JOURNAL OF COMPUTATIONAL PHYSICS **130,** 123–128 (1997)
ARTICLE NO. CP965567

A P-Stable Eighth-Order Method for the Numerical Integration of Periodic Initial-Value Problems

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An eighth-order P-stable two-step method for the numerical integration of second-order periodic initial-value problems is developed in this paper. This method has seven stages per iteration and an interval of periodicity equal to $(0, \infty)$; i.e., it is P-stable. Numerical and theoretical results obtained for several well-known problems show the efficiency of the new method.

1. INTRODUCTION

The last 10 years there has been much activity in the area of numerical solution of the second-order initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{1}$$

involving second-order ordinary differential equations in which the first derivative does not appear explicitly. Equations having periodical solutions are under investigation. Examples occur in celestial mechanics, in quantum mechanical scattering theory, in theoretical physics, and in electronics (see [1–2]).

There are two main categories of methods for the numerical solution of problems of the form (1) with periodical solutions. Category I consists of methods with coefficients dependent on the problem. The application of these methods is possible when the frequency of the solution of the problem is known a priori. Category II consists of methods with constant coefficients, i.e., with coefficients independent from the problem. These methods can be applied to any problem with periodical solution, even if the frequency of the problem is unknown initially. An appropriate requirement for these methods is that of P-stability. We note here that classical Runge–Kutta or Runge–Kutta–Nyström methods are not efficient for the solution of (1) since their interval of periodicity is empty.

Several methods have been developed for the solution of (1) belonging to Category I. We mention the works of Gautschi [3], Lyche [4], Raptis and Allison [5], Cash, Raptis, and Simos [6], Ixaru and Rizea [7], Simos [8], and Thomas, Simos, and Mitsou [9]. The main disadvantage of these methods is the requirement of the knowledge a priori of the frequency of the solution of the problem. The main areas of application of these methods are problems for which the above requirement is possible, such as the Schrödinger equation.

Numerous numerical techniques have been obtained for the solution of (1) belonging to Category II. Each method of this category must be P-stable, especially in the cases of the problems with high oscillatory solutions. The P-stability property has been first introduced by Lambert and Watson [10]. Several P-stable methods have been developed for the solution of (1), especially when we have an oscillatory solution. We refer to the works of Cash [11] and Chawla and Rao [12]. In these works sixth-order P-stable methods have been obtained. An important contribution for the P-stable methods is the work of Hairer [13] in which lower order P-stable methods have been developed.

The purpose of this paper is to develop an eighth-order P-stable method for the solution of (1). In Section 2 we will describe the basic theory of the stability of symmetric multistep methods. In Section 3 we will develop the P-stable method of order eight. In this section also, the computational implementation of the P-stable method is presented. Finally, in Section 4 an application of the new method on some well-known problems is presented. Theoretical and numerical results show that these new methods are more efficient than the other well-known P-stable methods.

2. BASIC THEORY

To investigate the stability properties of methods for solving the initial-value problem (1) Lambert and Watson [10] introduce the scalar test equation,

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0021-9991/97 $25.00

$$y'' = -w^2 y, \tag{2}$$

and the **interval of periodicity.**

When we apply a symmetric two-step method to the scalar test equation (2) we obtain a difference equation of the form

$$y_{n+1} - 2C(H)y_n + y_{n-1} = 0, \tag{3}$$

where $H = wh$, h is the step length, $C(H) = B(H)/A(H)$, where $A(H)$ and $B(H)$ are polynomials in H and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots$.

The characteristic equation associated with (3) is

$$s^2 - 2C(H)s + 1 = 0. \tag{4}$$

Bruca and Nigro [17] introduced the frequency distortion as an important property of a method for solving special second-order initial-value problems. For frequency distortion other authors [15, 16] use the terms of *phase-lag*, *phase error*, or *dispersion*. From now on we use the term **phase-lag.**

Following Coleman [14] when we apply a symmetric two-step method to the scalar test equation $y'' = -w^2 y$ then we have the difference equation (3). The characteristic equation associated with (3) is given by (4). The roots of the characteristic equation (4) are denoted as s_1 and s_2.

We have the following definitions.

DEFINITION 1. (See [15, 16]). The method (3) is unconditionally stable if $|s_1| \leq 1$ and $|s_2| \leq 1$ for all values of wh.

DEFINITION 2. Following Lambert and Watson [10] we say that the numerical method (3) has an interval of periodicity $(0, H_0^2)$, if, for all $H^2 \in (0, H_0^2)$, s_1 and s_2 satisfy

$$s_1 - e^{i\theta(H)}, \quad s_2 = e^{-i\theta(H)}, \tag{5}$$

where $\theta(H)$ is a real function of H. For any method corresponding to the characteristic equation (4) the phase-lag is defined (see [14]) as the leading term in the expansion of

$$t = H - \theta(H) = H - \cos^{-1}[C(H)]. \tag{6}$$

If the quantity $t = O(H^{q+1})$ as $H \to 0$, the order of phase-lag is q.

DEFINITION 3 [13]. The method (3) is **P-stable** if its **interval of periodicty** is $(0, \infty)$.

THEOREM 1 (For the proof see [16]). *A method which has the characteristic equation (4) has an interval of periodicity* $(0, H_0^2)$, *if for all* $H^2 \in (0, H_0^2)$ $|C(H)| < 1$.

THEOREM 2 (For the proof see [16]). *About the method which has an interval of periodicity* $(0, H_0^2)$ *we can write*

$$\cos[\theta(H)] = C(H), \quad \text{where } H^2 \in (0, H_0^2). \tag{7}$$

Based on this, Coleman [14] arrived at the following remark.

Remark 1. If the phase-lag order is $q = 2$, then we have

$$\begin{aligned} t = cH^{2r+1} + O(H^{2r+3}) &\Rightarrow \cos(H) - C(H) \\ &= \cos(H) - \cos(H - t) = cH^{2r+2} + O(H^{2r+4}). \end{aligned} \tag{8}$$

3. CONSTRUCTION OF THE NEW SCHEME

The construction of the new scheme is based on the following hypotheses. First, we construct approximations to $y_{n\pm1/2}$ of order four, i.e., with local truncation error (LTE) of the form $O(h^5)$. Then, we obtain approximations to $y_{n\pm1/3}$, which depend on the approximations to $y_{n\pm1/2}$. These approximations are of order six, i.e., with LTE of the form $O(h^7)$. We produce also approximations to $y_{n\pm1/4}$, which depend on the approximations to $y_{n\pm1/2}$ and $y_{n\pm1/3}$. These approximations are also of order six, i.e., with LTE of the for $O(h^7)$. Finally, the method depends on the approximations to $y_{n\pm1/4}$ and $y_{n\pm1/3}$ and is of order eight, i.e., with LTE of the form $O(h^{10})$. We want also the produced method to satisfy the condition of P-stability (see Definition 3) and to have minimal phase-lag (see Definition 2 and Theorem 2).

Consider now the new family of eighth-order methods:

$$\begin{aligned}
y_{n+1/2} &= a_0 y_{n+1} + a_1 y_n + a_2 y_{n-1} \\
&\quad + h^2(a_3 f_{n+1} + a_4 f_n + a_5 f_{n-1}) \\
y_{n-1/2} &= (b_0 y_{n+1} + b_1 y_n + b_2 y_{n-1}) \\
&\quad + h^2(b_3 f_{n+1} + b_4 f_n + b_5 f_{n-1}) \\
y_{n+1/3} &= c_0 y_{n+1} + c_1 y_n + c_2 y_{n-1} \\
&\quad + h^2(c_3 f_{n+1} + c_4 f_n + c_5 f_{n-1} + c_6 \bar{f}_{n+1/2} + c_7 \bar{f}_{n-1/2}) \\
y_{n-1/3} &= d_0 y_{n+1} + d_1 y_n + d_2 y_{n-1} \\
&\quad + h^2(d_3 f_{n+1} + d_4 f_n + d_5 f_{n-1} + d_6 \bar{f}_{n+1/2} + d_7 \bar{f}_{n-1/2}) \\
y_{n-1/4} &= k_0 y_{n+1} + k_1 y_n + k_2 y_{n-1} + h^2(k_3 f_{n+1} + k_4 f_n \\
&\quad + k_5 f_{n-1} + k_6 \bar{f}_{n+1/2} + k_7 \bar{f}_{n-1/2} + k_8 \bar{f}_{n+1/3} + k_9 \bar{f}_{n-1/3}) \\
y_{n+1/4} &= q_0 y_{n+1} + q_1 y_n + q_2 y_{n-1} + h^2(q_3 f_{n+1} + q_4 f_n \\
&\quad + q_5 f_{n-1} + q_6 \bar{f}_{n+1/2} + q_7 \bar{f}_{n-1/2} + q_8 \bar{f}_{n+1/3} + q_9 \bar{f}_{n-1/3}) \\
y_{n+1} &- 2y_n + y_{n-1} \\
&= h^2[r_0 f_{n+1} + r_1 f_n + r_0 f_{n-1} \\
&\quad + r_2(\bar{f}_{n+1/3} + \bar{f}_{n-1/3}) + r_3(\bar{f}_{n+1/4} + \bar{f}_{n-1/4})].
\end{aligned} \tag{9}$$

Based on the hypotheses described in the first paragraph of this section we have to solve a constraint optimization problem (maximization of the order of the local truncation error with the constraints described in the first paragraph of this section). The resulting method of this problem is given by

$$y_{n+1/2} = \frac{1}{239712}(878803y_{n+1} - 1398038y_n + 758947y_{n-1}) - \frac{h^2}{719136}(225319f_{n+1} + 1961041f_n + 180373f_{n-1})$$

$$y_{n-1/2} = \frac{1}{143136}(-485111y_{n+1} + 1041790y_n - 413543y_{n-1}) + \frac{h^2}{429408}(126869f_{n+1} + 1174757f_n + 100031f_{n-1})$$

$$y_{n+1/3} = \frac{1}{871155}(43981909y_{n+1} - 86802278y_n + 43691524y_{n-1}) - \frac{h^2}{156807900}(131962457f_{n+1} + 3411330282f_n + 131102057f_{n-1} + 2110634512f_{n+1/2} + 2096868112f_{n-1/2})$$

$$y_{n-1/3} = -\frac{1}{2485161}(-120398555y_{n+1} + 242453884y_n + 119570168y_{n-1}) + \frac{h^2}{223664490}(180558629f_{n+1} + 4690706274f_n + 179331389f_{n-1} + 2870393104f_{n-1/2} + 2890028944f_{n+1/2})$$

$$y_{n-1/4} = \frac{1}{4}(3y_n + y_{n-1}) + h^2\left(-\frac{89943719f_{n+1}}{8465056927} + \frac{5788502176f_n}{5986090661} - \frac{195941013f_{n-1}}{5606053162} + \frac{5067930924f_{n+1/2}}{12700799327} + \frac{4991835037f_{n-1/2}}{8409347486} - \frac{51803845403f_{n+1/3}}{61976870998} - \frac{8985997675f_{n-1/3}}{7667642701}\right.$$

$$y_{n+1/4} = \left(\frac{17386806546y_{n-1}}{13933002235} - \frac{12919590189y_n}{7400497639} + \frac{28693512895y_{n+1}}{19155998342}\right) + h^2\left(-\frac{372575949f_{n+1}}{25808146454} - \frac{22734104849f_n}{14603068705} + \frac{64650764f_{n-1}}{6536968275} - \frac{15248842460f_{n+1/2}}{19137892759} - \frac{6646351228f_{n-1/2}}{6704215949} + \frac{44995145483f_{n-1/3}}{38392587458} + \frac{6874422965f_{n+1/3}}{8224026249}\right)$$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{23520}[357f_{n+1} + 65632f_n + 357f_{n-1} + 60507(f_{n+1/3} + f_{n-1/3}) - 81920(f_{n+1/4} + f_{n-1/4})]. \quad (10)$$

The evaluation of LTE needs tedious algebra. The hybrid Numerov-type methods that have been used the last 15 years for the construction of high order P-stable methods are special forms of two-step Runge–Kutta–Nystrom methods. Unfortunately only two-step Runge–Kutta methods have been studied seriously until now; see Jackiewitz and Tracogna [20]. Since a comprehensive presentation of the related theory is a serious undertaking beyond the scope of this article, we give some restricted results that apply in our case.

Suppose that we have to solve the autonomous system $y'' = f(y)$, where $y \in R^m$. There is no need for the independent variable because we include it as a parameter in the system with the additional equation $x'' = 0$. Now according to the Runge–Kutta–Nystrom theory (see Hairer *et al.* [21]), we expand all the expressions of the method with respect to h around the central point x_n. If the order of the method is p, taking into account that $y'' = f$, $y^{(3)} = f' = \frac{9f}{9y}$ etc., we arrive at local truncation error of the form $h^{p+2}(c_1F_1 + c_2F_2 + \cdots + c_sF_s) + O(h^{p+3})$, where c are numbers and F are elementary differentials involving only y' and partial derivatives of f with respect to y. We must note here that, assuming a scalar case, compression of different F_i's may occur. For example, $f''f'y'^2 \neq f'f''y'^2$ for a system of equations since f', f'', y' are matrices, but this is not true if we have a simple scalar differential equation. Finally, for reasons of simplicity the local truncation error of the method given in this paper, follows for the scalar case:

$$t_n(h) = L.T.E. = h^{10}[3.9810^{-7}ff'^4 - 6.1310^{-7}f^2f'^2f'' - 0.003383f'^3y'^2f'' - 0.00001836f^3f''^2 - 0.01315ff'y'^2f''^2 - 0.0009871y'^4f''^3 - 0.00003394f^3f'f^{(3)} - 0.000103ff'^2y'^2f^{(3)} - 0.00315f^2y'^2f''f^{(3)} - 0.005432f'y'^4f''f^{(3)} - 0.00007344fy'^4f^{(3)^2} - 0.00002295f^4f^{(4)}$$

$$- 0.0002395f^2f'y'^2f^{(4)} - 0.00005709f'^2y'^4f^{(4)}$$
$$- 0.002094fy'^4f''f^{(4)} - 0.00001836y'^6f^{(3)}f^{(4)}$$
$$- 0.0000918f^3y'^2f^{(5)} - 0.0001257ff'y'^4f^{(5)}$$
$$- 0.0002112y'^6f''f^{(5)} - 0.0000459f^2y'^4f^{(6)}$$
$$- 0.00001144f'y'^6f^{(6)} - 6.1210^{-6}fy'^6f^{(7)}$$
$$- 2.18610^{-7}y'^8f^{(8)}] + O(h^{11}). \quad (11)$$

If we apply the resulting method (10) to the scalar test equation (2) we obtain (3) with

$$A(H) = 1 + \frac{998372429H^2}{21764679325} + \frac{15130876H^4}{11551329243} + \frac{376784H^6}{11339782961} + \frac{9999H^8}{7983242618},$$
$$B(H) = 1 - \frac{19767934467H^2}{43529358650} + \frac{357379975H^4}{17832497716} - \frac{1006329H^6}{10134009986} + \frac{2049H^8}{6629024168}. \quad (12)$$

Based on Definitions 2 and 3 and on Theorem 1 it is obvious that

$$\left|C(H)\right| = \left|\frac{B(H)}{A(H)}\right| < 1$$

for all $H^2 \in (0, \infty)$; i.e., the method is P-*stable*.

From Definition 2 and Theorem 3 we have that

$$t = -\frac{-13843H^{10}}{8696390501} \times \frac{1}{4}; \quad (14)$$

i.e., the method has a phase-lag of order 8. This is the high order phase-lag that can be obtained under the constraints described in the beginning of this section.

We note that for nonlinear problems the above-mentioned method is implicit and an iterative process must be obtained for computing the approximate solution at each step. Here we consider application of the modified Newton method.

Consider the method developed in (10). Then, the iteration matrix is given by

$$y_{n+1}^{p+1} = y_{n+1}^{p} + \left(1 - \frac{998372429h^2J}{21764679325} + \frac{15130876h^4J^2}{11551329243} - \frac{376784h^6J^3}{11339782961} + \frac{9999h^8J^4}{7983242618}\right)^{-1} F(y_{n+1}^{p}), \quad (15)$$

where $J = \partial f/\partial y$.

The new method needs for the initial guess for the iteration one extra function evaluation given below:

$$\bar{y}_{n+1} = -[16(y_{n+1} + y_{n-1}) - 34y_n + y_{n-2}] + \frac{h^2}{3}[8(f_{n+1} + f_{n-1}) + 44f_n] + O(h^7)$$
$$y_{n+1}^{0} = -\left[\frac{128}{31}(y_n + y_{n-2}) - \frac{318}{31}y_n + y_{n-3}\right] + \frac{h^2}{465}[23(\bar{f}_{n+1} + f_{n-3}) + 688(f_n + f_{n-2}) + 2358f_{n-1}] + O(h^9). \quad (16)$$

4. NUMERICAL RESULTS–CONCLUSION

In this section we illustrate the new P-stable eighth-order method by applying it to the numerical solution of three problems. The first is the well-known orbital problem of Stiefel and Bettis [18]. The second is the problem introduced by Lambert and Watson [10], and the third is a nonlinear example introduced by Chawla and Rao [19]

4.1. *The Orbital Problem of Stiefel and Bettis* [18]

We consider the following problem studied by Steifel and Bettis [18]

$$z'' + z = 0.001e^{ix}, \quad z(0) = 1, \quad z'(0) = 0.9995i, \quad z \in C, \quad (17)$$

whose theoretical solution is

$$z(x) = u(x) + iv(x), \quad u, v \in R,$$
$$u(x) = \cos(x) + 0.0005x\sin(x) \quad (18)$$
$$v(x) = \sin(x) - 0.0005x\cos(x).$$

The solution (18) represents motion on the perturbation of a circular orbit in the complex plane; the point $z(x)$ spirals slowly outward so that at time x its distance from the orbit is

$$g(x) = [u^2(x) + v^2(x)]^{1/2} = [1 + (0.0005x)^2]^{1/2}.$$

We write (17) in the equivalent form,

$$u'' + u = 0.001\cos(x), \quad u(0) = 1, \quad u'(0) = 0,$$
$$v'' + v = 0.001\sin(x), \quad v(0) = 0, \quad v'(0) = 0.9995. \quad (20)$$

The real system (20) has been solved numerically for $0 \leq x \leq 40\pi$ using exact starting values and the following methods:

TABLE I

Comparison of the Maximum Absolute Errors Throughout the Trajectory in the Approximations Obtained by Using Methods 1–3

Method	Steps	Error	Steps	Error	Steps	Error	Steps	Error
1	192	1.34e-4	288	1.18e-5	384	2.11e-6	480	5.54e-7
2	320	5.56e-4	480	4.92e-5	640	8.77e-6	800	2.31e-6
3	137	1.23e-5	206	4.74e-7	274	4.85e-8	343	8.05e-9

Method 1. Sixth order P-stable method of Cash [11]

Method 2. P-stable sixth-order method of Chawla and Rao [12].

Method 3. The new method (10).

In Table I we present the maximum absolute error over all points in $0 \leq x \leq 40\pi$. The steps are chosen so that the function evaluations are of equal size.

4.2. *A Problem of Lambert and Watson* [10]

We consider the following problem studied by Lambert and Watson [10]:

$$y_1'' + \lambda^2 y_1 = f''(x) + \lambda^2 f(x), \quad y_1(0) = a + f(0),$$
$$y_1'(0) = f'(0), \tag{21}$$
$$y_2'' + \lambda^2 y_2 = f''(x) + \lambda^2 f(x), \quad y_2(0) = f(0),$$
$$y_2'(0) = \lambda a + f'(0). \tag{22}$$

Assuming $f(x) = e^{-x/20}$, the theoretical solutions is given by

$$\begin{aligned} y_1(x) &= a \cos \lambda x + f(x) \\ y_2(x) &= a \sin \lambda x + f(x). \end{aligned} \tag{23}$$

The system (22) has been solved numerically for $0 \leq x \leq 20\pi$ using exact starting values and the methods mentioned in the previous example.

In Tables II–VII we present the maximum absolute error

TABLE II

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 1$ and $\lambda = 1$

Method	Steps	Error	Steps	Error	Steps	Error
1	96	6.73e-5	192	1.06e-6	384	1.66e-8
2	160	2.79e-4	320	4.40e-6	640	6.89e-8
3	69	5.82e-6	138	2.30e-8	276	8.90e-11

TABLE III

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 1$ and $\lambda = 10$

Method	Steps	Error	Steps	Error	Steps	Error
1	768	2.55e-3	1152	2.26e-4	1536	4.04e-5
2	1280	1.05e-2	1920	9.37e-4	2560	1.67e-4
3	550	3.54e-4	825	1.40e-5	1100	1.41e-6

TABLE IV

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 1$ and $\lambda = 20$

Method	Steps	Error	Steps	Error	Steps	Error
1	1152	2.83e-2	1536	5.10e-3	1920	1.30e-3
2	1920	1.16e-1	2560	2.11e-2	3200	5.57e-3
3	825	7.00e-3	1100	7.09e-4	1372	1.22e-4

TABLE V

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 50$ and $\lambda = 1$

Method	Steps	Error	Steps	Error	Steps	Error
1	144	2.97e-4	192	5.30e-5	288	4.66e-6
2	240	1.23e-3	320	2.20e-4	480	1.93e-5
3	103	1.19e-5	137	1.22e-6	206	4.67e-8

TABLE VI

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 50$ and $\lambda = 10$

Method	Steps	Error	Steps	Error	Steps	Error
1	1000	2.64e-2	1500	2.32e-3	2000	4.15e-4
2	1667	1.09e-1	2500	9.65e-3	3334	1.72e-3
3	714	2.22e-3	1071	8.71e-5	1428	8.75e-6

TABLE VII

Comparison of the Maximum Absolute Errors in the Approximations Obtained by Using Methods 1–3; $a = 50$ and $\lambda = 20$

Method	Steps	Error	Steps	Error	Steps	Error
1	1500	2.94e-1	2250	2.61e-2	3000	4.66e-3
2	2500	1.21e+0	3750	1.08e-1	5000	1.93e-2
3	1071	4.38e-2	1606	1.74e-3	2142	1.74e-4

TABLE VIII

Comparison of the Global Errors in the Approximations at $x = 20\pi$ Obtained by Using Methods 1–3

Method	Steps	Error	Steps	Error	Steps	Error	Steps	Error
1	480	5.69e-2	720	4.56e-3	960	7.74e-4	1200	1.00e-4
2	720	2.86e-2	1080	2.76e-3	1440	5.04e-4	900	1.33e-4
3	360	1.30e-3	540	6.41e-5	720	6.11e-6	1800	9.20e-7

over all points in $0 \leq x \leq 20\pi$ for several values of a and λ. The steps are chosen so that the function evaluations are of equal size.

4.3. *A Nonlinear Example* [19]

We consider the following nonlinear problem studied by Chawla and Rao [19]

$$y'' + 100y = \sin y, \quad y(0) = y_0 = 0, \quad y'(0) = y_0' = 1. \quad (24)$$

In this example, since there is not an analytical solution, we measure the global errors in the computation of $y(20\pi) = 0.000392823991$.

Equation (24) has been solved numerically for $0 \leq x \leq 20\pi$ using the methods mentioned in the previous examples. The steps were chosen so the function evaluations are of equal size. Generally we can use, for starting values $\mathbf{y}_1 = \mathbf{y}(\mathbf{h})$, the embedded Runge–Kutta–Nyström method of Dormand, El-Mikkawy, and Prince RKN8(6)9FM (see [22]).

Since the problem is nonlinear for all the methods compared in this example an iterative process must be obtained for computing the approximate solution at each step. For the methods of Cash (Method 1) and Chawla and Rao (Method 2) we use the iterative processes and the extra function evaluations (for the initial guess) fully described in [11, 12], respectively. For the new method we use the iterative process (15) with the extra function evaluation (for the initial guess) given by (16). For all the methods used the iteration scheme was allowed to perform once.

In Table VIII we present the global error at $x = 20\pi$. The steps are chosen so that the function evaluations are of equal size. From the theoretical and numerical results presented it is obvious that this paper's eighth-order P-stable method is more efficient than the previously developed P-stable methods in the literature.

All the computations were carried out on a PC i486 using double precision arithmetic (16 significant digit accuracy).

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