). From (3.1b) and (3.2) it is easy to see that (3.7b) can be derived by finding a polynomial approximation $P_{k+2}(t_n+\nu h)$ of degree $(k+2)$ to the solution such that (let $t_n=0,\ h=1$)

$$\begin{cases} P_{k+2}(\nu)\,|_{\nu=j}=y_{n+j}, \quad j=0(1)k, \\ P'_{k+2}(\nu)\,|_{\nu=(k-1)}=f_{n+k-1}, \\ P'_{k+2}(\nu)\,|_{\nu=k}=f_{n+k}, \end{cases} \tag{3.8}$$

namely

$$\begin{cases} \tilde{\alpha}_j^{(k)}(i)=\begin{cases}-1, & \text{for } i=j, \\ 0, & \text{for } i\neq j,\end{cases} \quad i,\ j=0(1)k, \\ \tilde{\beta}_{(k-1)}^{(k)}(i)=\tilde{\beta}_k^{(k)}(i)=0, \quad i=0(1)k, \\ \tilde{\alpha}_j^{(k)\prime}(i)=0, \quad i=(k-1), \quad j=0(1)k, \\ \tilde{\beta}_{k-1}^{(k)\prime}(k-1)=\tilde{\beta}_k^{(k)\prime}(k)=1, \\ \tilde{\beta}_{k-1}^{(k)\prime}(k)=\tilde{\beta}_k^{(k)\prime}(k-1)=0. \end{cases} \tag{3.9}$$

Similar to (3.2) we have

$$\begin{cases} \tilde{\alpha}_j^{(k)}(\nu)=\tilde{\alpha}_j^*(k)(\nu-k)(\nu-k+1)\prod_{\substack{l=0\\l\neq j}}^{k}(\nu-l), \quad j=0(1)(k-2), \\ \tilde{\alpha}_{k-1}^{(k)}(\nu)=\dfrac{\tilde{a}_{k-1}\nu^2+\tilde{b}_{k-1}\nu+\tilde{c}_{k-1}}{(k-1)!}(\nu-k)\prod_{l=0}^{k-2}(\nu-l), \\ \tilde{\alpha}_k^{(k)}(\nu)=\dfrac{a_k\nu^2+b_k\nu+c_k}{k!}\prod_{l=0}^{k-1}(\nu-l), \\ \tilde{\beta}_{k-1}^{(k)}(\nu)=\dfrac{(\nu-k)}{(k-1)!}\prod_{l=0}^{k}(\nu-l), \\ \tilde{\beta}_k^{(k)}(\nu)=\dfrac{1}{k!}(\nu-k+1)\prod_{l=0}^{k}(\nu-l), \end{cases} \tag{3.10}$$

where

$$\begin{cases} \tilde{\alpha}_j^*(k)=-\dfrac{1}{(j-k)(j-k+1)}\prod_{\substack{l=0\\l\neq j}}^{k}\dfrac{1}{(j-l)}, \quad j=0(1)(k-1) \\ \tilde{a}_{k-1}=\sum_{i=0}^{k-2}\dfrac{1}{[(k-1)-i]}-2, \quad \tilde{a}_0=-2, \\ \tilde{b}_{k-1}=(1-2k)\tilde{a}_{k-1}-1, \\ \tilde{c}_{k-1}=-k(k\cdot\tilde{a}_{k-1}+\tilde{b}_{k-1}), \\ a_k=1+\sum_{i=0}^{k-1}(k-i)^{-1}, \\ b_k=(1-2k)a_k-1, \\ c_k=-(1+k\cdot b_k+k^2\cdot a_k). \end{cases} \tag{3.11}$$

But we are interested in deriving the relationship between the coefficients of (3.7b) and of (3.1b). By calculations we obtain

$$\begin{cases} \tilde{\alpha}_j^{(k)}(\nu)=\hat{\alpha}_j^{(k)}(\nu)+\dfrac{(\nu-j)}{(j-k+1)}\hat{\alpha}_j^{(k)}(\nu)\equiv\hat{\alpha}_j^{(k)}(\nu)+\delta_j^{(k)}(\nu), \quad j=0(1)(k-2), \\ \tilde{\alpha}_{k-1}^{(k)}(\nu)=\hat{\alpha}_{k-1}^{(k)}(\nu)-(\nu+k+1)(\hat{a}_{k-2}-2)\hat{\alpha}_{k-1}^{(k)}(\nu)\equiv\hat{\alpha}_{k-1}^{(k)}(\nu)+\delta_{k-1}^{(k)}(\nu), \\ \tilde{\alpha}_k^{(k)}(\nu)=\hat{\alpha}_k^{(k)}(\nu)+\dfrac{(\hat{a}_k+1)(\nu-k)^2}{(\nu-k)\hat{a}_k-1}\hat{\alpha}_k^{(k)}(\nu)\equiv\hat{\alpha}_k^{(k)}(\nu)+\delta_k^{(k)}(\nu), \\ \tilde{\beta}_{k-1}^{(k)}(\nu)=k(\nu-k)\hat{\beta}_k^{(k)}(\nu), \\ \tilde{\beta}_k^{(k)}(\nu)=\hat{\beta}_k^{(k)}(\nu)+(\nu-k)\hat{\beta}_k^{(k)}(\nu). \end{cases} \tag{3.12}$$

Thus the k-step, $(k+3)$th order hybrid method (3.7) becomes

$$\begin{cases} \text{the principal formula (3.1a) with } \nu=\nu^*, \\ y_{n+\nu^*}+\sum_{j=0}^{k}\hat{\alpha}_j^{(k)}(\nu^*)y_{n+j}=h\hat{\beta}_k^{(k)}(\nu^*)f_{n+k}-\sum_{j=0}^{k}\delta_j^{(k)}(\nu^*)y_{n+j} \\ \qquad +h(\nu^*-k)\hat{\beta}_k^{(k)}(\nu^*)(kf_{n+k-1}+f_{n+k}). \end{cases} \tag{3.7$'$}$$

Assuming that the solutions values $y_n, y_{n+1}, \cdots, y_{n+k-1}$ are available, our algorithm, in which (3.1) is used in practice and which includes the local error estimate, is carried out in the following steps:

(1) Compute $\bar{y}_{n+k}$ as the solution of the stiffly stable hybrid method

$$\begin{cases} y_{n+k}=y_{n+k-1}+h\sum_{j=0}^{k}\bar{\beta}_j^{(k)}(\nu^*)f_{n+j}+h\beta_{\nu^*}^{(k)}f_{n+\nu^*}, \\ y_{n+\nu^*}+\sum_{j=0}^{k}\hat{\alpha}_j^{(k)}(\nu^*)y_{n+j}=h\hat{\beta}_k^{(k)}(\nu^*)f_{n+k}. \end{cases}$$

Here the nonlinear algebraic equations defining $\bar{y}_{n+k}$ are solved using a modified Newton-Raphson technique iterated to convergence.

(2) Compute $\bar{f}_{n+k}=f(t_{n+k}, \bar{y}_{n+k})$ and

$$g_{n+k}\equiv-\sum_{j=0}^{k-1}\delta_j^{(k)}(\nu^*)y_{n+j}-\delta_k^{(k)}(\nu^*)\bar{y}_{n+k}+h(\nu^*-k)\hat{\beta}_k^{(k)}(\nu^*)(k\cdot f_{n+k-1}+\bar{f}_{n+k}).$$

(3) Compute y_{n+k} as the solution of k-step, $(k+3)$th order hybrid method

$$y_{n+k}=y_{n+k-1}+h\sum_{j=0}^{k}\bar{\beta}_j^{(k)}(\nu^*)f_{n+j}+h\beta_{\nu^*}^{(k)}f_{n+\nu^*} \tag{3.7a)*}$$

$$y_{n+\nu^*}+\sum_{j=0}^{k}\hat{\alpha}_j^{(k)}(\nu^*)y_{n+j}=h\hat{\beta}_k^{(k)}(\nu^*)f_{n+k}+g_{n+k}. \tag{3.7b)*}$$

Note that it is easy to see $y_{n+\nu^*}=y(t_n+\nu^*h)+O(h^{k+3})$ in (3.7b)*, therefore the solution y_{n+k} of (3.7)* still has the accuracy order $(k+3)$. Here again the nonlinear algebraic equations defining y_{n+k} are solved using the same technique iterated to convergence. Note also that there is a little difference between the algebraic equations defining respectively y_{n+k} and $\bar{y}_{n+k}$, and practical experience has shown that, since the value $\bar{y}_{n+k}$ usually serves as a very good initial approximation to y_{n+k}, this iterated procedure almost invariably converges in one iteration.

(4) Compute the quantity $\eta_{n+k}=\|y_{n+k}-\bar{y}_{n+k}\|_\infty$ as an estimate of the local error in $\bar{y}_{n+k}$ and control the steplength of integration on the basis of this estimate. If η_{n+k} is less than a prescribed local tolerance, the solution $\bar{y}_{n+k}$ is acceptable; otherwise the steplength or order will be changed.

In a word, our complete algorithm requires to evaluate at most once the coefficient matrix W_{n+k} and LU factorization.

We will not discuss the computational aspects of our algorithm any further, Theoretical analysis indicates that the hybrid method has all the advantages of Enright's method but not its principal disadvantages. The numerical results given in the next section show that a well-implemented version of the hybrid method (3.1) will be useful for the numerical integration of stiff systems.

4. Numerical Results

We present some preliminary numerical results which can be used to make a comparison between the second derivative multistep method, namely Enright's method (E2M), and the two-stage implicit hybrid method (H2M). The aim of this investigation is to demonstrate numerically the generally superior performance ot H2M of a given fixed steplength over E2M with the same steplength, for a small selection of test problems. At the present we do not claim that our numerical results demonstrate the superiority of our method over Enright's. However, as stated in the previous section at least, we do feel that our results indicate that a properly implemented version of our method should be useful for the numerical integration of stiff systems.

All the numerical test problems were implemented on a FELIX C-512 machine. Numerical results are obtained for linear and nonlinear stiff problems using double precision arithmetic. For comparison the problems were also solved by Enright's method (E2M). The numerical integration formulas which we considered are respectively

H2M$(k=1)$

$$\begin{cases} y_{n+1}=y_n+h\left[\left(\frac{1}{2}-\frac{1}{6\nu}\right)f_n+\left(\frac{1}{2}-\frac{1}{6(\nu-1)}\right)f_{n+1}\right] \\ \qquad -\frac{h}{6\nu(\nu-1)}f_{n+\nu}, \qquad\qquad \text{for } \nu=\frac{1}{2},\ \frac{3}{2},\ 2, \\ y_{n+\nu}=(\nu-1)^2y_n-\nu(\nu-2)y_{n+1}+\nu(\nu-1)hf_{n+1}. \end{cases}$$

H2M$(k=3)$

$$\begin{cases} y_{n+3}=y_{n+2}+\frac{h}{360}\left[\left(15-\frac{38}{\nu}\right)f_n-\left(75-\frac{114}{(\nu-1)}\right)f_{n+1}+\left(285-\frac{114}{(\nu-2)}\right)f_{n+2}\right. \\ \qquad \left.+\left(135+\frac{38}{(\nu-3)}\right)f_{n+3}-\frac{228}{\nu(\nu-1)(\nu-2)(\nu-3)}f_{n+\nu}\right] \\ \qquad\qquad\qquad \text{for } \nu=1.5,\ 2.5,\ 4, \\ y_{n+\nu}=-\frac{1}{18}(\nu-1)(\nu-2)(\nu-3)^2y_n+\frac{1}{4}\nu(\nu-2)(\nu-3)^2y_{n+1} \\ \qquad -\frac{1}{2}\nu(\nu-1)(\nu-3)^2y_{n+2}+\frac{1}{36}\nu(\nu-1)(\nu-2)(11\nu-39)y_{n+3} \\ \qquad +\frac{1}{6}\nu(\nu-1)(\nu-2)(\nu-3)hf_{n+3}. \end{cases}$$

E2M($k=1$)

$$y_{n+1}=y_n+h\left(\frac{1}{3}y'_n+\frac{2}{3}y'_{n+1}\right)-\frac{1}{6}h^2y''_{n+1}$$

and E2M($k=3$)

$$y_{n+3}=y_{n+2}+h\left(\frac{7}{1080}y'_n-\frac{1}{20}y'_{n+1}+\frac{19}{40}y'_{n+2}+\frac{307}{540}y'_{n+3}\right)-\frac{19}{180}h^2y''_{n+3}.$$

These formulas were implemented with the fixed steplength $h=0.1$.

The two test problems ([7], problems B and E2) in the interval $0\leqslant t\leqslant 1$ are respectively

$$(\mathrm{P1})\begin{cases} y'_1=-10y_1+\mu y_2, \\ y'_2=-\mu y_1-10y_2 \\ y'_3=-4y_3 \\ y'_4=-y_4 \\ y'_5=-\dfrac{1}{2}y_5 \\ y'_6=-\dfrac{1}{10}y_6, \end{cases} \qquad \text{for } \mu=3,\ 8,\ 25,\ 50,\ 100, \quad y_i(0)=1,\ i=1(1)6,\ t_f=1.$$

$$(\mathrm{P2})\begin{cases} y'_1=y_2, \\ y'_2=5(1-y_1^2)\cdot y_2-y_1, \quad y_1(0)=2,\ y_2(0)=0,\ t_f=1. \end{cases}$$

In order to save space in Tables 1 and 2 we give only part of the numerical results obtained for the integration of (P1) using E2M ($k=1$) and H2M ($k=1$) with $\nu=0.5$, 1.5, 2, where L denotes the number of times of the iteration.

As can be seen from the two tables, the iterated scheme of H2M($k=1$) converges

Table 1. Partial results for the integration of (P1) with $\mu=8$

Exact sol.	H2M ($k=1$)	E2M ($k=1$)		
	$\nu=0.5$, 1.5, 2, $L=1$	$L=1$	$L=3$	$L=5$
$0.383111*10^{-4}$	$0.393271*10^{-4}$	$0.879544*10^{-3}$	$0.189080*10^{-3}$	$0.188477*10^{-3}$
$-0.515225*10^{-4}$	$-0.727544*10^{-4}$	$-0.747251*10^{-3}$	$0.403636*10^{-4}$	$0.316680*10^{-4}$
$0.183156*10^{-1}$	$0.182564*10^{-1}$	$0.219211*10^{-1}$	$0.224850*10^{-1}$	$0.224852*10^{-1}$
0.367879	0.367874	0.373623	0.373663	0.373663
0.606530	0.606530	0.608976	0.608980	0.608980
0.904837	0.904837	0.904837	0.904837	0.904837

Table 2. Partial results for the integration of (P1) with $\mu=50$

Exact sol.	H2M ($k=1$)	E2M ($k=1$)		
	$\nu=0.5$, 1.5, 2, $L=1$	$L=1$	$L=2$	$L=3$
$0.318976*10^{-4}$	$0.183124*10^{-4}$	$\doteq -2*10^5$	$\doteq 10^2$	$\doteq 10$
$0.557212*10^{-4}$	$0.417560*10^{-5}$	$\doteq -7*10^5$	$\doteq 4*10^2$	$\doteq 3*10$
The remaining are the same with Table 1				

in only one iteration but E2M ($k=1$) can not, and for (P1) with $\mu=50$ (including $\mu=100$) the solution of H2M ($k=1$) is stable but E2M ($k=1$) is not.

In Tables 3 and 4 we give details of the numerical results obtained for the integration of (P2) using H2M ($k=1$, 3) and E2M ($k=1$, 3). Where ER_L ($L=1(1)4$) denotes greatest ralative error at $t=1$.

Table 3. Results for the integration of (P2)

L	Exact sol.	E2M ($k=1$)	H2M ($k=1$)		
			$\nu=0.5$	$\nu=1.5$	$\nu=2$
1	$y_1=1.869409210$ $y_2=-0.1482399437$	1.86932736 −0.14823453	1.86961334 −0.14821197	1.86959285 −0.14821464	1.86946621 −0.14823196
ER_1		$4.38*10^{-5}$	$1.89*10^{-4}$	$1.71*10^{-4}$	$5.39*10^{-5}$
2		1.86915116 −0.14828214	1.8693798 −0.14823609	1.86942872 −0.14823725	1.86941763 −0.14823871
ER_2		$2.85*10^{-4}$	$2.60*10^{-5}$	$1.82*10^{-5}$	$8.32*10^{-6}$
3		1.86914305 −0.14828383	1.86943690 −0.14823624	1.86942681 −0.14823751	1.86941655 −0.14823886
ER_3		$2.96*10^{-4}$	$2.50*10^{-5}$	$1.64*10^{-5}$	$7.31*10^{-6}$
4		1.86914217 −0.14828404	1.86943689 −0.14823624	1.86942679 −0.14823751	1.86941653 −0.14823886
ER_4		$2.98*10^{-4}$	ER_3	ER_3	ER_3
5					
ER_5		ER_3	ER_3	ER_3	ER_3

Table 4. Results for the integration of (P2)

L	E2M ($k=3$)	H2M ($k=3$)		
		$\nu=1.5$	$\nu=2.5$	$\nu=4$
1	1.869195544 −0.148238475	1.869401661 −0.148241053	1.869377504 −0.148244414	1.869288182 −0.148256711
ER_1	$1.14*10^{-4}$	$7.48*10^{-6}$	$3.02*10^{-5}$	$1.13*10^{-4}$
2	1.869240757 −0.148268008	1.869409982 −0.148239874	1.869408653 −0.148240069	1.869403162 −0.148240828
ER_2	$1.89*10^{-4}$	$4.72*10^{-7}$	$8.43*10^{-7}$	$5.96*10^{-6}$
3	1.869247190 −0.148267030	1.869410010 −0.148239870	1.869408898 −0.148240029	1.869404779 −0.148240603
ER_3	$1.83*10^{-4}$	$5.00*10^{-7}$	$5.73*10^{-7}$	$4.45*10^{-6}$
4	1.869247962 −0.148266907		1.869408900 −0.148240028	1.869404830 −0.148240600
ER_4	$1.82*10^{-4}$	ER_3	$5.67*10^{-7}$	$4.43*10^{-6}$

Where the exact solutions are given in Table 3.

As can be seen from these two tables, the solutions of H2M ($k=1$, 3) are more accurate than those of E2M ($k=1$, 3), and the iterated schemes of H2M converge more rapidly than E2M.

Table 5. Error constant C_{k+3}

k	1	2	3	4	5	6	7
C_{k+3}	$\frac{1}{72}$	$\frac{7}{1440}$	$\frac{17}{7200}$	$\frac{41}{30240}$	$\frac{731}{846720}$	$\frac{8563}{14515200}$	$\frac{27719}{65318400}$

We conclude by a remark concerning the multistage implicit hybrid method which does not involve multiderivative. If the stability for the linear system $y'=Ay$ is analyzed the multistage implicit hybrid method can have the stability properties of a multiderivative method. The multiderivative and equivalent multistage hybrid methods require the solution of a linear equation involving a polynomial in the Jacobian. If this polynomial is chosen to have equal roots, an LU factorization of a linear polynomial can be performed, followed by multiple back substitutions. This makes maximum use of the sparsity by avoiding powers of the Jacobian. For example, the optimal second derivative methods developed by Enright in [11] corresponds to the "optimal" two-stage implicit hybrid method which comprises two-parameters.

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