

# ***A New Explicit Singularly P–Stable Four–Step Method for the Numerical Solution of Second–Order IVPs***

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## **ABSTRACT**

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In this paper, we introduce a new symmetric explicit four-step method with variable coefficients for the numerical solution of second-order linear periodic and oscillatory initial value problems of ordinary differential equations. For the first time in the literature, we generate an explicit method with the most important singularly P-stability property. The method is multiderivative and has algebraic order eight and infinite order of phase-lag. The numerical results for some chemical (e.g. orbit problems of Stiefel and Bettis) as well as quantum chemistry problems (i.e. systems of coupled differential equations) indicated that the new method is superior, efficient, accurate and stable.

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## **1. INTRODUCTION**

In this paper, the numerical solution of the special second-order initial value problems with periodical and/or oscillating solutions of the form:

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y_0'(x_0) = y_0', \quad (1)$$

is discussed where we assume that  $f$  is sufficiently differentiable. These equations are used as the mathematical model for problems in celestial mechanics, physical chemistry, chemical physics, quantum mechanics, electronics, materials sciences and some others. Numerous problems such as chemical kinetics, orbital dynamics, orbital problem, circuit and control theory and Newton's second law applications involve second-order ODEs as discussed by [7,8,9].

The class of the above equations with oscillatory and/or periodic solutions (see [1,2]) deserves special attention. In the past decades, various classes of methods have been designed for solving Equation (1) numerically: Runge-Kutta, linear multistep, predictor-

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corrector, trigonometrically or exponentially methods [19,20]. One of the most important properties of the numerical methods for solving Equation (1) is the P-stability property; if a method has this property, then it is more suitable for solving Equation (1).

In a paper [5], Lambert and Watson claimed that the P-stable methods must be implicit; explicit methods cannot be P-stable and all of the linear multistep P-stable methods are implicit. Of course, we know that the implicit methods are not applicable alone and to compute the implicit terms, it is required to use another suitable explicit method. In 2003, Li and Wu [6] designed the explicit P-stable method that had nonlinear form. Following that, some modified explicit P-stable methods were presented but all of them had the same nonlinear structures [26,28,29]. But in this paper, for the first time in the literature, we develop a new explicit linear four-step method that has the most important P-stability property. Firstly, since the new method is explicit, we do not need the other predictor method; thus it has less computational complexity in the numerical implementations. The other hand this method can be recognized as a suitable predictor method for other predictor-corrector methods. The other important point about the new method is that, with regard to its linear structure, it can be used directly in the vector form for solving differential equations systems and there is no need for vector product and quotient that was highly necessary to implement the nonlinear P-stable method of Li and Wu [6] etc. Generally, the solution of (1) is periodic, so it is expected that the results produced by some numerical methods be of the periodicity of the analytic solution. In 1976, Lambert and Watson [5] proposed the concepts of periodicity interval and P-stability which can be used to discuss the stability of the numerical method for second-order initial value problems. Although many P-stable methods have been proposed, the earliest method to solve (1) numerically is the Numerov's method. Recently, Shokri et al [10,18,22] have developed Obrechhoff type methods of various algebraic orders. The methods based on vanishing of phase-lag and some of its derivatives [21,24], Runge-Kutta methods [14,31,34], multistep methods [20,23], multiderivative methods [27], and hybrid methods [25,26] are some of the approaches that can be used for solving a second-order differential equation. We know that the numerical methods of second-order initial value problems are divided into two classes: The methods with constant coefficients and the methods with coefficients depending on the frequency of the problem. The new method is from the second class. The purpose of this paper is the construction of more efficient methods for the numerical solution of second-order initial value problems with highly oscillatory solutions. More specifically, the aim of this paper is to develop a new four-step predictor P-stable method which has the phase-lag and some of its derivatives equal to zero.

## 2. BASIC THEORY

For the numerical solution of the initial value problem (1), multistep methods of the form

$$\sum_{i=1}^k c_i (y_{n+i} + y_{n-i}) + c_0 y_n = h^2 [\sum_{i=1}^k b_i (f_{n+i} + f_{n-i}) + b_0 f_n], \quad (2)$$

with  $2k$  steps can be used over the equally spaced intervals  $\{x_i\}_{i=-k}^k \in [a, b]$  and  $h = |x_{i+1} - x_i|, i = -k(1)k - 1$ . When the symmetric  $2k$ -step method (2) is applied to the scalar test equation

$$y''(x) = -\omega^2 y(x), \quad (3)$$

a difference equation  $A_0(v)y_n + \sum_{i=1}^k A_i(v)(y_{n-i} + y_{n+i}) = 0$  is obtained, where  $v = \omega h$ ,  $h$  is the step length and  $A_0(v), A_1(v), \dots, A_k(v)$  are polynomials of  $v$  and hence the characteristic equation of (2) will be

$$A_0(v) + \sum_{i=1}^k A_i(v)(s^{-i} + s^i) = 0.$$

**Definition 2.1.** The interval  $(0, v_0^2)$  is called the periodicity interval of method (2) if the roots  $\tau_j, j = 1, 2, \dots, 2k$ , satisfy

$$\tau_{1,2} = \exp(\pm i\theta(v)), \quad |\tau_j| \leq 1, \quad j = 3, 4, \dots, 2k, \quad (4)$$

where  $\theta(v)$  is a real function of  $v$ . A method is called P-stable if its interval of periodicity is equal to  $(0, \infty)$ .

**Definition 2.2.** A multistep method is called singularly almost P-stable if its interval of periodicity is equal to  $(0, \infty) - S$  where  $S$  is a set of distinct points.

**Definition 2.3.** The phase-lag error of method (2) is defined by  $PL = v - \theta(v)$ . Then if the quantity  $PL = O(v^{q+1})$  as  $v \rightarrow \infty$ , the order of phase-lag is  $q$ .

**Theorem 2.4.** The symmetric  $2k$ -step method (2) has phase-lag order  $q$  and phase-lag constant  $c$  given by

$$-c v^{q+2} + O(v^{q+4}) = \frac{\sum_{i=1}^k 2A_i(v) \cos(iv) + A_0(v)}{\sum_{i=1}^k 2i^i A_i(v)} \quad (5)$$

**Proof.** See [32].

### 3. DEVELOPMENT AND ANALYSIS

To solve numerically (1), we define explicit four-step, symmetric, multiderivative method of the form:

$$y_{n+2} + y_{n-2} + a_1(y_{n+1} + y_{n-1}) + a_0 y_n = h^2 [b_1(f_{n+1} + f_{n-1}) + b_0 f_n] + h^4 [c_1(g_{n+1} + g_{n-1}) + c_0 g_n], \quad (6)$$

where  $y'' = f(x, y)$  and  $y^{(4)} = g(x, y)$ . Note that  $a_j, b_j$  and  $c_j, j=0, 1$  are six arbitrary parameters that must be calculated. Applying (6) to the scalar test Equation (3), one gets its difference and characteristic equations, respectively of the form

$$A^2(v)(y_{n+2} + y_{n-2}) + A_1(v)(y_{n+1} + y_{n-1}) + A_0(v)y_n = 0, \quad (7)$$

where  $A_i(v) = a_i + v^2 b_i - v^4 c_i$ ,  $i = 0, 1, 2$ , where  $v = \omega h$  and

$$A_2(v)(\lambda^4 + 1) + A_1(v)(\lambda^3 + \lambda) + A_0(v)\lambda^2 = 0. \quad (8)$$

Now, if we assume that  $A_1(v) = 0$ , then (8) is reduced to  $A_2(v)(\lambda^4 + 1) + A_0(v)\lambda^2 = 0$ . In addition, to calculate the phase-lag of the method (6), we apply the direct formula (5) for  $k = 2$  and for  $A_j(v)$ ,  $j = 0(1)2$ . This leads to the following equation:

$$PL = \frac{-2 \cos(2v) + (2v^4 c_1 - 2v^2 b_1 - 2a_1) \cos(v) + v^4 c_0 - v^2 b_0 - a_0}{2v^4 c_1 - 2v^2 b_1 - 2a_1 - 8}. \quad (9)$$

In the new method (6), there are six arbitrary parameters that we have to calculate. To calculate these coefficients we produce a system of six equations as follow:

$$\begin{cases} A_1(v) = 0 \\ PL^{(i)} = 0, \quad i = 0(1)4 \end{cases}$$

Solving the above system will produce the coefficients of the new method. To save space, the formulas of the new method with their figures are shown in Appendix. But, for small values of  $|v|$ , these coefficients may be subject to heavy cancellations. In this case, we should use the following Taylor series expansions:

$$\begin{aligned} a_0 &= -2 + \frac{64}{63}v^2 + \frac{1504}{19845}v^4 - \frac{345368}{13752585}v^6 + \dots, \\ a_1 &= -\frac{32}{63}v^2 - \frac{752}{19845}v^4 + \frac{172684}{13752585}v^6 + \dots, \\ b_0 &= \frac{188}{63} - \frac{3392}{3969}v^2 + \frac{52072}{2750517}v^4 + \frac{22943456}{2252673423}v^6 - \dots, \\ b_1 &= \frac{32}{63} + \frac{688}{3969}v^2 + \frac{390748}{13752585}v^4 + \frac{13355458}{11263367115}v^6 + \dots, \\ c_0 &= \frac{524}{945} - \frac{10952}{59535}v^2 + \frac{4948568}{206288775}v^4 - \frac{294945008}{168950506725}v^6 + \dots, \\ c_1 &= \frac{128}{945} - \frac{944}{59535}v^2 + \frac{130616}{206288775}v^4 - \frac{1935806}{16895050672}v^6 + \dots, \end{aligned}$$

where  $v = \omega h$ , and the local truncation error of the new method is

$$LTE_{ex4sp} = \frac{97}{595350} h^{10} [\omega^{10} y + 5\omega^8 y^{(2)} + 10\omega^6 y^{(6)} + 10\omega^4 y^{(6)} + 5\omega^2 y^{(8)} + y^{(10)}]. \quad (10)$$

Since the new method is explicit, it is most important to show its stability property. In two ways, the singularly P-stability of the new method can be demonstrated: by its figure and the theorem. For this purpose, the application of the new method (6) to the scalar test equation

$$y'' = -\phi^2 y(x), \quad (11)$$

leads to the following difference equation

$$A_2(s, v)(y_{n+2} + y_{n-2}) + A_1(s, v)(y_{n+1} + y_{n-1}) + A_0(s, v)y_n = 0, \quad (12)$$

where  $A_0(s, v) = \frac{1}{6} \frac{A_{00}}{A}$ ,  $A_1(s, v) = \frac{2}{3} \frac{A_{10}}{A}$ ,  $A_2(s, v) = 1$  where  $v = \omega h$ ,  $s = \phi h$  and  $A_{i0}$ ,  $i = 0, 1$  and

$$A = v^4((v^2 + 3) \cos(v)^2 + 2v^2 - 3), \quad (13)$$

$$\begin{aligned}
A_{00} = & (4v^8 + (-8s^2 - 78)v^6 + (4s^4 + 60s^2 + 27)v^4 \\
& + (-6s^4 - 90s^2)v^2 - 9s^4)\cos(v)^4 \\
& - (6(-5v^4 + (s^2 + \frac{27}{2})v^2 - \frac{3}{2}s^2))(s + v)v\sin(v)(s - v)\cos(v)^3 \\
& + (-10v^8 + (20s^2 + 135)v^6 + (-10s^4 - 222s^2 + 9)v^4 \\
& + (51s^4 + 90s^2)v^2 + 9s^4)\cos(v)^2 \\
& + 48((s + v)(-v^4 + (s^2 + \frac{21}{16})v^2 - \frac{9}{16}s^2)v\sin(v)(s - v)\cos(v) \\
& + 12v^2(v^6 + (-2s^2 - 1)v^4 + (s^4 + 6s^2 - 3)v^2 - 3s^4), \tag{14}
\end{aligned}$$

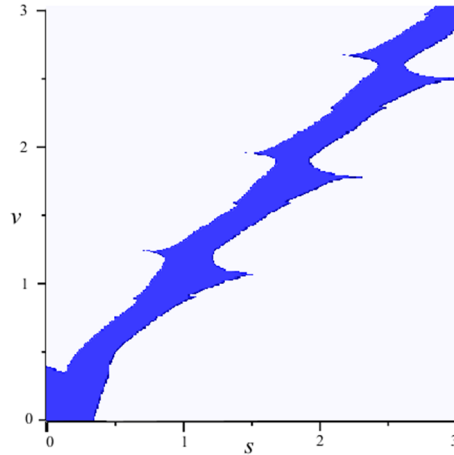
$$\begin{aligned}
A_{10} = & (s + v)(s - v)(v^6 + (-\frac{9}{4} + s^2)v^4 + (\frac{99}{8} - \frac{15}{4}s^2)v^2 + \frac{9}{8}s^2)\cos(v)^3 \\
& - (3(-v^4 + (s^2 - \frac{39}{8})v^2 - \frac{9}{8}s^2))v\sin(v)\cos(v)^2 \\
& + (-\frac{1}{2}v^6 + (\frac{99}{8} + \frac{1}{2}s^2)v^4 + (\frac{21}{8}s^2 - \frac{99}{8})v^2 - \frac{9}{8}s^2)\cos(v) \\
& - (\frac{9}{8}(-\frac{16}{3}v^4 + s^2 + 11v^2))v\sin(v). \tag{15}
\end{aligned}$$

A linear multistep method is said to be P-stable if the first quadrant of the  $s$ - $v$  plane is completely shadowed. It is said to be singularly P-stable if the method is P-stable when  $\omega = \phi$ , i.e. only when the frequency of the scalar test equation for the stability analysis is equal to the frequency of the scalar test equation for the phase-lag analysis, i.e. the shadowed area contains the bisector of the first quadrant of the  $s$ - $v$  plane. The stability region ( $s$ - $v$  plane) of the new method is plotted in Figure 1. A shadowed area denotes the region where the method is stable, while a white area denotes the region where the method is unstable. According to Figure 1, we can say that the new method is singularly P-stable. Of course, in the following theorem, we prove algebraically that the new method is singularly P-stable.

**Theorem 3.1.** The new explicit four-step Obrechhoff method with vanished phase-lag and its first, second, third and fourth derivatives (6) is singularly P-stable.

**Proof.** The stability function of the new method is

$$ST = A_2(s, v)(\lambda^4 + 1) + A_1(s, v)(\lambda^3 + \lambda) + A_0(s, v)\lambda^2, \tag{16}$$



**Figure 1:** The periodicity region of the new singularity P-stable Oberchekoff method.

where  $A_i(s, v), i = 0, 1, 2$  are mentioned after (12). In the case  $s = v$  we have

$$\begin{aligned} A_0 &= 2 - 4\cos^2(v), \\ A_1 &= 0, \\ A_2 &= 1. \end{aligned}$$

Then the characteristic equation (ChE) for the new method (6) is given by:

$$ChE = \lambda^4 - 2(2\cos^2(v) - 1)\lambda^2 + 1, \quad (17)$$

Since  $\cos(2v) = 2\cos^2(v) - 1$ , we have

$$\begin{aligned} \lambda_{1,2} &= \exp(\pm iv), \\ \lambda_{3,4} &= -\exp(\pm iv). \end{aligned}$$

So, our new method has a characteristic equation that can be written as (17), then all of its characteristic roots satisfy the necessary condition:  $|\lambda_1| = |\lambda_2| - 1$  and  $|\lambda_i| \leq 1$  with  $i = 3, 4$  for  $h\omega < \infty$ . Therefore, the interval of periodicity of the new method is  $(0, \infty)$ , and thus when  $s = v$ , the new method is P-stable, i.e. the new explicit eighth algebraic order four-step Obrechhoff method with vanished phase-lag and its first, second, third and fourth derivatives (6) is singularly P-stable. ■

## 4. NUMERICAL RESULTS

### 4.1 THE METHODS

We have used several multistep methods for the integration of the four test problems. These methods are

- The Numerov's method which is indicated as Method I.
- The Exponentially-fitted two-step method developed by Raptis and Allison [16] which is indicated as Method II.

- The Exponentially-fitted four-step method developed by Raptis [15] which is indicated as Method III.
- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [13] which is indicated as Method IV.
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [13] which is indicated as Method V.
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [13] which is indicated as Method VI.
- An exponentially-fitted eight-order method obtained in [31] which is indicated as XII.
- The new explicit four-step P-stable Obrechhoff method with vanished phase-lag and its first, second, third, fourth and fifth derivatives developed in this paper which indicated as New.

## 4.2. THE PROBLEMS

The efficiency of the new optimized symmetric explicit four-step (predictor) method will be measured through the integration of four chemical initial value problems with oscillating solution.

**Example 4.1.** Consider the almost periodic orbital problem studied by Franco and Palacios [3], as  $y'' + y = \varepsilon e^{i\psi x}$  where  $y \in \mathbb{C}$  and  $y(0) = 1, y'(0) = i, \varepsilon = 0.001, \psi = 0.01$ . The theoretical solution of the this problem is given by  $y(x) = u(x) + iv(x)$ , where  $u(x) = \frac{1-\varepsilon-\psi^2}{1-\psi^2} \cos(x) + \frac{\varepsilon}{1-\psi^2} \cos(\psi x)$  and  $v(x) = \frac{1-\varepsilon\psi-\psi^2}{-\psi^2} \sin(x) + \frac{\varepsilon}{1-\psi^2} \sin(\psi x)$ . This system of equations has been solved for  $x \in [0, 1000\pi]$ . For this problem we use  $\omega = 1$ .

**Example 4.2.** Consider the almost periodic orbital problem studied by Stiefel and Bettis [33], that can be described by  $y'' + y = 0.001e^{ix}$ , where  $y \in \mathbb{C}$  and  $y(0) = 1, y'(0) = 0.9995i$ . The theoretical solution of this problem is given by  $y(x) = u(x) + iv(x)$ , where  $u(x) = \cos(x) + 0.0005 \sin(x), v(x) = \sin(x) - 0.0005x$ . This system has been solved for  $x \in [0, 1000\pi]$  and for this problem we use  $\omega = 1$ .

**Example 4.3.** Consider the initial value problem  $y'' = -100y + 99\sin(t)$  where  $y(0) = 1, y'(0) = 11$  and  $t \in [0, 1000\pi]$  with the exact solution  $y(x) = \cos(10t) + \sin(10t) + \sin t$ . This equation is called inhomogeneous equation. For this problem we use  $\omega = 1$ .

**Example 4.4.** Let us consider the nonlinear undamped Duffing's equation  $y'' = -y - y^3 + B\cos(\omega x)$ , where

$$y(0) = 0.200426728067, \quad y'(0) = 0, \quad B = 0.002, \quad \omega = 1.01,$$

and  $x \in \left[0, \frac{40.5\pi}{1.01}\right]$ .

We use the following exact solution from [12],

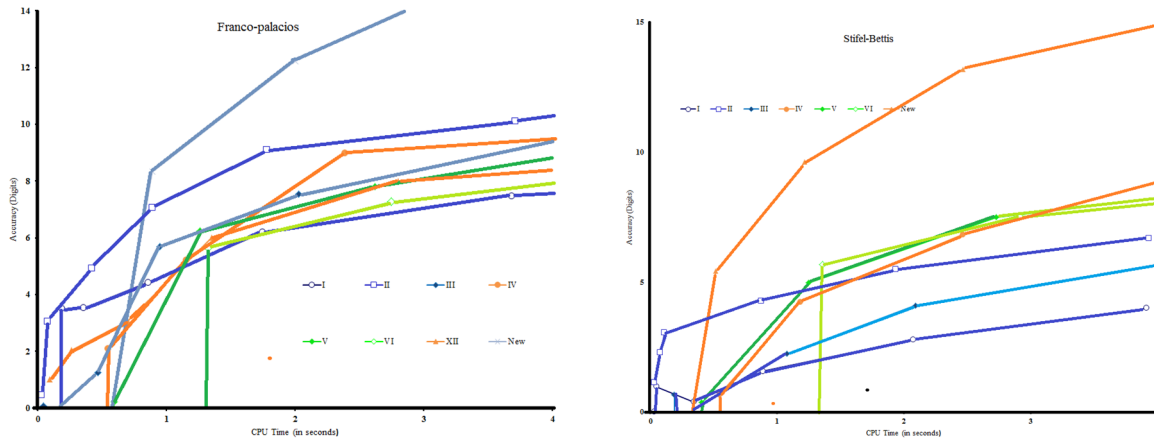
$$g(x) = \sum_{i=0}^3 K_{2i+1} \cos((2i + 1)\omega x),$$

where

$$K_1 = 0.200179477536, \quad K_3 = 0.246946143 \times 10^{-3}, \quad K_5 = 0.304016 \times 10^{-6},$$

and

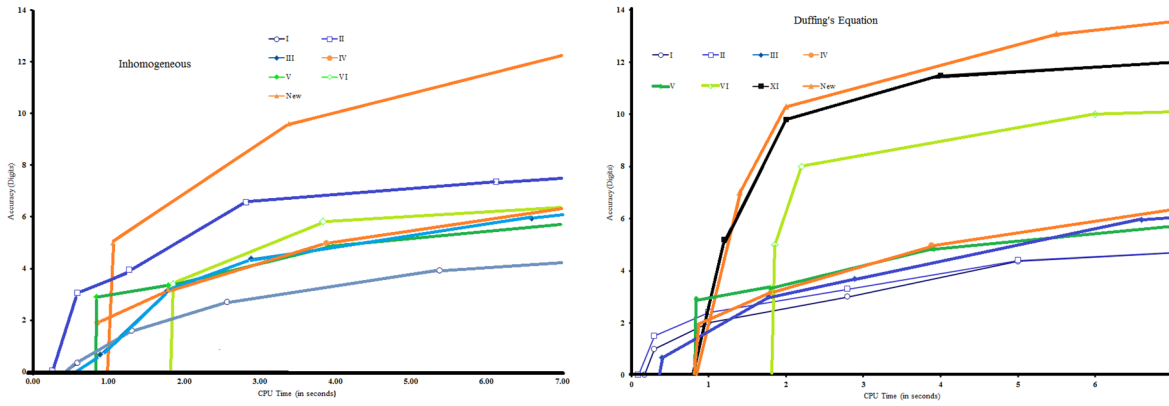
$$K_7 = 0.374 \times 10^{-9}.$$



**Figure 2:** Efficiency for the Franco and Palacios equation (left) and the orbital problem by Stiefel and Bettis (right).

In Figure 2, we see the results for the Franco-Palacios almost periodic problem (left) and the Stiefel-Bettis almost periodic problem (right) and in Figure 3, we see the results for the inhomogeneous equation (left) and the undamped Duffing’s (right) equation for several values of CPU time (in seconds). Among all the methods used, the new symmetric explicit four-step method of eighth algebraic order was the most efficient. We concluded that the new method is highly efficient compared to other similar methods it also indicates the importance of phase-lag when solving ordinary differential equations with oscillating solutions.





**Figure 3:** Efficiency for the Inhomogeneous equation (left) and the Duffing’s Equation (right).

**Example 4.5.** The close-coupling differential equations of the Schrödinger type have the form:

$$\left[ \frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^N V_{im} y_{mj}, \quad (18)$$

For  $1 \leq i \leq N$  and  $m \neq i$ . In this paper, the case in which all channels are open is studied. So, the boundary conditions are  $y_{ij} = 0$  at  $x = 0$  and

$$y_{ij} \sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left( \frac{k_i}{k_j} \right)^{\frac{1}{2}} K_{ij} k_i x n_{l_i}(k_i x),$$

where  $j_l(x)$  and  $n_l(x)$  are the spherical Bessel and Neumann functions, respectively. Of course, the new method can also be used for the case of closed channels. For this example, we use a variable stepsize technique. For this purpose, we will use embedded pairs that will be based on an LTEE process. To save space, only the numerical results are given in Table 1. For more details, we invite the readers to see the paper [35]. For the approximate solution of the above presented problem, we have used the following methods:

- The iterative Numerov method of Allison [1] which is indicated as Method A.
- The variable-step method of Raptis and Cash [17] which is indicated as Method B.
- The embedded Runge-Kutta method developed in [2] which is indicated as Method C.
- The embedded Runge-Kutta method ERK4(2) developed in [30] which is indicated as Method D.
- The embedded symmetric two-step method developed in [11] which is indicated as Method E.
- The embedded symmetric two-step method developed in [4] which is indicated as Method F.

- The developed embedded symmetric two-step method developed in [36] which is indicated as Method G.
- The developed six-step P-stable method developed in [27] which is indicated as Method H.
- The new four-step singularly P-stable method developed in this paper which is indicated as Method New.

## 5. CONCLUSION

In this paper, we have presented a new explicit singularly P-stable four-step Obrechhoff method for the numerical solution of periodic or high oscillatory initial value problems. From the numerical test to the well-known chemical problems, we found that the new method is advantageous its simplicity, accuracy, stability and efficiency.

**Table 1.** Coupled differential equations.

Method	N	$h_{max}$	RTC	$ME_{rr}$
Method A	4	0.014	3.25	$1.2 \times 10^{-3}$
	9	0.014	23.51	$5.7 \times 10^{-2}$
	16	0.014	99.15	$6.8 \times 10^{-1}$
Method B	4	0.056	1.55	$8.9 \times 10^{-4}$
	9	0.056	8.43	$7.4 \times 10^{-3}$
	16	0.056	43.32	$8.6 \times 10^{-2}$
Method C	4	0.007	45.15	$9.0 \times 10^0$
	9			
	16			
Method D	4	0.112	0.39	$1.1 \times 10^{-5}$
	9	0.112	3.48	$2.8 \times 10^{-4}$
	16	0.112	19.31	$1.3 \times 10^{-3}$
Method E	4	0.448	0.14	$3.4 \times 10^{-7}$
	9	0.448	1.37	$5.8 \times 10^{-7}$
	16	0.448	9.58	$8.2 \times 10^{-7}$
Method F	4	0.448	0.07	$2.8 \times 10^{-7}$
	9	0.448	1.14	$4.3 \times 10^{-7}$
	16	0.448	8.39	$7.1 \times 10^{-7}$
Method G	4	0.448	0.04	$9.7 \times 10^{-8}$
	9	0.448	1.01	$1.2 \times 10^{-7}$
	16	0.448	7.15	$2.3 \times 10^{-7}$
Method H	4	0.896	0.03	$5.2 \times 10^{-8}$
	9	0.896	0.96	$8.3 \times 10^{-8}$
	16	0.896	6.37	$9.1 \times 10^{-8}$
Method New	4	0.896	0.02	$4.3 \times 10^{-8}$
	9	0.896	0.83	$6.2 \times 10^{-8}$
	16	0.896	5.21	$7.1 \times 10^{-8}$

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**APPENDIX**

$$a_0 = 1/6(4(\cos(v))^4 v^4 - 30(\cos(v))^3 \sin(v) v^3 - 78(\cos(v))^4 v^2 - 10(\cos(v))^2 v^4 + 81(\cos(v))^3 \sin(v) v + 48 \cos(v) \sin(v) v^3 + 27(\cos(v))^4 + 135(\cos(v))^2 v^2 + 12v^4 - 63 \cos(v) \sin(v) v + 9((\cos(v))^2 - 12v^2 - 36)/((\cos(v))^2 v^2 + 3(\cos(v))^2 + 2v^2 - 3),$$

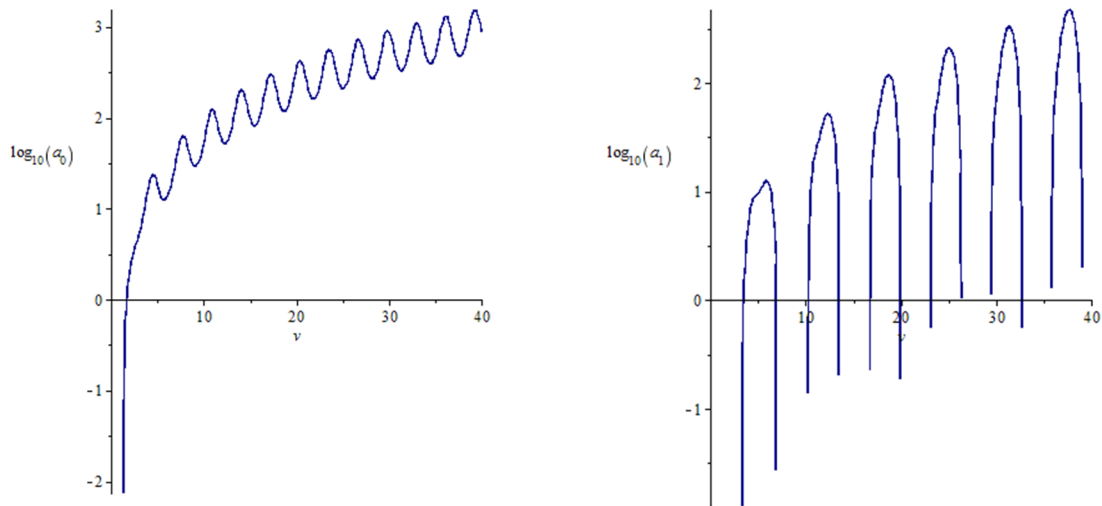
$$a_1 = 1/12(8(\cos(v))^3 v^4 - 24(\cos(v))^2 \sin(v) v^3 + 18(\cos(v))^3 v^2 + 4 \cos(v) v^4 - 117(\cos(v))^2 \sin(v) v - 48v^3 \sin(v) - 99(\cos(v))^3 - 99 \cos(v) v^2 + 99v \sin(v) + 99\cos(v))/((\cos(v))^2 v^2 + 3((\cos(v))^2 + 2v^2 - 3),$$

$$b_0 = 1/3((-4v^4 + 30v^2 - 45)((\cos(v))^4 + (18v^3 - 45v) \sin(v) (\cos(v))^3 + (10v^4 - 111v^2 - 45) \cos(v) + (24v^3 - 45v)\sin(v))/((v^2 + 3)((\cos(v))^2 + 2v^2 - 3)v^2),$$

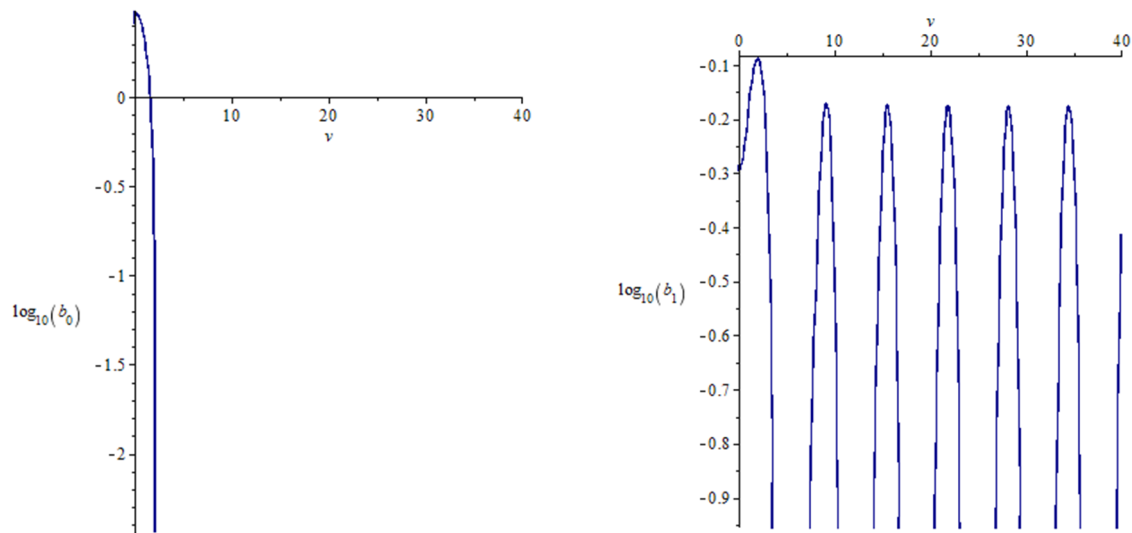
$$b_1 = 1/6((-8v^4 + 6v^2 + 45)(\cos(v))^3 + (24v^3 + 45v) \sin(v) (\cos(v))^2 + (-4v^4 + 39v^2 - 45) \cos(v) + (24v^3 - 45v)\sin(v)) / ((v^2 + 3)(\cos(v))^2 + 2v^2 - 3)v^2,$$

$$c_0 = -1/6(4(\cos(v))^4 v^4 - 6(\cos(v))^3 \sin(v) v^3 - 6(\cos(v))^4 v^2 - 10(\cos(v))^2 v^4 + 9(\cos(v))^3 \sin(v) v + 48 \cos(v) \sin(v) v^3 - 9(\cos(v))^4 + 51(\cos(v))^2 v^2 + 12v^4 - 27 \cos(v) \sin(v) v + 9(\cos(v))^2 - 36v^2)/(v^4((\cos(v))^2 v^2 + 3(\cos(v))^2 + 2v^2 - 3)),$$

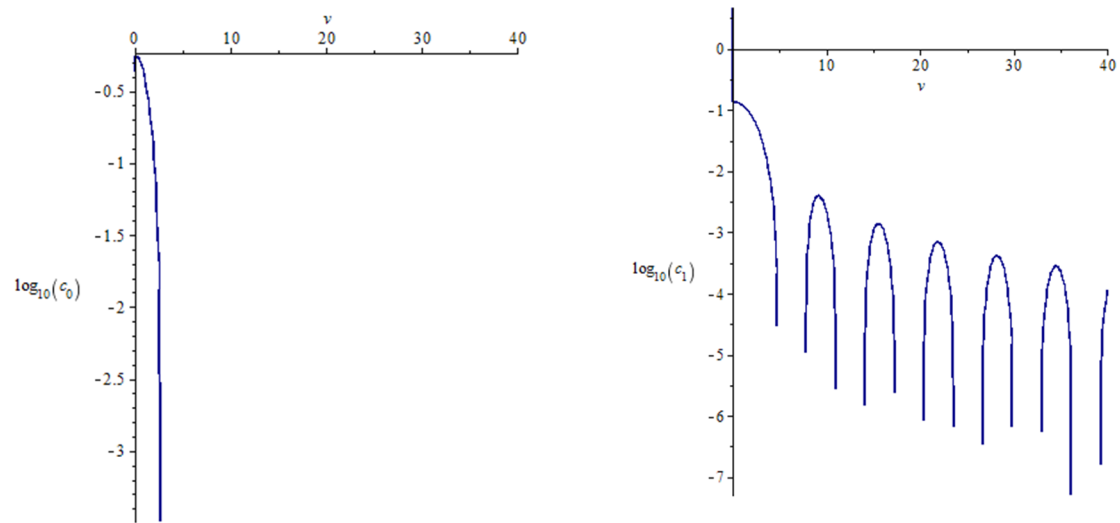
$$c_1 = -1/12(8(\cos(v))^3 v^4 - 24(\cos(v))^2 \sin(v) v^3 - 30(\cos(v))^3 v^2 + 4 \cos(v) v^4 + 27(\cos(v))^2 \sin(v) v + 9(\cos(v))^3 + 21 \cos(v) v^2 - 9v \sin(v) - 9\cos(v))/ (v^4((\cos(v))^2 v^2 + 3(\cos(v))^3 + 2v^2 - 3)).$$



**Figure 4:** Behavior of the coefficients  $a_0$  and  $a_1$  of new method.



**Figure 5:** Behavior of the coefficients  $b_0$  and  $b_1$  of new method.



**Figure 6:** Behavior of the coefficients  $d_0$  and  $d_1$  of new method.

## REFERENCES

1. A. C. Allison, The numerical solution of coupled differential equations arising from the Schrödinger equation, *J. Comput. Phys.* **6** (1970) 378–391.
2. J. R. Dormand and P. J. Prince, A family of embedded Runge-Kutta formulae, *J. Comput. Appl. Math.* **6** (1) (1980) 19–26.

3. J. M. Franco and M. Palacios, High-order P-stable multistep methods, *J. Comput. Appl. Math.* **30** (1) (1990) 1–10.
4. F. Hui and T. E. Simos, A new family of two stage symmetric two-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **53** (10) (2015) 2191–2213.
5. J. D. Lambert and I. A. Watson, Symmetric multistep methods for periodic initial value problems, *J. Inst. Math. Appl.* **18** (1976) 189–202.
6. Q. Li and X. Y. Wu, A two-step explicit P-stable method for solving second-order initial value problems, *Appl. Math. Comput.* **138** (2-3) (2003) 435–442.
7. Q. Li and X. Y. Wu, A two-step explicit P-stable method of high phase-lag order for second order IVPs, *Appl. Math. Comput.* **151** (1) (2004) 17–26.
8. Q. Li and X. Y. Wu, A two-step explicit P-stable method of high phase-lag order for linear periodic IVPs, *J. Comput. Appl. Math.* **200** (1) (2007) 287–296.
9. M. Mehdizadeh Khalsaraei, A. Shokri and M. Molayi, The new high approximation of stiff systems of first order IVPs arising from chemical reactions by k-step L-stable hybrid methods, *Iranian J. Math. Chem.* **10** (2) (2019) 181–193.
10. M. Mehdizadeh Khalsaraei and A. Shokri, An explicit six-step singularly P-stable Obrechhoff method for the numerical solution of second-order oscillatory initial value problems, *Numer. Algor.* (2019), DOI:10.1007/s11075-019-00784-w.
11. K. Mu and T. E. Simos, A Runge-Kutta type implicit high algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of coupled differential equations arising from the Schrödinger equation, *J. Math. Chem.* **53** (5) (2015) 1239–1256.
12. B. Neta, P-stable symmetric super-implicit methods for periodic initial value problems, *Comput. Math. Appl.* **50** (5-6) (2005) 701–705.
13. G. D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits, *The Astro. J.* **100** (5) (1990) 1694–1700.
14. H. Ramos, Development of a new Runge-Kutta method and its economical implementation, *Comput. Math. Methods* **1** (2) (2019) e1016.
15. A. D. Rapits, Exponentially-fitted solutions of the eigenvalues Schrödinger equation with automatic error control, *Comput. Phys. Commun.* **28** (1983) 427–431.
16. A. D. Rapits and A. C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation, *J. Comput. Phys. Commun.* **14** (1978) 1–5.
17. A. D. Raptis and J. R. Cash, A variable step method for the numerical integration of the one-dimensional Schrödinger equation, *Comput. Phys. Commun.* **36** (2) (1985) 113–119.

18. A. Shokri, A new eight-order symmetric two-step multiderivative method for the numerical solution of second-order IVPs with oscillation solutions, *Numer. Algor.* **77** (1) (2018) 95–109.
19. A. Shokri, An explicit trigonometrically fitted ten-step method with phase-lag of order infinity for the numerical solution of the radial Schrödinger equation, *Appl. Comput. Math.* **14** (1) (2015) 63–74.
20. A. Shokri, The symmetric two-step P-stable nonlinear predictor-corrector methods for the numerical solution of second order initial value problems, *Bull. Iranian Math. Soc.* **41** (2015) 191–205.
21. A. Shokri, M. Mehdizadeh Khalsaraei, M. Tahmourasi and R. Garcia-Rubio, A new family of three-stage two-step P-stable multiderivative methods with vanished phase-lag some of its derivatives for the numerical solution of radial Schrödinger equation and IVPs with oscillating solutions, *Numer. Algor.* **80** (2) (2018) 557–593.
22. A. Shokri, M.Y. Rahimi Ardabili, S. Shahmorad and G. Hojjati, A new two-step P-stable hybrid Obrechhoff method for the numerical integration of second-order IVPs., *J. Comput. Appl. Math.* **235** (2011) 1706–1712.
23. A. Shokri and H. Saadat, High phase-lag order trigonometrically fitted two-step Obrechhoff methods for the numerical solution of periodic initial value problems, *Numer. Algor.* **68** (2015) 337–354.
24. A. Shokri and M. Tahmourasi, A new two-step Obrechhoff method with vanished phase-lag and some of its derivatives for the numerical solution of radial Schrödinger equation and related IVPs with oscillating solutions, *Iranian J. Math. Chem.* **8** (2) (2017) 137–159.
25. A. Shokri, J. Vigo-Aguiar, M. Mehdizadeh Khalsaraei and R. Garcia-Rubio, A new class of two-step P-stable TFPL methods for the numerical solution second order IVPs with oscillating solutions, *J. Comput. Appl. Math.* **354** (2019) 551–561.
26. A. Shokri, J. Vigo-Aguiar, M. Mehdizadeh Khalsaraei and R. Garcia-Rubio, A new four-step P-stable Obrechhoff method with vanished phase-lag and some of its derivatives for the numerical solution of Schrödinger equation, *J. Comput. Appl. Math.* **354** (2019) 569–586.
27. A. Shokri, J. Vigo-Aguiar, M. Mehdizadeh Khalsaraei and R. Garcia-Rubio, A new implicit six-step P-stable method for the numerical solution of Schrödinger equation, *Int. J. Comput. Math.* (2019), DOI: 10.1080/00207160.2019.1588257.
28. S. Stavroyiannis and T. E. Simos, A nonlinear explicit two-step algebraic order method of order infinity for linear periodic initial value problems, *Comput. Phys. Commun.* **181** (8) (2010) 1362–1368.

29. S. Stavroyiannis and T. E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs, *Appl. Numer. Math.* **59** (10) (2009) 2467–2474.
30. T. E. Simos, Exponentially fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation and related problems, *Comput. Mater. Sci.* **18** (3-4) (2000) 315–332.
31. T. E. Simos and J. Vigo-Aguiar, An exponential fitted high order method for long-time integration of periodic initial-value problems, *Comput. Phys. Commun.* **140** (3) (2001) 358–365.
32. T. E. Simos and P. S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.*, **79** (2) (1997) 189–205.
33. E. Steifel and D. G. Bettis, Stabilization of Covell's methods, *Numer. Math.* **13** (1969) 154–175.
34. J. Vigo-Aguiar and H. Ramos, Variable stepsize implementation of multistep methods for  $y'' = f(x, y, y_0)$ , *J. Comput. Appl. Math.* **192** (2006) 114–131.
35. X. Xi and T. E. Simos, A new four-stages twelfth algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **77** (2) (2017) 333–392.
36. Z. Zhou and T. E. Simos, A new two stage symmetric two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the radial Schrödinger equation, *J. Math. Chem.* **54** (2) (2016) 442–465.