

ONE-STEP METHODS FOR THE NUMERICAL SOLUTION OF STIFF ORDINARY DIFFERENTIAL SYSTEMS

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1. INTRODUCTION

This paper deals with the numerical solution of the values problem for stiff systems of ordinary differential equations. Throughout we shall use

$$(1.1) \quad y'(t) = f(y(t)), \quad 0 \leq t \leq T, \quad y(0) = y_0$$

to denote problems or classes of problems under consideration. Here $y(t)$ is a real vector of N elements and f , a real-valued vector nonlinear function. We assume that f is a Lipschitz function. This implies that for all initial vectors, y_0 , the problem possesses a unique solution for all $t \in [0, T]$.

Stiff problems occur in many fields of applications including chemical kinetics, reactor kinetics, control theory, dynamics of missile guidance, electronic circuit theory, biomathematics etc.

The essence of stiffness is the solution to be computed is slowly varying, but perturbations exist which are rapidly damped. The presence of such perturbations complicates the numerical computation of the solution.

Example 1 : We consider the scalar equation :

$$y'(t) = \lambda y(t) + g'(t) - \lambda g(t), \quad t \geq 0, \quad y(0) = y_0, \quad \lambda \ll 0 \quad (1.2)$$

where g is slowly varying as a function of t only, the solution $y(t)$ is given by

$$y(t) = g(t) + e^{\lambda t} [y_0 - g(y_0)]$$

Because $\lambda \ll 0$, after a very short time distance the transient $e^{\lambda t} [y_0 - g(y_0)]$, which is also called the stiff component or strongly varying solution component, is no longer present in the solution $y(t)$. The function $g(t)$ dominates the solution to be computed on the larger part of the integration interval $[0, T]$. The explicit Euler method

$$y_{n+1} = y_n + hf(y_n), \quad n = 0(1)M, \quad Mh = T$$

is damped only if $-2 < h\lambda < 0$. This condition of numerical stability imposes a severe restriction of the stepsize h if $\lambda \ll 0$, even when $y_n - g(t_n)$ is negligibly small. This situation is typically when we apply an explicit linear method to a stiff problem. The stepsize is restricted by numerical stability rather than by accuracy.

Example 2: For the general linear problem

$$y'(t) = Ay(t) + r(t), \quad t \geq 0, \quad y(0) = y_0$$

where A is a constant $N \times N$ matrix and r is a time dependent forcing term, the most obvious way of defining stiffness is to impose conditions on the eigenvalues of A . Different solution components occur when the Jacobian matrix possesses eigenvalues which differ greatly in magnitude. Let $\lambda_1, \dots, \lambda_N$ denote these eigenvalues. Then (1.5) may be called *stiff* if

- (i) there exist λ_i with $\operatorname{Re}(\lambda_i) \ll 0$;
- (ii) there exist λ_i of moderate size, i.e., $|\lambda_i|$ is small when compared with the modulus of the eigenvalues satisfying (i);
- (iii) no λ_i exist with a large positive real part;
- (iv) no λ_i exist with a large imaginary part, unless $\operatorname{Re}(\lambda_i) \ll 0$.

It is assumed here that the forcing term $r(t)$ is as smooth as the slowly varying exponentials in the solution.

Stiffness for a nonlinear problem is usually described in terms of the eigenvalues of the Jacobian matrix. The argument is based on local linearization.

In the literature, stiff problems are also called problems with large Lipschitz constants, because the property of those is the presence of a large classical Lipschitz constant

$$TL = T \sup_u \|f'_y(u)\| \gg 1$$

The main requirement for a good stiff method is that it should have strong stability properties. The concept of absolute stability is connected with the scalar equation

$$(1.2) \quad y'(t) = \lambda y(t), \quad \lambda \in C, \quad t \geq 0, \quad y(0) = y_0$$

Though this equation is very simple, its use as a model to predict the stability behaviour of numerical methods for general nonlinear systems. An one-step method applied to this test equation reduces to

$$(1.3) \quad y_{n+1} = R(z)y_n, \quad z = h\lambda$$

where R is called the *stability function*. The method is said to be *absolutely stable* at $z \in C$ if, for this z , $|R(z)| \leq 1$. The set of all points z which satisfies this requirement is called *the absolute stability region*. If the half-plane $\operatorname{Re}(z) \leq 0$ is contained in the absolute stability region, the method is said to be *A-stable*. A condition which ensures that the method has the correct damping at $z = -\infty$, is *stability at infinity*: $\lim_{z \rightarrow -\infty} R(z) = 0$. Then, a one-step numerical method is said to be *L-stable* if it is *A-stable* and stable at infinity. In the case of *A-stability* and only $\lim_{z \rightarrow -\infty} |R(z)| < 1$, we have *strong A-stability*.

The *A-stability* criterion was originally developed for linear multistep methods, but has been widely applied to Runge-Kutta formula. It is well known from a famous results of Dahlquist, that the highest attainable order of an *A-stable* implicit linear multistep method is limited to two. The explicit methods do not have property of *A-stability*. Among the class of implicit Runge-Kutta formula we have the possibility of deriving *A-stable* methods of high order. One of the main arguments against

the use of these was on the grounds of the amount of computational effort required to solve the resulting systems of algebraic equations. Research into finding efficient stiff methods has followed some main directions:

- (1) inside the Runge-Kutta class, the investigation of the use of transformation methods to obtain a solution of algebraic equations in an efficient manner of the derivation of different classes of implicit Runge-Kutta formula which do not call for the solution of a system of simultaneous equations;
- (2) the generalization of linear methods by formula with high derivations, cyclic and composite methods, hybrid methods, pseudo Runge-Kutta, etc.;
- (3) the construction of nonlinear methods such as that of rational Runge-Kutta type (see on this subject an author's paper [12]);

The aim of this paper is to analyse the possibility to replace second derivative multistep formula by hybrid methods with same stability properties. We make a first step with the support of one-step methods. Examples for some classes are given in the following sections.

In section 3 we deal with second derivative methods and in section 4 with hybrid methods connected to those. We examine carefully the stability properties and the performance. Our purpose is to derive *A-stable* formula. Finally, in section 5, numerical comparisons of some new methods with the classical ones are given. The efficiency of the new integrations is demonstrated by solving a series of challenging test problems.

2. BACKGROUNDS

One-leg methods were introduced by Dahlquist in 1975 (see reference [7]). The characteristic of these is the presence of only one value of f in each step. This made possible a certain theoretical stability analysis for stiff nonlinear problems (*G-stability*, contractivity). Every linear k -step method

$$\sum_{i=0}^k \alpha_{k-i} y_{n+1-i} = h \sum_{i=0}^k \beta_{k-i} f_{n+1-i}, \quad f_{n+1} = f(t_n + ih, y_{n+1}), \quad \sum_{i=0}^k \beta_{k-i} = 1$$

has a „one-leg twin”

$$(2.1) \quad \sum_{i=0}^k \alpha_{k-i} y_{n+1-i} = hf \left(\sum_{i=0}^k \beta_{k-i} t_{n+1-i}, \sum_{i=0}^k \beta_{k-i} y_{n+1-i} \right)$$

The point in which the function is evaluated is named *collocation point*.

For linear autonomous problem the one-leg difference equation is identical to the linear multistep equation. Hence, the stability regions are the same for a linear multistep method and its one-leg twin.

It was realized that, for fixed step size, the one-leg implementation of the equivalent linear k -step method would be advantageous with regard to storage economy. For variable stepsize, in which case they are not equivalent, the one-leg methods seem to have superior stability properties, in stiff problems. On the other side, Dahlquist methods are particularly easy to apply to implicit differential equations.

The disadvantage is the decrease of the maximum order versus the multistep formula. In [7], Dahlquist shows that the maximum order of a one-leg formula with k steps is $k + 1$. Therefore, in the case of one-step method the maximum order is 2.

Second derivative multistep formula. Iteration schemes that have been proposed for stiff equations are usually based on a modified Newton-Raphson technique. The usual predictor-corrector iteration scheme is not feasible since $\|h df/dy\|$ must remain small to ensure the convergence. Realizing that the Jacobian matrix might be used for the iteration scheme, Enright in 1974 (see reference [9]) consider the possibility of developing a class of formula that explicitly uses the Jacobian matrix. Since $y'' = (df/dy)y'$ for autonomous systems, the above-mentioned author considers the following class of second derivative formula :

$$\sum_{i=0}^k \alpha_i y_{n+i} - h \sum_{i=0}^k \beta_i f_{n+i} - h^2 \sum_{i=0}^k \gamma_i f'_{n+i} = 0, f'_{n+i} = J_{n+i} f_{n+i}, J_{n+i} = \frac{df}{dy}(y_{n+i}) \quad (2.2)$$

If the coefficients γ_i are zero, except for the last, the condition of stability at infinity is ensured and the maximum order of the formula with k steps is $k + 2$.

Example: For the one-step case, the method is L -stable as well and of order 3:

$$(2.3) \quad y_{n+1} = y_n + \frac{h}{3}(2f_{n+1} + f_n) - \frac{h^2}{6}f'_{n+1}$$

The local truncation error $TE = y(t_{n+1}) - y(t_n)$ is

$$TE = \frac{h^4}{72} \frac{d^3 f}{dt^3}(y(t_n)) + O(h^5)$$

Problem 1: Is it possible to build similar one-leg formula for second derivative multistep methods? How great is the loss in the accuracy order of such a formula?

England's hybrid method. England (see reference [8]) gives a partial answers to this question. He built up a θ -class of hybrid methods with the same stability properties as those of the Enright's formula.

Example: For the one-step case, the methods of order 3 have the following form :

$$(2.4) \quad \begin{cases} y_{n+1} = y_n + h \frac{3\theta - 1}{6\theta} f_n + h \frac{3\theta - 2}{6(\theta - 1)} f_{n+1} - \frac{h}{6\theta(\theta - 1)} f'_{n+1} \\ y_{n+0} = (\theta - 1)^2 y_n - \theta(\theta - 2) y_{n+1} + h\theta(\theta - 1) f_{n+1} \end{cases}$$

The particular member taken into implementation by the author of the above mention paper is in accordance to the condition of a zero coefficient

in the first equation for f_n :

$$(2.5) \quad \begin{cases} y_{n+1} = y_n + \frac{h}{4} f_{n+1} + \frac{3h}{4} f_{n+1/3}, \\ y_{n+1/3} = \frac{5}{9} y_{n+1} + \frac{4}{9} y_n - \frac{2h}{9} f_{n+1} \end{cases}$$

$$TE = -\frac{h^4}{216} \left(\frac{d^3 f}{dt^3} - 4 \frac{d^2 f}{dt^2} \frac{df}{dt} \right) (y(t_n)) + O(h^5)$$

The formula certainly is L -stable and of order 3.

The derivative calculus is replaced by a function evaluation in a new point.

Highest order. It is possible to derive a second derivative method with upper order than 3. Obrechhoff's formula is of order 4, but it is only A -stable :

$$(2.6) \quad y_{n+1} = y_n + \frac{h}{2}(f_{n+1} + f_n) - \frac{h^2}{12}(f'_{n+1} - f'_n)$$

$$TE = \frac{h^5}{720} \frac{d^4 f}{dt^4}(y(t_n)) + O(h^6)$$

Problem 2: Is it possible to build up hybrid methods of order 4 similar to Obrechhoff's second derivative formula? Preserving the convention of only one implicit equation to solve in y_{n+1} , is it possible to reach better stability properties?

Exponential fitting. The idea of using exponentially fitted formula for the approximate numerical integration of certain classes of stiff systems has received considerable attention. The basic idea is to derive integration formula containing free parameters, other than the step length of integration, and then choose these parameters so that a given exponential function satisfies the integration formula exactly. It needs to be emphasized that exponential fitting is really applicable to only a limited class of stiff systems, i.e., to systems having a Jacobian which is in some sense slowly varying, with all the eigenvalues of large modulus, lying in two or fewer clusters. However, for systems for which exponential fitting integration formula are substantially more efficient than conventional ones.

When the method is applied to the test equation, the approximation error is related to

$$T(z) = R(z) - e^{-z}, \quad z = h\lambda$$

If for some $q = h\lambda_0$ we have $T(q) = 0$, then the numerical solution of the test equation is exact in the discrete meaning. If q is a zero of $d + 1$ multiplicity, we note that $R(z)$ is exponential fitted of order d at $z = q$. In the stiff case the exponential fitting points are the biggest eigenvalues multiplied by the stepsize.

Pseudo-Runge-Kutta methods. Bokhoven's formula. Pseudo Runge-Kutta process are generalization of the classical methods with the same name. Bokhoven in 1980 (see reference [1]) describes such methods named by the author *Implicit Endpoint Quadrature Formula*. They have the following form :

$$(2.7) \quad y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i, \quad k_i = (1 - \theta_i) y_n + \theta_i y_{n+1} + h \sum_{j=0}^s a_{ij} k_j, \quad i = 1(1)s$$

Also, the same author established the order conditions.

Example 1: Among other formula, we see some *A-stable* ones of order 3 and 4. The formula of order 4 is the following :

$$(2.8) \quad \begin{cases} y_{n+1} = y_n + \frac{h}{6}(f_{n+1} + f_n) + \frac{2h}{3} f_{n+\frac{1}{2}}, \\ y_{n+\frac{1}{2}} = \frac{1}{2}(y_{n+1} + y_n) - \frac{h}{8}(f_{n+1} - f_n) \end{cases}$$

$$TE = -\frac{h^5}{2880} \left(\frac{d^4 f}{dt^4} - 5 \frac{d^3 f}{dt^3} \frac{df}{dt} \right) (y(t_n)) + O(h^6)$$

Example 2: For order 3 are given England's one-step scheme and :

$$(2.9) \quad \begin{cases} y_{n+1} = y_n + \frac{h}{2}(f_{n+\theta_1} + f_{n+\theta_2}), \\ y_{n+\theta_1} = \frac{2 + \sqrt{3}}{6} y_n + \frac{4 - \sqrt{3}}{6} y_{n+1} - \frac{h}{6} f_{n+1}, \quad \theta_1 = \frac{3 - \sqrt{3}}{6}, \quad \theta_2 = \frac{3 + \sqrt{3}}{6} \\ y_{n+\theta_2} = \frac{4 - \sqrt{3}}{6} y_n + \frac{2 + \sqrt{3}}{6} y_{n+1} + \frac{h}{4} f_n \end{cases}$$

$$TE = -\frac{h^3}{24} \left(\frac{d^2 f}{dt^2} \frac{df}{dt} \right) (y(t_n)) + O(h^5)$$

3. ONE LEG METHODS ASSOCIATED TO SECOND DERIVATIVE FORMULA

We consider the class of integration formula (OLS 1)

$$\sum_{i=0}^k \alpha_{k-i} y_{n+1-i} - hf \left(\sum_{i=0}^k \beta_{k-i} t_{n+1-i}, \sum_{i=0}^k \beta_{k-i} y_{n+1-i} \right) - \frac{h^2}{2} \delta f', \left(\sum_{i=0}^k \gamma_{k-i} t_{n+1-i}, \sum_{i=0}^k \gamma_{k-i} y_{n+1-i} \right) = 0$$

where $\sum_{i=0}^k \gamma_{k-i} = \sum_{i=0}^k \beta_{k-i} = 1$.

Order. A statement about the order can be proved similar to that for one-leg methods (like in [7]).

PROPOSITION 1. *The maximum order of a method (OLS 1) is $k+2$ and there are at least $k+1$ distinct methods with this property. For these only one coefficient β_i is not zero.*

Proof. We introduce operator notation

$$\rho y_n = \sum_{i=0}^k \alpha_{k-i} y_{n+1-i}, \quad \sigma y_n = \sum_{i=0}^k \beta_{k-i} y_{n+1-i}, \quad \gamma y_n = \sum_{i=0}^k \gamma_{k-i} y_{n+1-i}$$

The differentiation error operator L_a and the interpolation error L_i are

$$(L_a \varphi)(t_n) = \rho \varphi(t_n) - h \varphi'(t_n) - \frac{\delta h^2}{2} \varphi''(\gamma t_n)$$

$$(L_i \sigma \varphi)(\sigma t_n) = \sigma \varphi(t_n) - \varphi(\sigma t_n), \quad (L_i \gamma \varphi)(\gamma t_n) = \gamma \varphi(t_n) - \varphi(\gamma t_n)$$

where φ is a sufficiently smooth function. Then, the local truncation error is

$$\begin{aligned} Ly(t_n) &= \rho y(t_n) - hf(\sigma t_n, \sigma y(t_n)) - \frac{h^2 \delta}{2} f'(\gamma t_n, \gamma y(t_n)) = \\ &= (L_a y)(t_n) + h[f(\sigma t_n, y(\sigma t_n)) - f(\sigma t_n, \sigma y(t_n))] + \frac{h^2 \delta}{2} [f(\gamma t_n, y(\gamma t_n)) - \\ &\quad - f(\gamma t_n, \gamma y(t_n))] \approx (L_a y)(t_n) - hf'(\sigma t_n, y(\sigma t_n)) (L_i \sigma y)(\sigma t_n) - \\ &\quad - \frac{h^2 \delta}{2} f''(\gamma t_n, y(\gamma t_n)) (L_i \gamma y)(\gamma t_n) \end{aligned}$$

If

$$L\varphi = O(h^p), \quad L_a \varphi = O(h^{p_a}), \quad L_i \sigma \varphi = O(h^{p_1}), \quad L_i \gamma \varphi = O(h^{p_1})$$

then

$$p = \min\{p_a, p_1 + 1, p_2 + 2\}$$

Dahlquist shows in [7] that

$$\max p_1 = \begin{cases} \infty & \text{if } \exists j : \sigma t_n = t_{n+1-j}, \quad 0 \leq j \leq k \\ k, & \text{otherwise} \end{cases}$$

A similar statement holds for p_2 . If $p_1 = p_2 = \infty$ we don't have a one-leg methods. Then the maximum order is obtained when $p_1 = \infty$ and $p_2 = \infty$. If we note $\theta = (t_{n+1} - \gamma t_n)/h$, p_2 is maximized when

$$\gamma_{k-i}(\theta) = \frac{\omega(\gamma t_n)}{(\gamma t_n - t_{n+1-i}) \omega'(t_{n+1-i})}, \quad \omega(t) = \prod_{j=0}^k (t - t_{n+1-j})$$

For each j we have $k+2$ free parameters: $\theta, \delta, \alpha_1, \dots, \alpha_k$. In these conditions, $\max p_a = k+2$ and, in conclusion, $\max p = k+2$. For each j , the linear system of condition for order $p_a = k+2$ has at least one solution.

One-step method. We study the particular case of the *one-step formula* with minimum order 2:

$$y_{n+1} = y_n + hf \left(\frac{1+u}{2} y_{n+1} + \frac{1-u}{2} y_n \right) - h^2 \frac{u}{2} f' \left(\frac{1+v}{2} y_{n+1} + \frac{1-v}{2} y_n \right).$$

Maximum order. We note that it is possible to eliminate the $O(h^3)$ terms from the truncation error by choosing $u = 1, v = \frac{1}{3}$ or $u = -1, v = -\frac{1}{3}$. Then the formula has the optimal order 3. One from these is the following (for an autonomous system):

$$(3.1) \quad y_{n+1} = y_n + hf(y_{n+1}) - \frac{h^2}{2} f' \left(\frac{2}{3} y_{n+1} + \frac{1}{3} y_n \right)$$

$$TE = -\frac{h^3}{72} \left[\frac{d^3 f}{dy^3} f^3 - 3 \left(\frac{df}{dy} \right)^3 f \right] (y(t_n)) + O(h^5)$$

This truncation error is comparable with the error produced by Enright's one-step method.

Stability properties. In order to examine the stability properties of our formula, we use the maximum modulus theorem. Applying the method of order 2 to the scalar test equation, we obtain the stability function

$$R(z) = \frac{1 + z(1-u)/2 - z^2 u(1-v)/4}{1 - z(1+u)/2 + z^2 u(1+v)/4}$$

We notice that $|R(ip)| \leq 1, \forall p \in \mathbf{R}$ if and only if $v \geq 0$. Under this circumstance, the requirement that $R(z)$ may be analytic in $Re(z) < 0$, i.e., that there are not zero of the denominator of $R(z)$ in the left complex half-plane, is equivalent with $u > 0$. The inequality $\lim_{z \rightarrow -\infty} |R(z)| < 1$ is reduced to $v > 0$. Thus, the method is *strong A-stable if and only if* $u > 0, v > 0$ and *L-stable when* $v = 1, u > 0$. The method of maximum order 3 is only *strong A-stable*.

One-leg associated to second derivative formula. If we consider a second derivative formula of minimum order 2.

$$y_{n+1} = y_n + h \left(\frac{1+a}{2} f_{n+1} + \frac{1-a}{2} f_n \right) - h^2 \left(\frac{b+a}{4} f'_{n+1} - \frac{b-a}{4} f'_n \right)$$

we can associated a twin formula of the new class with the same stability function for $u=a, v=b/a$. We exclude the case of $a=0$. Thus, if the second derivative method is L-stable and order 2, we can associate to it a formula (3.1) also L-stable and of order 2.

Example: In the particular case of the 3th-order Enright's method and for an autonomous system, the associated formula is of order 2 and has

the following from

$$(3.2) \quad y_{n+1} = y_n + hf \left(\frac{2}{3} y_{n+1} + \frac{1}{3} y_n \right) - \frac{h^2}{6} f'(y_{n+1})$$

The error produced at each step by this method is

$$TE = \frac{h^3}{9} \left(\frac{d^2 f}{dy^2} f^2 \right) (y(t_n)) + O(h^4)$$

In the above class of methods the maximum order is obtained when only one β_i is not zero. The following class of methods does not suffer this restriction.

$$(OLS 2) \quad \sum_{i=0}^k \alpha_{k-i} y_{n+1-i} - h \sum_{i=0}^k \beta_{k-i} f_{n+1-i} - \frac{h^2 \delta}{2} f' \left(\sum_{i=0}^k \gamma_{k-i} t_{n+1-i}, \sum_{i=0}^k \gamma_{k-i} y_{n+1-i} \right) = 0$$

The maximum order is also $k+2$, but there are k free parameters in the set of α_i or β_i .

One-step case. If we take into account the one-step case, we can write the method of minimum order 2

$$(3.3) \quad y_{n+1} = y_n + h \left(\frac{1+u}{2} f_{n+1} + \frac{1-u}{2} f_n \right) - h^2 \frac{u}{2} f' \left(\frac{1+v}{2} y_{n+1} + \frac{1-v}{2} y_n \right)$$

Order. Unfortunately, it is not possible to reach order 4 with such a method, but the formula of order 3 forms a class depending on a free parameter since the unique restriction is $uv = \frac{1}{3}$.

Stability. The *A*- and *L*-stability conditions are the same for the above mentioned class, because the stability function is the same. If the free parameter is chosen in such a way that the method is stable at infinity, we get Enright's one-step formula. If the free parameter is chosen for exponential fitting at $q \in C_- = \{z \in C \mid Re z < 0\}$: $R(q) = e^q$, then

$$u = w = \frac{1}{3v} = \frac{1}{3} \frac{(-q^2 + 6q - 12)e^q + q^2 + 6q + 12}{(q^2 - 2q)e^q + q^2 + 2q}$$

Enright's method can be seen thus as an exponential fitting to $-\infty$ of the formula in discussion, because $\lim_{q \rightarrow -\infty} u(q) = \frac{1}{3}$. The exponential fitting to zero is not possible since $\lim_{q \rightarrow 0} u(q) = 0$. It is easy to verify analytically that the exponentially fitted formula is *A-stable* for any $q \in \mathbf{R}^*$ because $u(q) > 0$.

4. HYBRID METHODS

We pose the problem to find new hybrid methods which can replace the Jacobian, which is necessary to calculate for a formula of the above section. We search for a scheme with the following form

$$(HM 1) \begin{cases} y_{n+1} = y_n + \frac{1+u}{2} hf(vy_{n+1} + (1-v)y_n) + \frac{1-u}{2} hf_{n+0} \\ y_{n+0} = wy_{n+1} + (1-w)y_n + \frac{h}{2}(\theta - w + x)f_{n+1} + \frac{h}{2}(\theta - w - x)f_n \end{cases}$$

The first equation is known as the *quadrature formula* and the second, as the *interpolation formula*.

Order. The maximum order of these schemes is 3. If we take into account the conditions of order 3 for the quadrature formula and of order 2 for the interpolation formula, the hybrid scheme preserves the order 3 of the quadrature formula. We get two classes that depend each on a parameter of the second equation. The coefficients are given by $u = \pm \frac{1}{2}$, $x = -\frac{2}{9}$ and in a *first case* $v = 0$, $\theta = \frac{2}{3}$ or in a *second case* $v = 1$, $\theta = \frac{1}{3}$, where w remains a free parameter. The condition of order 3 for the interpolation formula give two methods with the error coefficient equal to that of the quadrature formula. One, for $\theta = \frac{2}{3}$, is

$$(4.1) \begin{cases} y_{n+1} = y_n + \frac{h}{4}f_n + \frac{3h}{4}f_{n+2/3} \\ y_{n+2/3} = \frac{20}{27}y_{n+1} + \frac{7}{27}y_n - \frac{4h}{27}f_{n+1} + \frac{2h}{27}f_n \end{cases}$$

$$TE = \frac{h^4}{216} \left(\frac{d^3f}{dt^3} \right) (yt_n) + O(h^4)$$

The local truncation error is lower than the one of Enright's one-step formula and for some system functions f , lower than the one of England's method.

Stability. Strong A -stability takes place, in the first case, if $w > \frac{2}{3}$, and, in the second case, if $w > \frac{1}{3}$. Thus, the above method is an example of strongly A -stable class member.

Exponential fitting. In the case of order 2, the free parameter w may be used for exponential fitting. In the first case we get

$$w(q) = \frac{4(q^2 - 6)e^q + 2q^2 + q + 6}{9(q^2 - 2q)e^q + q^2 + 2q}, \quad \lim_{q \rightarrow -\infty} w(q) = \frac{8}{9}, \quad \lim_{q \rightarrow 0} w(q) = \frac{2}{3}$$

and the formula is *strongly A-stable* for any $q \in \mathbb{R}^*$. In the second case

$$w(q) = \frac{1(q^2 + 6q - 24)e^q + 5q^2 + 18q + 24}{9(q^2 - 2q)e^q + q^2 + 2q}, \quad \lim_{q \rightarrow -\infty} w(q) = \frac{5}{9}, \quad \lim_{q \rightarrow 0} w(q) = \frac{1}{3}$$

Also in this case the corresponding formula is *strongly A-stable* for any $q \in \mathbb{R}^*$.

If, instead of the exponential fitting we put the condition of stability at infinity, then we get two methods. One is England's one-step method for $w = \frac{5}{9}$ and is the last formula exponentially fitted at $-\infty$. Another, in the case $\theta = \frac{2}{3}$, $w = \frac{8}{9}$ is also a formula exponentially fitted at $-\infty$

$$(4.2) \begin{cases} y_{n+1} = y_n + \frac{h}{4}f_n + \frac{3h}{4}f_{n+2/3} \\ y_{n+2/3} = \frac{8}{9}y_{n+1} + \frac{1}{9}y_n - \frac{2h}{9}f_{n+1} \end{cases}$$

$$TE = \frac{h^4}{216} \left(\frac{d^3f}{dt^3} + 2 \frac{d^2f}{dt^2} \frac{df}{dt} \right) (yt_n) + O(h^5)$$

Thus, the formula is comparable with England's one step scheme and Enright's formula. It is a better alternative than (4.1), because it has the property of L -stability. Formula (4.2) is also included in the θ -class described by England, which successfully replaces Enright's method and contains only L -stable methods.

England's θ -class contains all L -stable methods with the minimum order 1 in both equations of the following formula class

$$(HM 2) \begin{cases} y_{n+1} = y_n + h \left(\frac{v+u}{2} f_{n+1} + \frac{v-u}{2} f_n \right) - h v f_{n+0} \\ y_{n+0} = w y_{n+1} + (1-w)y_n + h \frac{\theta-w+x}{2} f_{n+1} + h \frac{\theta-w-x}{2} f_n \end{cases}$$

It is easier to see that for this class there is an increasing in maximum order of accuracy versus the class (HM 1). The conditions of order 4 lead to

Bokhoven's formula (2.8), which has the same stability function as Obrechhoff's method, thus it is only A -stable.

To improve the performance of Bokhoven's 3th-order scheme (2.9), we study the class :

$$\begin{cases} y_{n+1} = y_n + h \frac{1+u}{2} f_{n+0_1} + h \frac{1-u}{2} f_{n+0_2} \\ y_{n+0_1} = w_1 y_{n+1} + (1-w_1) y_n + \frac{h}{2} (\theta_1 - w_1 + x_1) f_{n+1} + \frac{h}{2} (\theta_1 - w_1 - x_1) f_n \\ y_{n+0_2} = w_2 y_{n+1} + (1-w_2) y_n + \frac{h}{2} (\theta_2 - w_2 + x_2) f_{n+1} + \frac{h}{2} (\theta_2 - w_2 - x_2) f_n \end{cases}$$

(HM 3)

Order. If we require the conditions of order 3, the methods depend on three free parameters : u, w_1, w_2

$$\theta_1 = \frac{1}{2} \pm \frac{\sqrt{3(1-u^2)}}{6(1+u)}, \quad \theta_2 = \frac{1}{2} \mp \frac{\sqrt{3(1-u^2)}}{6(1-u)},$$

$$x_1 = -\frac{1+2u}{6(1+u)}, \quad x_2 = \frac{2u-1}{6(1-u)}$$

Stability. We consider the case of order 3. The stability function is the following

$$R(z) = \frac{1 + (1-2t)z + (1/3-t)z^2}{1 - 2tz - (1/6-t)z^2}, \quad t = \frac{1+u}{4} w_1 + \frac{1-u}{4} w_2$$

The condition of *strong A-stability* is $t > \frac{1}{4}$. Bokhoven's method of order

3 is only A -stable, because $t = \frac{1}{4}$. When $t = \frac{1}{3}$, we get a class which de-

pends on two parameters (for example w_1, w_2) with the same linear stability properties as Enright's method. If we take into account the case $w_1 = w_2 = \frac{2}{3}$, then u is a free parameter and it can be chosen for minimising error.

Example 1. In the case of L -stability, if the parameters are chosen such that all equations of (HM 3) are of order 3, then one of the solutions

is the next :

$$\begin{cases} y_{n+1} = y_n + \frac{2+\sqrt{3}}{4} h f_{n+\sqrt{3}/3} + \frac{2-\sqrt{3}}{4} h f_{n-\sqrt{3}/3} \\ y_{n+\sqrt{3}/3} = \left(1 - \frac{2\sqrt{3}}{9}\right) y_{n+1} + \frac{2\sqrt{3}}{9} y_n - \frac{\sqrt{3}}{9} (\sqrt{3}-1) h f_{n+1} + \frac{2\sqrt{3}}{9} (2-\sqrt{3}) h f_n \\ y_{n-\sqrt{3}/3} = \left(1 + \frac{2\sqrt{3}}{9}\right) y_{n+1} - \frac{2\sqrt{3}}{9} y_n - \frac{\sqrt{3}}{9} (\sqrt{3}+1) h f_{n+1} - \frac{2\sqrt{3}}{9} (2+\sqrt{3}) h f_n \end{cases}$$

(4.3)

$$TE = \frac{h^4}{72} \frac{d^3 f}{dt^3}(y(t_n)) + O(h^5)$$

This method is an important one. We observe the identity of the local truncation error and of the form of stability function with Enright's method. Similar effects with the classical one-step method are obtained, but the evaluation of the Jacobian matrix to each Newton iteration step is replaced with 2 function evaluations. Here we did not find in the form of the local truncation error some perturbations produced by the interpolation equations, like in Bokhoven's one-step method.

Example 2. For such methods it is possible to reach order 4. The unique method is the following :

$$\begin{cases} y_{n+1} = y_n + \frac{h}{2} f_{n+1/2+\sqrt{3}/6} + \frac{h}{2} f_{n+1/2-\sqrt{3}/6} \\ y_{n+1/2+\sqrt{3}/6} = \left(\frac{1}{2} \pm \frac{2\sqrt{3}}{9}\right) y_{n+1} + \left(\frac{1}{2} \mp \frac{2\sqrt{3}}{9}\right) y_n - \frac{h}{6} \left(\frac{1}{2} \pm \frac{\sqrt{3}}{6}\right) f_{n+1} + \frac{h}{6} \left(\frac{1}{2} \mp \frac{\sqrt{3}}{6}\right) f_n \end{cases}$$

(4.4)

$$TE = \frac{h^5}{4320} \left(\frac{d^4 f}{dt^4} + 5 \frac{d^3 f}{dt^3} \frac{df}{dt} \right) + O(h^6)$$

Analysing the stability function, we can see that this is the same as for Obrechhoff's formula. Thus, the method is only A -stable. We observe that, for the majority of the system functions f , the level of local truncation error is lowest than the one of Obrechhoff's formula or Bokhoven's scheme (2.8). The computational effort is the same as for (2.8).

In Bokhoven's scheme (2.9) 3 function evaluations per Newton step are needed : in $y_{n+0_1}, y_{n+0_2}, y_{n+1}$. One step needs $3m+1$ function evaluations, where m is the iteration number taken to solve the implicit equation ; m is relatively small if the starting value is good.

We now consider a different class for which 3 evaluations are also necessary :

$$\begin{cases} y_{n+1} = y_n + ahf(uy_{n+1} + (1-u)y_n) + bhf(y_{n+0}) + chf(vy_{n+1} + (1-v)y_n) \\ y_{n+0} = wy_{n+1} + (1-w)y_n + hdf(uy_{n+1} + (1-u)y_n) + hef(vy_{n+1} + (1-v)y_n) \end{cases}$$

(HM4)

Order. The conditions of 3-order are :

$$a + b + c = 1, \theta = w + d + e, \theta^2 = w + 2(du + ev)$$

$$au + b\theta + cv = \frac{1}{2}, au^2 + b\theta^2 + cv^2 = \frac{1}{3}, au + b\theta^2 + cv = \frac{1}{3}$$

Under these circumstances, a formula of order 3 has three free parameters, u, v, θ .

The local error produced by the quadrature formula is

$$TE_1 = -\frac{h^4}{36} \left[\left(\frac{1}{2} - \theta \right) \frac{d^3f}{dt^3} + uv \frac{3\theta^2 - 4\theta + 1}{\theta^2 - \theta} \frac{d^3f}{dy^3} f^3 \right] (y(t_n)) + O(h^5)$$

To this is added the error produced by the approximation of y_{n+1} with the integration formula

$$TE_2 = \frac{h^4}{36} \left[(1 - \theta) \frac{d^2f}{dt^2} - \right.$$

$$\left. \frac{(u + v - 1)\theta - [6(\theta^2 - \theta) + 1]uv}{\theta^2 - \theta} \left(\frac{df}{dy} \right)^2 f \right] \frac{df}{dy} f (y(t_n)) + O(h^5)$$

We observe that the error formula introduced by England's one-step method is a particular case of the above. The advantage of using this class is the dependence on more parameters and the possibility of formulate reach order 4. The method of maximum order in this class is Bokhoven's formula (2.8).

Stability. If we impose the supplementary condition of stability at infinity, the new equation is

$$d(1 - u) + e(1 - v) = 0$$

Then the coefficients are

$$a = \frac{v - \frac{1}{2}}{v - u} + \frac{v - \theta}{6(\theta^2 - \theta)(v - u)}, \quad c = \frac{u - \frac{1}{2}}{u - v} + \frac{u - \theta}{6(\theta^2 - \theta)(u - v)}, \quad b = -\frac{1}{6(\theta^2 - \theta)}$$

$$d = \frac{(\theta^2 - \theta)(v - 1)}{v - u}, \quad e = \frac{(\theta^2 - \theta)(u - 1)}{u - v}, \quad w = 2\theta - \theta^2$$

where θ is the solution of the equation

$$[6uv - 3(u + v) + 3]\theta^2 - [6uv - 2(u + v) + 2]\theta + uv = 0$$

These methods, depending on u and v , are all L -stable because the stability function is the same as that of Enright's method and that of the θ -class of England.

Examples

1) $u = 0, v = 1$ or $u = 1, v = 0$ gives the England's θ -class ;

2) $v = 0, \theta = \frac{2}{3}$ gives a class of formula depending on u :

$$(4.5) \begin{cases} y_{n+1} = y_n + \frac{3h}{4} f_{n+2/3} + \frac{h}{4} f_n, \\ y_{n+2/3} = \frac{8}{9} y_{n+1} + \frac{1}{9} y_n - \frac{2h}{9u} f(u y_{n+1} + (1 - u)y_n) + \frac{2(1-u)h}{9u} f_n, \end{cases}$$

$$TE = \frac{h^4}{216} \left(\frac{d^3f}{dt^3} + 2 \frac{d^2f}{dt^2} \frac{df}{dt} + 18(u - 1) \frac{d^2}{dy^2} f^2 \frac{df}{dt} \right) (y(t_n)) + O(h^5)$$

For $u = 1$ we get scheme (4.2).

3) $v = 1, \theta = \frac{1}{3}$ gives England's one-step method ;

4) if $u + v = 1$, then

$$\theta = \frac{1}{2} \pm \frac{\sqrt{3}}{6}, \quad b = 1, \quad d = \frac{u}{6(u - x)}, \quad e = \frac{x}{6(u - v)},$$

$$w = \frac{1}{6} + \theta, \quad a = \frac{\theta - \frac{1}{2}}{x - u}, \quad e = \frac{\theta - \frac{1}{2}}{u - v}$$

The local truncation error is

$$TE = -\frac{h^4}{36} \left[\pm \frac{\sqrt{3}}{6} \left(\frac{d^3f}{dt^3} + 6u(1 - u) \frac{d^3f}{dy^3} f^3 \right) - \left(\frac{1}{2} \mp \frac{\sqrt{3}}{6} \right) \frac{d^2f}{dt^2} \frac{df}{dy} f \right] (y(t_n)) + O(h^5)$$

If we consider $1 - 6u(1 - u) = 0$ and if by convention $u > x$, then for

$u = \frac{1}{2} + \frac{\sqrt{3}}{6}$ the formula is the following :

$$(4.6) \begin{cases} y_{n+1} = y_n + hf(y_{n+\frac{1}{2} \pm \frac{\sqrt{3}}{6}}) \mp \\ \mp \frac{1}{2} hf\left(\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)y_{n+1} + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)y_n\right) \pm \\ \pm \frac{1}{2} hf\left(\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)y_{n+1} + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)y_n\right) \\ y_{n+\frac{1}{2} \pm \frac{\sqrt{3}}{6}} = \left(\frac{2}{3} \pm \frac{\sqrt{3}}{6}\right)y_{n+1} + \left(\frac{1}{3} \mp \frac{\sqrt{3}}{6}\right)y_n - \\ - \frac{1 + \sqrt{3}}{12} hf\left(\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)y_{n+1} + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)y_n\right) + \\ + \frac{\sqrt{3} - 1}{12} hf\left(\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)y_{n+1} + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)y_n\right) \end{cases}$$

$$TE = \mp \frac{\sqrt{3}h^4}{216} \left(\frac{d^4f}{dt^4} + \frac{d^3f}{dy^3} f^3\right)(y(t_n)) + \frac{3 \mp \sqrt{3}}{216} \left(\frac{d^2f}{dt^2} \frac{df}{dy} f\right)(y(t_n)) + O(h^5)$$

which for some functions f may produce a lower error than the one of Enright's one-step method.

5. NUMERICAL RESULTS

We have been testing the following schemes

Nr.	Name of the scheme	Stability Order 3	Minimal effort per step
(2.3)	— Enright's second derivative formula	L—stable	1 Function, 1 Derivative
(2.5)	— England's hybrid one-step scheme	L—stable	2 Function, 0 Derivative
(3.1)	— from class (OLS 1)	strongly A—stable	1 Function, 1 Derivative
(4.1)	— from class (HM 1)	strongly A—stable	2 Function, 0 Derivative
(4.2)	— from class (HM 1)	L—stable	2 Function, 0 Derivative
(4.6.1)	— for $\theta = 1/2 + \sqrt{3}/6$, from class (HM 4)	L—stable	3 Function, 0 Derivative
(4.6.2)	— for $\theta = 1/2 - \sqrt{3}/6$, from class (HM 4)	L—stable	3 Function, 0 Derivative
Order 4			
(2.6)	— Obrechhoff's second derivative formula	A—stable	1 Function, 1 Derivative
(2.8)	— Bokhoven's hybrid scheme	A—stable	2 Function, 0 Derivative
(4.4)	— from class (HM 3)	A—stable	3 Function, 0 Derivative

These formulas have been implemented in a constant stepsize method. The above methods suppose to solve some equation in y_{n+1} :

$$F(y_{n+1}) = 0$$

where F depends on the chosen method. The iteration scheme adapted to solve the implicit set of equations is a modified Newton-Raphson technique

$$F^i(y_n)(y_{n+1}^{(i)} - y_n^{(i)}) = -F(y_n^{(i)}), i \geq 0, y_{n+1}^{(0)} = y_n + hf_n$$

The starting value is given by the Euler explicit formula.

The numerical process consists in the following stages at each step :

Stage 1.1. The evaluation of the specific linear matrix system $F'(y_n) = I - ahJ_n + bh^2J_n^2$, with specific couple (a, b) : $a = 2/3, b = 1/6$ for (2.3), (2.5), (4.2), (4.6), $a = 5/9, b = 1/9$ for (4.1), $a = 1, b = 1/3$ for (3.1) and $a = 1/2, b = 1/12$ for (2.6), (2.8), (4.4).

Stage 1.2. Evaluate $y_{n+1}^{(0)}$; $i = 0$;

Stage 2.1. Compute $F(y_{n+1}^{(i)})$;

Stage 2.2. Solve the linear system :

(0) the decomposition $LU = F'(y_n)$, U upper triangular matrix, L lower triangular matrix ;

(1) solve the system $Lx = -F(y_{n+1}^{(i)})$;

(2) solve the system $Ud = x$;

(3) compute $y_{n+1}^{(i+1)} = y_n^{(i)} + d, i \leftarrow i + 1$;

Stage 2.3. If $\|d\|_2 \geq tolerance$ and if the iteration number exceeds a certain limit, then Go To *stage 2.1.* ; in the opposite case, if the maximal number of iteration steps has been over-passed, an error message is printed and *final step*, otherwise continue ;

Stage 3. Evaluate function at the approximation $y_{n+1}^{(i)}$ necessary for the following step and store the values and the Jacobian if the method asks for it.

Final step. Continue with the next step.

The efficiency of the methods has been measured by independent machine statistics like the number of function calls, Jacobian evaluations, and matrix inversions.

The numerical results appear in the following tables. We have noted : xxF = the function evaluation number, xxD = the derivative evaluation number, xxS = the number of linear systems solved. By* we have indicated the method with the lowest error for a certain choice of the step and component system.

The comparison was drawn between the exact solution and the solutions given by the methods for each system, at the point $t = 1$.

The number of iterations depends on the chosen steplength. The stepsize is indicated in the headtable. The possible values are 0.1, 0.05 or 0.01, depending on the required condition of convergence of the methods in discussion.

The following testing systems are known to be stiff :

System (S1) :

$$\begin{cases} y_1'(t) = -4498y_1(t) - 5996y_2(t) + 0.006 - t \\ y_2'(t) = 2248.5y_1(t) + 2997y_2(t) - 0.503 + 3t, \\ y_3'(t) = -y_3(t) \end{cases}, y(0) = \begin{pmatrix} 25498/1500 \\ -16499/1500 \\ 1 \end{pmatrix}$$

Exact :

$$\begin{cases} y_1(t) = -2e^{-t} + 7e^{-1500t} + \frac{17998-14991t}{1500} \\ y_2(t) = 1.5e^{-t} - 3.5e^{-1500t} - \frac{13499-11245.5t}{1500}, \\ y_3(t) = e^{-t} \end{cases}, y(1) = \begin{pmatrix} -1.268908 \\ 0.9505142 \\ 0.3678795 \end{pmatrix}$$

System (S2) :

$$\begin{cases} y_1'(t) = -6y_1(t) + 5y_2(t) + 2\sin t \\ y_2'(t) = 94y_1(t) - 95y_2(t) \\ y_3'(t) = -1000y_3(t) - y_3^2(t) \end{cases}, y(0) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$$

Exact :

$$\begin{cases} y_1(t) = \frac{94}{99}e^{-t} + \frac{1}{10001} \left(\frac{10}{99}e^{-1000t} - 9496\cos t + 9506\sin t \right) \\ y_2(t) = \frac{94}{99}e^{-t} + \frac{1}{10001} \left(-\frac{108}{99}e^{-1000t} - 9494\cos t + 9506\sin t \right) \\ y_3(t) = \frac{1000}{1 - (1 + 1000)e^{1000t}} \end{cases}$$

$$y(1) = \begin{pmatrix} 0.6361023 \\ 0.6193826 \\ 0 \end{pmatrix}$$

System (S3) :

$$\begin{cases} y_1'(t) = -0.013y_1(t) - 1000y_1(t)y_3(t) \\ y_2'(t) = -2500y_2(t)y_3(t) \\ y_3'(t) = -0.013y_1(t) - 1000y_1(t)y_3(t) - 2500y_2(t)y_3(t) \end{cases}, y(0) = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

Exact [10] : $y(1) = \begin{pmatrix} 0.99073192 \\ 1.00926441 \\ -0.00000367 \end{pmatrix}$

Analysing the results, we can see that the proposed methods in the paper present all have good stability properties and implementation performances. Some methods are indicated for solving special stiff systems like methods (4.1) and (4.4) for the system (S1) or (S3) and (4.2) for the system (S2).

Although it is difficult to draw any definite conclusions from these limited results, a general pattern is indicated. It appears that our methods are at least comparable to the classical ones and therefore worth considering in a comprehensive comparison. However, we do feel that our results

Method	(S1)	Effort	(S2)	Effort	(S3)	Effort
	$h = 0.01$		$h = 0.05$		$h = 0.1$	
Enright (2.3)	1.195369	302F	.6904017	64F	.9916564	23F
	-.8953443	302D	.6731095	64D	1.00834	23D
	.3690993	202S	-6.539034E-30*	44S	-3.670194E-6*	14S
England(2.5)	1.205755	504F	.6834468	114F	.9916568	39F
	-.9031347	100D	.6661996	20D	1.00834	9D
	.3678792	202S	-6.546161E-30	47S	-3.670197E-6	15S
OLS1 (3.1)	1.174317	510F	.7059933	124F	.9916567	67F
	-.8795553	305D	.6886706	72D	1.008339	38D
	.3715501	205S	-2.77061E-7	52S	-3.676911E-6	29S
HM1(4.1)	1.205853*	506F	.6830078	128F	.9916446*	67F
	-.9032077*	100D	.6657606	20D	1.008352*	9D
	.3678793*	203S	-4.812774E-9	54S	-3.662948E-6	29S
HM 1(4.2)	1.205848	504F	.683005*	114F	.9916566	41F
	-.9032041	100D	.6657568*	20D	1.00834	9D
	.3678792	202S	-6.539737E-30	47S	-3.670196E-6	16S
HM 4(4.6.1)	1.205755	706F	.6834486	158F	.9916787	48F
	-.9031349	100D	.6661998	20D	1.008318	9D
	.3678792	202S	-6.579986E-30	46S	-3.670312E-6	9S
HM 4(4.6.2)	1.205758	706F	.6834486	158F	.9916565	54F
	-.9031366	100D	.6661998	20D	1.00834	9S
	.3678792	202S	-6.568837E-30	46S	-3.670195E-6	15S
	$h=0.01$		$h=0.01$		$h=0.01$	
Obrechhoff (2.6)	1.196627	304F	.6464161	296F	.9907243	202F
	-.8962881	304D	.6295791	296D	1.009272	202D
	.3678732	204S	0*	196S	1.009272	202D
Bokhoven (2.8)	1.205815*	510F	.645691*	464F	-3.665286E-6	102S
	-.931796*	100D	.6288624*	100D	.9907317	310F
	.3678794*	205S	0*	182S	-3.665327E-6*	105S
HM 3(4.4)	1.205753	712F	.6457027	646F	.9907318*	415F
	-.9031334	100D	.6288741	100D	1.009264*	100D
	.3678794*	204S	0*	182S	-3.665327E-6*	105S

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indicate that a properly implementation version of our algorithms should be useful for the numerical integration of stiff differential systems. We expect that, in the case of a variable steplength, those new methods have better properties than the classical methods.

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