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A New Two Step Hybrid Singularly P–Stable Method for the Numerical Solution of Second Order IVPs with Oscillating Solutions

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ABSTRACT

In this paper, a new two-step hybrid method of twelfth algebraic order is constructed and analyzed for the numerical solution of initial value problems of second-order ordinary differential equations. The proposed methods are symmetric and belong to the family of multiderivative methods. Each methods of the new family appear to be hybrid, but after implementing the hybrid terms, it will continue as a multiderivative method. Therefore, the name semi-hybrid is used. The consistency, convergence, stability and periodicity of the methods are investigated and analyzed. The numerical results for some quantum chemistry problems such as. undamped Duffing's equation and orbit problems of Stiefel and Bettis indicated that the new method is superior, efficient, accurate and stable.

1. INTRODUCTION

Let us consider the initial value problems of second-order ordinary differential equations:

$$y'' = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1.1}$$

where we presume that $f(x, y)$ is sufficiently differentiable and that the first derivative does not appear explicitly in $f(x, y)$. Second-order linear differential equations are used to model many situations in physics and engineering. Here, we look at how this works for systems of an object with mass attached to a vertical spring and an electric circuit containing a resistor, an inductor, and a capacitor connected in series. Models such as these

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can be used to approximate other more complicated situations; e.g., bonds between atoms or molecules are often modeled as springs that vibrate. Generally, the solution to (1.1) is periodic, so it is expected that the results produced by suitable numerical methods be of the same periodicity of the analytic solution. Numerical methods of second-order initial value problems are divided into two classes:

- The methods with constant coefficients.
- The methods with coefficients depending on the frequency of the problem.

The analytical methods for solving differential equations are only applicable to a limited set of equations. The differential equations that appear in physics problems are almost never among these well-known categories of equations and one needs to use numerical methods to solve these problems. The rapid advancements in computational resources such as memory and processing speed of modern computers have also increased the importance of numerical methods. In the following, we mention some references. The methods based on vanishing of phase-lag and some of its derivatives [24], trigonometrically or exponentially fitted methods [4,20,23], Runge-Kutta methods [8,10], multistep methods [3,5,22], multiderivative methods [14,15], numerical methods for the fractional initial value problems [1,7,19] and hybrid methods [12,13,16] are some of the approaches that can be used for solving a second-order differential equation. The Stormer-Cowell multistep procedure with more than two steps suffered from orbital instability issues. However, these methods required prior knowledge of frequency values. Higher-order or multiderivative methods would avoid using small steps in approximating the analytical methods. Several researchers have introduced new methods via adaptation of higher-order methods, among them are the Obrechkoff methods [18]. Lambert and Watson [11] have introduced the interval of periodicity and P-stability concepts in 1976, which can be used in the stability analysis of such methods. The hybrid methods can be viewed as a predictor-corrector multistep procedure with an additional predictor at an off-step point. Consider multiderivative method of the form

$$\sum_{i=0}^{k} \alpha_i y_{n-j+1} = \sum_{i=1}^{l} h^{2i} \sum_{j=0}^{k} \beta_{ij} y_{n-j+1}^{(2i)}, \tag{1.2}$$

for the numerical integration of the problem (1.1). The method (1.2) is symmetric when $\alpha_j = \alpha_{k-j}$, $\beta_j = \beta_{k-j}$, $j = 0,1,2,\dots,k$, and it is of order q if the truncation error associated with the linear difference operator is given as

$$TE = C_{q+2} h^{q+2} y^{(q+2)}, x_{n-k+1} < \eta < x_{n+1},$$

where C_{q+2} is a constant dependent on h. In order to investigate the stability properties of the methods for solving the initial value problem (1.1) Lambert and Watson [11] introduced the scalar test equation

$$y'' = \omega^2 y,\ \omega \in \mathbb{R}. \tag{1.3}$$

When a symmetric two-step method is applied to the scalar test equation (1.3), we obtain a difference equation of the form

$$A(v)y_{n+1} - 2B(v)y_n + A(v)y_{n-1} = 0, \tag{1.4}$$

or equivalently

$$A(v)y_{n+1} - 2C(v)y_n + y_{n-1} = 0, \tag{1.5}$$

where $v = \omega h$, h is the step length and $C(v)$ is a function of v independent of y_{n+1}, y_n and y_{n-1}. So, the characteristic equation of the method is defined by

$$\xi^2 - 2C(v)\xi + 1 = 0, \tag{1.6}$$

Definition 1.1. The interval $(0, v_0^2)$ is said to be the periodicity interval of method (1.5), if for all $v^2 \in (0, v_0^2)$, the roots of (1.6) satisfy $\xi_1 = \bar{\xi}_2 = e^{i\theta(v)}$, where $\theta(v)$ is a real function of *v*.

Definition 1.2. The method (1.5) is called P-stable if its periodicity interval is $(0, +\infty)$.

Definition 1.3. For any method corresponding to the characteristic equation (1.6), the quantity $P(v) = v - cos^{-1}[C(v)]$ is called the phase-lag of the method.

Anantha Krishnaiah [6], gives an equivalent definition of the phase-lag error as follow:

Definition 1.4. The phase-lag of a numerical method is the leading term in the expression of

$$P(v) = \left|\frac{\cos(v) - C(v)}{v^2}\right|. \tag{1.7}$$

Now, if *P*(*v*) = $0(v^{t+1})$ as $v \to 0$, the order of phase-lag is *t*.

Definition 1.5. A method is said to be phase-fitted, if it has phase-lag of order infinity.

This article is organized as follows. The presentation and production of the new method is presented in Section 2. In Section 3, the numerical experiments are reported. Finally, we provide some concluding remarks.

2. Development and Analysis

2.1. Development

For the numerical integration of (1.1), we consider the new two-step method as follow

$$y_{n+1} - 2y_n + y_{n-1} = h^2[\alpha_1 f_n + \alpha_2(f_{n+1} + f_{n-1})]$$

$$+h^4[\alpha_3 g_n + \alpha_4(g_{n+1} + g_{n-1})]$$
$$+h^4\beta_1\left[\bar{g}_{n+\frac{1}{2}} + \hat{g}_{n-\frac{1}{2}}\right].$$
$$+h^6\beta_2\left[\overline{w}_{n+\frac{1}{2}} + \widehat{w}_{n-\frac{1}{2}}\right], \tag{2.1}$$

where

$$\bar{y}_{n+\frac{1}{2}} = h^2(f_{n+1} + f_{n-1}) + \frac{1}{2}h^2 f_n,$$
$$\hat{y}_{n-\frac{1}{2}} = h^2(f_{n+1} + f_{n-1}) + \frac{1}{2}h^2 f_n,$$

where h is the step length of the method, $y'' = f(x,y), y^{(4)} = g(x,y), y^{(6)} = w(x,y)$, and $\alpha_i, i = 1(1)4$ and $\beta_j,\ j = 1,2$ are six arbitrary parameters. For this method, we assume four of the free parameters are calculated through Taylor's series and the rest of the free parameters by the manufacturer system through vanishing of phase-lag and its first derivative. So, the coefficients $\alpha_1, \alpha_2, \alpha_3$ and α_4 will be as

$$\alpha_1 = \frac{115}{126} - 800\beta_1 - 1920\beta_2,$$
$$\alpha_2 = 400\beta_1 + 960\beta_2 + \frac{11}{252},$$
$$\alpha_3 = -\frac{976}{3}\beta_1 - 800\beta_2 + \frac{313}{7560},$$
$$\alpha_4 = -\frac{112}{3}\beta_1 - 80\beta_2 - \frac{13}{15120}.$$

Now, we apply the above method to the scalar test equation (1.3) and we get the following difference equation:

$$A(v)y_{n+1} - 2B(v)y_n + A(v)y_{n-1} = 0, \tag{2.2}$$

where $C(v)$ is a function of v independent of y_{n+1}, y_n and y_{n-1}. Then the characteristic equation associated with (2.2) can be written as:

$$\xi^2 - 2C(v)\xi + 1 = 0, \tag{2.3}$$

So, according to (1.7), the phase-lag of the method (2.1) is as follows:

$$\begin{aligned} PL = {} & -(30240\cos(v)\,v^8\beta_2 - 30240\cos(v)\,v^6\beta_1 - 564480\cos(v)\,v^4\beta_1 \\ & -1209600\cos(v)\,v^4\beta_2 - 13\cos(v)\,v^4 - 2459520v^4\beta_1 - 6048000v^4\beta_2 \\ & -6048000\cos(v)\,v^2\beta_1 - 14515200\cos(v)\,v^2\beta_2 + 313v^4 - 660\cos(v)\,v^2 \\ & +6048000v^2\beta_1 - 14515200v^2\beta_2 - 6900v^2 - 6900v^2 - 15120\cos(v) + 15120)/ \\ & ((30240\beta_2 v^8 - 30240\beta_1 v^6 - 564480v^4\beta_1 - 1209600v^4\beta_2 \\ & -13v^4 - 6048000v^2\beta_1 - 14515200v^2\beta_2 - 660v^2 - 15120)v^2). \end{aligned}$$

We demand that the phase-lag and its first derivative to be equal to zero. Based on the above we obtain the coefficients of the first method. To save space, the coefficients of the method are given in the Appendix. The following Taylor series expansions should be used in the cases that the coefficients are subject to heavy cancelations for some values of $|v|$:

$$\alpha_1 = \frac{11405}{12639} - \frac{27282982}{273429029445}v^2 - \frac{1586736771}{8601275207853328}v^4 + \frac{104275129825222497941}{5124584829913877700838065600}v^6 + \cdots,$$

$$\alpha_2 = \frac{617}{12639} + \frac{13641491}{273429029445}v^2 + \frac{1586736771}{17202550415706656}v^4 - \frac{104275129825222497941}{10249169659827755401676131200}v^6 - \cdots,$$

$$\alpha_3 = \frac{28213}{758340} - \frac{61945787}{1531202564892}v^2 - \frac{3340484369329}{46446886122407971200}v^4 + \frac{64145009945443436 81}{7686877244870816551257098 40}v^6 + \cdots,$$

$$\alpha_4 = -\frac{1019}{758340} - \frac{72232813}{15312025648920}v^2 - \frac{72592685567}{7145674788062764800}v^4 + \frac{3308549981993749799}{361735399758626661235628160 0}v^6 + \cdots,$$

$$\beta_1 = \frac{9}{674080} + \frac{5143513}{36748861557408}v^2 + \frac{229673365421}{371575088979263769600}v^4 - \frac{15648703928695229}{9370669403271090652961034 24}v^6 - \cdots,$$

$$\beta_2 = -\frac{37}{203841792} - \frac{69996503}{11024658467222400}v^2 - \frac{143989579787}{891780213550233047040}v^4 - \frac{1989558340954492837}{5466223818574802880893936 64000}v^6 - \cdots,$$

where $v = \omega h$. The local truncation error of the new proposed method is given by:

$$LTE_{New} = \frac{223631h^{14}}{918205352064000}\left[\omega^4 y^{(10)} + 2\omega^2 y^{(12)} + y^{(14)}\right].$$

The behavior of the coefficients are shown in Figures 2.1 – 2.3.

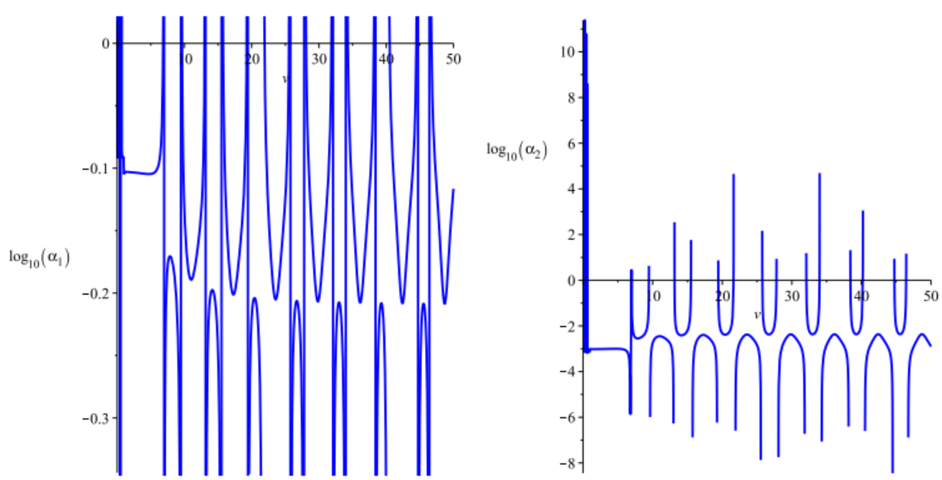

Figure 2.1: Behavior of the coefficients α_1 and α_2 of the new method.

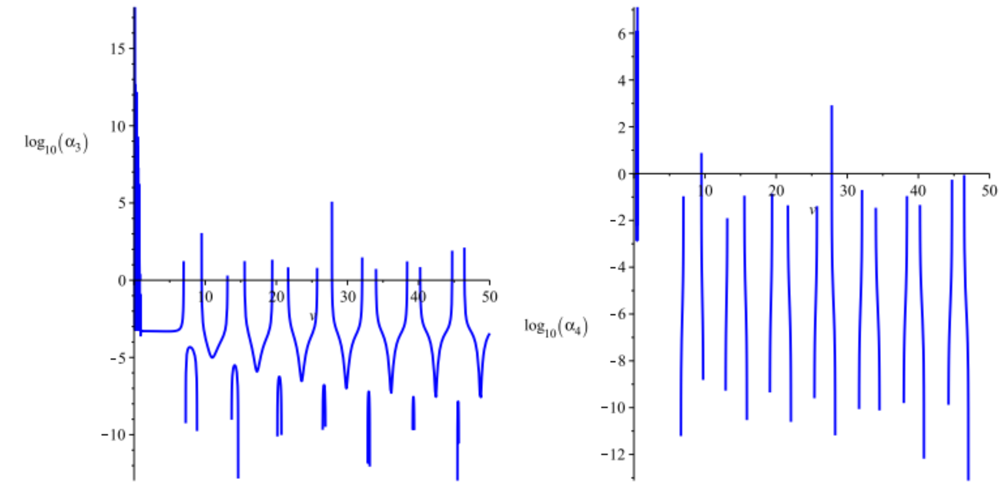

Figure 2.2: Behavior of the coefficients α_3 and α_4 of the new method.

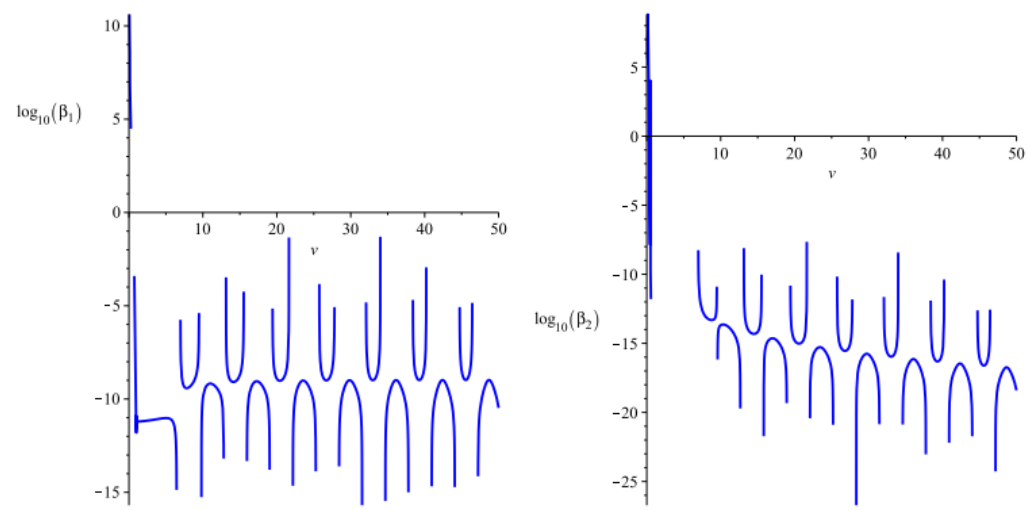

Figure 2.3: Behavior of the coefficients β_1 and β_2 of the new method.

2.2. PERIODICITY ANALYSIS

In order to investigate and calculate the interval of periodicity and the stability region of the new method (2.1), we use the following scalar test equation:

$$y''(x) = -\phi y(x) \cdot \tag{2.4}$$

Note that the frequency used in the scalar test equation for the stability analysis (ϕ) is not equal to the frequency of the scalar test equation used for the phase-lag analysis (1.3), (ϕ), i.e. $\phi \neq \omega$. For this purpose, applying the new method to the scalar test equation (2.4), leads to the following difference equation

$$A_1(s,v)(y_{n+1}+y_{n-1})+A_0(s,v)y_n=0, \tag{2.5}$$

where

$$A_0(s,v)=\frac{1}{7560}\frac{A_{00}}{A},$$
$$A_1(s,v)=\frac{1}{30240}\frac{A_{10}}{A},$$

where $v = \omega h$ and $s = \phi h$ and

$$\begin{aligned}A_{00} =\ &((-313s^4+6900s^2-15120)v^{12}+(-13800s^4+262800s^2-564480)v^{10}\\ &+(-363960s^4+4818240s^2-9676800)v^8+(-5483520s^4+19353600s^2\\ &-14515200)v^6+(-9676800s^4+29030400s^2-14515200)v^4\\ &-14515200s^2(s^2-2)v^2-14515200s^4)\cos(v)^2+((997200s^2-2459520)v^{10}\\ &+(-1495800s^4+1229760s^2+6048000)v^8+(2459520s^4-12096000s^2\\ &+14515200)v^6+(6048000s^4-29030400s^2+29030400)v^4+(14515200s^4\\ &-58060800s^2)v^2+29030400s^4)\cos(v)+(249300((s^2\\ &-3416/1385)v^9\sin(v)-(16128/277)s^2+(16128/277)v^2))(s-v)(s+v)\end{aligned}$$

$$\begin{aligned}A_{10} =\ &(26((15120/13+s^4+(660/13)s^2)v^8+((49680/13)s^2\\ &+(1320/13)s^4+564480/13)v^6+((55080/13)s^4+(1149120/13)s^2\\ &+9676800/13)v^4+((564480/13)s^4+14515200/13+(7257600/13)s^2)v^2\\ &+(7257600/13)s^2+14515200/13+(3024000/13)s^4)(s+v)^2(s-v)^2\cos(v)^2\\ &+((1252s^6+27600s^4+465120s^2+4919040)v^{10}+(-626s^8-41400s^6\\ &-758160s^4-8507520s^2-12096000)v^8+(27600s^8+120960s^6+1128960s^4\\ &+9676800s^2-29030400)v^6+(404640s^8+1128960s^6+4838400s^4\\ &+29030400s^2-58060800)v^4+(3790080s^8+9676800s^6+29030400s^4\\ &+116121600s^2)v^2-12096000s^4((12/5)s^2+24/5+s^4))\cos(v)\\ &+313v^9(s+v)(s-v)(s^6+(6900/313)s^4+(116280/313)s^2\\ &+1229760/313)\sin(v)+(997200s^8+2459520s^6+6048000s^4+14515200s^2\\ &+29030400)v^4+(-4919040s^8-12096000s^6-29030400s^4-58060800s^2)v^2\\ &+6048000s^4((12/5)s^2+24/5+s^4),\end{aligned}$$

and

$$\begin{aligned}A =\ &v^4((v^8+(112/3)v^6+640v^4+960v^2+960)\cos(v)^2\\ &+((488/3)v^6-400v^4-960v^2-1920)\cos(v)-(122/3)\sin(v)v^7+960).\end{aligned}$$

In Figure 2.4, we present the $s-v$ plane for the method developed in this paper. A shadowed area denotes the $s-v$ region where the method is stable, while a white area denotes the region where the method is unstable. A linear multistep method is said to be P-stable if the first quadrant of the $s-v$ plane is completely shadowed.

Definition 2.1. A method is called singularly P-stable if its interval of periodicity is equal to $(0,+\infty)$ only when the frequency used in the scalar test equation for the stability analysis ϕ is equal to the frequency used for the scalar test equation for the phase lag analysis ϕ, i.e., $\phi=\omega$.

Based on the Definition 2.1, we can say that a method is said to be singularly P-stable if the first diagonal of the $s-v$ plane is completely shadowed. Based on this study and Figure 2.4, we conclude that the new two-step method is singularly P-stable, i.e. P-stable when $s=v$. Of course, in the following theorem, we prove algebraically that the new method is singularly P-stable.

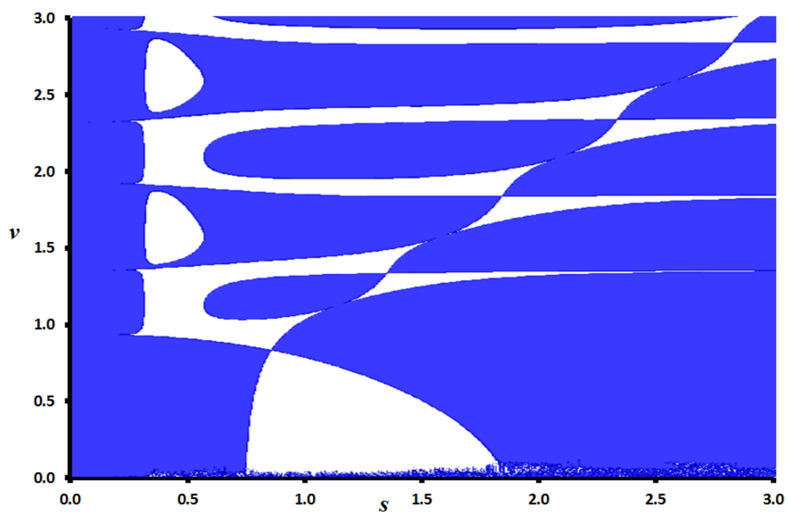

Figure 2.4: The periodicity region of the new method.

Theorem 2.1 *The new two-step hybrid method* (2.1) *is singularly P-stable.*

Proof. If we take $s=v$ in (2.5), the characteristic equation of the new method can be written as $\text{Char}=313\frac{C_1}{C_2}(\lambda^2-2\cos(v)\,\lambda+1)$, where

$$C_1=((v^6+(116280/313)v^2+1229760/313+(6900/313)v^4)\cos(v)$$
$$-1229760/313+(498600/313)v^2)v^6$$

and

$$C_2 = (15120v^8 + 564480v^6 + 9676800v^4 + 14515200v^2 + 14515200)\cos(v)^2$$
$$+(2459520v^6 - 6048000v^4 - 14515200v^2 - 29030400)\cos(v)$$
$$-614880\sin(v)v^7 + 14515200$$

So, the interval of periodicity is $(0, +\infty)$, and then the new method is singularly P-stable.

3. Numerical Results

In this section, we are going to calculate some numerical results obtained by the new hybrid method (2.1), and compare them with those from other multistep methods. The methods used in the comparison have been denoted by:

- The multiderivative method of Shokri [21], which is indicated as Method A.
- The multiderivative method of Simos [25], which is indicated as Method B.
- The multiderivative method of Van Daele [27], which is indicated as Method C.
- The multiderivative method of Achar [2], which is indicated as Method D.
- The multiderivative method of Wang [28], which is indicated as Method E.
- The first method developed in this paper, which indicated as New

Example 3.1. Let us consider the nonlinear undamped Duffing's equation

$$y'' = -y - y^3 + B\cos(\omega x), \qquad y(0) = 0.200426728067, \qquad y'(0) = 0, \tag{3.1}$$

where $B = 0.002, \omega = 1.01$ and $x \in \left[0, \frac{40.5\pi}{1.01}\right]$, We use the following exact solution for (3.1) from [17], $g(x) = \sum_{i=0}^{3} K_{2i+1}\cos((2i+1)\omega x)$, where

$$\{K_1, K_3, K_5, K_7\} = \{0.200179477536, 0.246946143 \times 10^{-3}, 0.304016 \times 10^{-6}, 0.374 \times 10^{-9}\}.$$

In order to integrate this equation by an Obrechkoff method, one needs the values of y', which occur in calculating $y^{(4)}$. These higher order derivatives can all be expressed in terms of $y(x)$ and $y'(x)$ through (3.1), i.e.

$$y^{(3)}(x) = -\left(1 + 3y^2(x)\right)y'(x) - B\omega\sin(\omega x),$$
$$y^{(4)}(x) = -(1 + 3y^2(x))y''(x) - 6y(x)y'(x)^2 - B\omega^2\cos(\omega x),$$

The absolute errors at $x = \frac{40.5\pi}{1.01}$, are given in Table 3.1, where $M = \frac{40.5\pi}{1.01}$ and the CPU times are listed in Table 3.2.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	$8.26e-11$	$9.31e-11$	$3.15e-4$	$4.06e-5$	$4.09e-5$	$4.08e-5$
$\frac{M}{1000}$	$9.52e-12$	$8.03e-12$	$1.81e-5$	$1.87e-6$	$1.27e-6$	$1.27e-6$
$\frac{M}{2000}$	$3.74e-12$	$5.52e-12$	$1.07e-6$	$3.84e-8$	$3.94e-8$	$3.93e-8$
$\frac{M}{3000}$	$7.16e-13$	$7.25e-12$	$2.09e-7$	$5.13e-9$	$5.18e-9$	$5.17e-9$
$\frac{M}{4000}$	$2.18e-13$	$6.99e-12$	$6.55e-8$	$3.19e-9$	$1.23e-9$	$1.23e-9$
$\frac{M}{5000}$	$9.65e-14$	$6.65e-12$	$2.67e-8$	$9.89e-10$	$4.09e-10$	$4.07e-10$

Table 3.1: Comparison of the end-point absolute error in the approximations obtained for Example 3.1.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	1.42	1.45	1.44	1.48	1.19	1.41
$\frac{M}{1000}$	2.25	2.87	2.89	2.94	2.31	2.89
$\frac{M}{2000}$	5.12	6.27	6.23	6.36	4.81	6.24
$\frac{M}{3000}$	7.61	9.86	9.86	9.72	7.55	9.55
$\frac{M}{4000}$	10.25	13.42	13.55	13.39	9.99	13.06
$\frac{M}{5000}$	14.81	16.86	16.92	16.97	12.86	16.50

Table 3.2: CPU time for the example 3.1.

Example 3.2. Consider the initial value problem

$$y'' = -100y + 99\sin(x), y(0) = 1, y'(0) = 11,$$

with the exact solution $y(t) = \sin(t) + \sin(10t) + \cos(10t)$. This equation has been solved numerically for $0 \leq x \leq 10\pi$ using exact starting values. In the numerical experiment, we take the step lengths $h = \pi/50, \pi/100, \pi/200, \pi/300, \pi/400$ and $\pi/500$. The absolute errors at the end point are given in Table 3.3, and the CPU times are listed in Table 3.4.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{\pi}{50}$	$8.32\text{e}-27$	$1.76\text{e}-26$	$3.03\text{e}-06$	$3.64\text{e}-06$	$2.23\text{e}-08$	$1.76\text{e}-16$
$\frac{\pi}{100}$	$4.61\text{e}-31$	$4.50\text{e}-30$	$1.15\text{e}-08$	$6.79\text{e}-09$	$7.98\text{e}-11$	$4.54\text{e}-20$
$\frac{\pi}{200}$	$3.69\text{e}-36$	$1.91\text{e}-34$	$4.50\text{e}-11$	$1.07\text{e}-12$	$5.24\text{e}-14$	$1.92\text{e}-24$
$\frac{\pi}{300}$	$9.04\text{e}-38$	$4.61\text{e}-37$	$1.76\text{e}-12$	$8.13\text{e}-15$	$6.38\text{e}-16$	$4.65\text{e}-27$
$\frac{\pi}{400}$	$7.81\text{e}-40$	$6.28\text{e}-39$	$1.76\text{e}-13$	$2.56\text{e}-16$	$2.74\text{e}-17$	$6.34\text{e}-29$
$\frac{\pi}{500}$	$5.02\text{e}-41$	$2.23\text{e}-40$	$2.95\text{e}-14$	$1.79\text{e}-17$	$2.38\text{e}-18$	$2.25\text{e}-30$

Table 3.3: Comparison of the end-point absolute error in the approximations obtained for Example 3.2.

Example 3.3. Consider the initial value problem

$$y'' = \frac{8y^2}{1+2x}, y(0) = 1,\ y'(0) = -2,\ x \in [0,4.5],$$

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{\pi}{50}$	0.19	0.26	0.17	0.25	0.19	0.11
$\frac{\pi}{100}$	0.43	0.58	0.51	0.53	0.45	0.28
$\frac{\pi}{200}$	0.92	1.14	0.86	0.83	0.75	0.58
$\frac{\pi}{300}$	1.35	1.81	1.14	1.15	0.95	0.92
$\frac{\pi}{400}$	1.52	2.50	1.39	1.40	1.23	1.26
$\frac{\pi}{500}$	1.76	2.95	1.70	1.78	1.47	1.56

Table 3.4: CPU time for the example 3.2.

with the exact solution $y = \frac{1}{1+2x}$. The absolute errors at $x = 4.5$ are given in the Table 3.5, and the CPU times are listed in Table 3.6.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{4.5}{500}$	4.36e − 22	2.14e − 21	1.07e − 09	1.31e − 17	7.46e − 14	2.74e − 21
$\frac{4.5}{1000}$	1.37e − 25	1.23e − 24	9.24e − 12	1.77e − 20	5.36e − 16	1.55e − 24
$\frac{4.5}{2000}$	7.86e − 29	3.36e − 28	5.45e − 14	2.20e − 23	2.88e − 18	5.84e − 28
$\frac{4.5}{3000}$	8.14e − 31	1.81e − 30	2.45e − 15	4.23e − 25	1.25e − 19	5.22e − 30
$\frac{4.5}{4000}$	4.05e − 32	1.02e − 31	2.63e − 16	2.52e − 26	1.32e − 20	1.78e − 31
$\frac{4.5}{5000}$	6.14e − 33	1.11e − 32	4.60e − 17	2.80e − 27	2.29e − 21	1.28e − 32

Table 3.5: Comparison of the end-point absolute error in the approximations obtained for Example 3.3.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{4.5}{500}$	0.19	0.36	0.36	0.34	0.19	0.31
$\frac{4.5}{1000}$	0.75	0.61	0.62	0.61	0.76	1.23
$\frac{4.5}{3000}$	1.14	1.28	1.23	1.92	1.20	1.87
$\frac{4.5}{4000}$	1.51	1.93	1.89	2.59	1.62	2.56
$\frac{4.5}{5000}$	2.03	2.56	2.59	3.29	2.06	3.24

Table 3.6: CPU time for Example 3.3.

Example 3.4. Consider the almost periodic orbital problem studied by Franco and Palacios [9], can be described by

$$y'' = \varepsilon e^{i\psi x}, \qquad y(0) = 1, \qquad y'(0) = i, \qquad y \in \mathbb{C},$$

or equivalently by

$$u'' + u = \varepsilon cos(\psi x), \qquad u(0) = 1, \qquad u'(0) = 0,$$
$$v'' + v = \varepsilon sin(\psi x), \qquad v(0) = 0, \qquad v'(0) = 1,$$

where $\varepsilon = 0.001$ and $\psi = 0.01$. The theoretical solution of the this problem is given by

$$y(x) = u(x) + iv(x), \qquad u, v \in \mathbb{R}, \tag{3.2}$$

where

$$u(x) = \frac{1-\varepsilon-\psi^2}{1-\psi^2}\cos(x) + \frac{\varepsilon}{1-\psi^2}\cos(\psi x),$$
$$v(x) = \frac{1-\varepsilon\psi-\psi^2}{-\psi^2} sin(x) + \frac{\varepsilon}{1-\psi^2} sin(\psi x),$$

This system of equations has been solved for $x \in [0,1000\pi]$. For this problem we use $\omega = 1$. The absolute errors at the end point are given in Table 3.7, and the CPU times are listed in Table 3.8, where $M = \frac{40.5\pi}{1.01}$.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	2.53e − 10	1.35e − 09	2.04e − 06	5.19e − 06	1.07e − 04	2.58e − 09
$\frac{M}{1000}$	1.02e − 11	4.53e − 11	2.40e − 07	1.59e − 07	1.52e − 05	7.43e − 11
$\frac{M}{1500}$	3.08e − 12	6.17e − 12	5.87e − 08	9.03e − 08	1.12e − 06	8.03e − 12
$\frac{M}{2000}$	8.39e − 13	1.05e − 12	2.64e − 08	1.45e − 08	4.96e − 07	2.01e − 12
$\frac{M}{2500}$	1.09e − 13	6.19e − 13	1.60e − 08	2.43e − 09	1.25e − 07	7.80e − 13
$\frac{M}{3000}$	7.98e − 14	2.05e − 13	1.13e − 08	1.82e − 09	3.45e − 08	3.80e − 13

Table 3.7: Comparison of the end-point absolute error in the approximations obtained for Example 3.4.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	0.36	0.39	0.36	0.42	0.37	0.37
$\frac{M}{1000}$	0.65	0.78	0.76	0.80	0.78	0.78
$\frac{M}{1500}$	0.93	1.15	1.17	1.19	1.20	1.17
$\frac{M}{2000}$	1.24	1.56	1.59	1.61	1.58	1.47
$\frac{M}{2500}$	1.67	1.98	1.95	2.00	1.98	1.97
$\frac{M}{3000}$	2.05	2.32	2.37	2.34	2.39	2.40

Table 3.8: CPU time for Example 3.4.

Example 3.5. The almost periodic orbital problem studied by Stiefel and Bettis [26], can be described by

$$y'' + y = 0.001e^{ix}, \qquad y(0) = 1, \qquad y'(0) = 0.9995i, \qquad y \in \mathbb{C},$$

or equivalently by

$$u'' + u = 0.001\cos(\psi x), \qquad u(0) = 1, \qquad u'(0) = 0,$$
$$v'' + v = 0.001\sin(\psi x), \qquad v(0) = 0, \qquad v'(0) = 0,$$

The theoretical solution of this problem is given by $y(x) = u(x) + iv(x)$, where $u, v \in \mathbb{R}$ and

$$u(x) = cos(x) + 0.0005sin(x),$$
$$u(x) = sin(x) - 0.0005cos(x),$$

This system has been solved for $x \in [0,1000\pi]$ and for this problem we use $\omega = 1$.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	4.09e − 06	2.36e − 05	1.86e − 03	1.91e − 03	2.55e − 02	3.54e − 05
$\frac{M}{1000}$	5.18e − 07	1.07e − 06	4.32e − 04	7.44e − 04	4.94e − 02	2.05e − 06
$\frac{M}{1500}$	1.61e − 18	1.03e − 07	1.08e − 04	1.89e − 05	8.74e − 04	1.28e − 07
$\frac{M}{2000}$	2.51e − 09	2.38e − 09	2.69e − 05	2.61e − 07	1.21e − 05	7.94e − 09
$\frac{M}{2500}$	4.03e − 10	1.09e − 10	6.70e − 06	4.48e − 09	1.96e − 07	4.96e − 10
$\frac{M}{3000}$	1.47e − 11	1.12e − 11	1.46e − 06	8.55e − 11	4.36e − 09	2.71e − 11

Table 3.9: Comparison of the end-point absolute error in the approximations obtained for Example 3.5.

h	New	Method A	Method B	Method C	Method D	Method E
$\frac{M}{500}$	0.05	0.05	0.05	0.06	0.05	0.05
$\frac{M}{1000}$	0.09	0.11	0.11	0.12	0.11	0.14
$\frac{M}{1500}$	0.24	0.30	0.31	0.30	0.30	0.23
$\frac{M}{2000}$	0.58	0.80	0.72	0.62	0.80	0.75
$\frac{M}{2500}$	1.24	1.58	1.47	1.34	1.39	1.42
$\frac{M}{3000}$	2.06	2.59	2.71	2.64	2.66	2.84

Table 3.10: CPU time for Example 3.5.

4. CONCLUSIONS

In this paper, we have presented the new two-step symmetric hybrid method of order 12. The details of the procedure adapted for the applications have been given in section two. With vanishing of phase-lag and its derivative, we have improved the local truncation error, phase-lag error, interval of periodicity and CPU time for the classes of two-step multiderivative methods. The numerical results obtained by the new method for some chemical problems show its superiority in efficiency, accuracy and stability.

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APPENDIX: The Coefficients of the new Method

$$\alpha_1 = \frac{115}{126} + \frac{1}{1134}((780(v^4 + \frac{56}{3}v^2 + 200)(v^{10} + \frac{990}{13}v^8 + \frac{30240}{13}v^6 - \frac{10080}{13}v^4 - \frac{604800}{13}v^2$$
$$- \frac{3628800}{13})\cos(v) - 18780v^{14} + 333880v^{12} + 10696800v^{10} + 209088000v^8 - 1236211200v^6$$
$$-8491392000v^4 - 31352832000v^2 + 130636800000)(\sin(v))^2$$
$$-4695(v^2 - \frac{6900}{313})((v^4 + \frac{56}{3}v^2 + 200)\cos(v) - 200 + \frac{244}{3}v^2)v^9\sin(v)$$
$$+(-780v^{14} + 1453480v^{12} - 57343200v^{10} + 263520000v^8$$
$$+1206374400v^6 + 13644288000v^4 - 85349376000v^2$$
$$+174182400000)\cos(v) + 18780v^{14} - 333880v^{12} - 10696800v^{10}$$
$$-209088000v^8 + 4236825600v^6 - 13644288000v^4 + 85349376000v^2 - 174182400000)v^{-4}$$
$$(((v^8 + \frac{112}{3}v^6 + 640v^4 + 960v^2 + 960)(v^4 + \frac{56}{3}v^2 + 200)\cos(v) + \frac{206080}{3}v^6 - 149760v^4$$
$$-341760v^2 + \frac{49256}{9}v^8 - 576000 + 244v^{10})(\sin(v))^2 + \frac{122}{3}v^7((v^4 + \frac{56}{3}v^2 + 200)\cos(v)$$
$$-200 + \frac{244}{3}v^2)\sin(v) + (-768000 - 263680v^2 - 56v^{10} - \frac{132904}{9}v^8$$
$$-149760v^4 - v^{12} + \frac{134080}{3}v^6)\cos(v) + 768000 + 263680v^2 + 149760v^4$$
$$-244v^{10} - \frac{206080}{3}v^6 - \frac{49256}{9}v^8)^{-1} + \frac{1}{63}((52v^8 + 5280v^6 + 220320v^4$$
$$+2257920v^2 + 12096000)(\sin(v))^2 - 626\sin(v)v^9 + (1252v^8 - 55200v^6$$
$$-809280v^4 - 7580160v^2 + 24192000)\cos(v) - 52v^8 - 5280v^6$$
$$-2214720v^4 + 7580160v^2 - 24192000)((v^8 + \frac{112}{3}v^6 + 640v^4$$
$$+960v^2 + 960)(\sin(v))^2 + \frac{122}{3}\sin(v)v^7 + (1920 + 960v^2 + 400v^4$$
$$-\frac{488}{3}v^6)\cos(v) - 640v^4 - v^8 - 1920 - 960v^2 - \frac{112}{3}v^6)^{-1}v^{-4},$$

$$\alpha_2 = \frac{11}{252} + \frac{1}{2268}((-780(v^4 + \frac{56}{3}v^2 + 200)(v^{10} + \frac{990}{13}v^8 + \frac{30240}{13}v^6$$
$$-\frac{10080}{13}v^4 - \frac{604800}{13}v^2 - \frac{3628800}{13})\cos(v) + 18780v^{14} - 333880v^{12}$$
$$-10696800v^{10} - 209088000v^8 + 1236211200v^6 + 8491392000v^4$$
$$+31352832000v^2 - 130636800000)(\sin(v))^2$$
$$+4695(v^2 - \frac{6900}{313})((v^4 + \frac{56}{3}v^2 + 200)\cos(v)$$
$$-200 + \frac{244}{3}v^2)v^9\sin(v) + (780v^{14} - 1453480v^{12} + 57343200v^{10}$$

$$-263520000v^8 - 1206374400v^6 - 13644288000v^4 + 85349376000v^2$$
$$-174182400000)\cos(v) - 18780v^{14} + 333880v^{12} + 10696800v^{10}$$
$$+209088000v^8 - 4236825600v^6 + 13644288000v^4 - 85349376000v^2$$
$$+174182400000)v^{-4}(((v^8 + \frac{112}{3}v^6 + 640v^4 + 960v^2 + 960)(v^4$$
$$+\frac{56}{3}v^2 + 200)\cos(v) + \frac{206080}{3}v^6 - 149760v^4 - 341760v^2$$
$$+\frac{49256}{9}v^8 - 576000 + 244v^{10})(\sin(v))^2 + \frac{122}{3}v^7((v^4 + \frac{56}{3}v^2$$
$$+200)\cos(v) - 200 + \frac{244}{3}v^2)\sin(v) + (-768000 - 263680v^2$$
$$-56v^{10} - \frac{132904}{9}v^8 - 149760v^4 - v^{12} + \frac{134080}{3}v^6)\cos(v)$$
$$+768000 + 263680v^2 + 149760v^4 - 244v^{10} - \frac{206080}{3}v^6$$
$$-\frac{49256}{9}v^8)^{-1} + \frac{1}{63}((-26v^8 - 2640v^6 - 110160v^4$$
$$-1128960v^2 - 6048000)(\sin(v))^2 + 313\sin(v)v^9$$
$$+(-626v^8 + 27600v^6 + 404640v^4 + 3790080v^2 - 12096000)\cos(v)$$
$$+26v^8 + 2640v^6 + 1107360v^4 - 3790080v^2 + 12096000)((v^8$$
$$+\frac{112}{3}v^6 + 640v^4 + 960v^2 + 960)(\sin(v))^2 + \frac{122}{3}\sin(v)v^7$$
$$+(1920 + 960v^2 + 400v^4 - \frac{488}{3}v^6)\cos(v) - 640v^4 - v^8$$
$$-1920 - 960v^2 - \frac{112}{3}v^6)^{-1}v^{-4},$$

$$\alpha_3 = \frac{1}{34020}((9516(v^4 + \frac{56}{3}v^2 + 200)(v^{10} + \frac{990}{13}v^8 + \frac{30240}{13}v^6$$
$$-\frac{10080}{13}v^4 - \frac{604800}{13}v^2 - \frac{3628800}{13})\cos(v) - 229116v^{14}$$
$$+4073336v^{12} + 130500960v^{10} + 2550873600v^8$$
$$-15081776640v^6 - 103594982400v^4 - 382504550400v^2$$
$$+1593768960000)(\sin(v))^2 - 57279(v^2 - \frac{6900}{313})((v^4 + \frac{56}{3}v^2$$
$$+200)\cos(v) - 200 + \frac{244}{3}v^2)v^9\sin(v) + (-9516v^{14}$$
$$+17732456v^{12} - 699587040v^{10} + 3214944000v^8$$
$$+14717767680v^6 + 166460313600v^4 - 1041262387200v^2$$
$$+2125025280000)\cos(v) + 229116v^{14} - 4073336v^{12}$$
$$-130500960v^{10} - 2550873600v^8 + 51689272320v^6$$
$$-166460313600v^4 + 1041262387200v^2$$
$$-2125025280000)v^{-4}(((v^8 + \frac{112}{3}v^6 + 640v^4$$
$$+960v^2 + 960)(v^4 + \frac{56}{3}v^2 + 200)\cos(v) + \frac{206080}{3}v^6$$
$$-149760v^4 - 341760v^2 + \frac{49256}{9}v^8 - 576000$$
$$+244v^{10})(\sin(v))^2 + \frac{122}{3}v^7((v^4 + \frac{56}{3}v^2 + 200)\cos(v)$$
$$-200 + \frac{244}{3}v^2)\sin(v) + (-768000 - 263680v^2 - 56v^{10}$$
$$-\frac{132904}{9}v^8 - 149760v^4 - v^{12} + \frac{134080}{3}v^6)\cos(v) + 768000$$
$$+263680v^2 + 149760v^4 - 244v^{10} - \frac{206080}{3}v^6 - \frac{49256}{9}v^8)^{-1}$$
$$+\frac{1}{378}((130v^8 + 13200v^6 + 550800v^4 + 5644800v^2$$
$$+30240000)(\sin(v))^2 - 1565\sin(v)v^9 + (3130v^8$$

$$-138000v^6 - 2023200v^4 - 18950400v^2 + 60480000)\cos(v)$$
$$-130v^8 - 13200v^6 - 5536800v^4 + 18950400v^2$$
$$-60480000)((v^8 + \tfrac{112}{3}v^6 + 640v^4 + 960v^2 + 960)(\sin(v))^2$$
$$+\tfrac{122}{3}\sin(v)v^7 + (1920 + 960v^2 + 400v^4 - \tfrac{488}{3}v^6)\cos(v)$$
$$-640v^4 - v^8 - 1920 - 960v^2 - \tfrac{112}{3}v^6)^{-1}v^{-4} + \tfrac{313}{7560},$$

$$\alpha_4 = \tfrac{1}{4860}(((156v^{14} + 14792v^{12} + 615840v^{10}$$
$$+9028800v^8 + 63060480v^6 - 203212800v^4 - 2264371200v^2$$
$$-8709120000)\cos(v) - 3756v^{14} + 66776v^{12} + 2139360v^{10}$$
$$+41817600v^8 - 247242240v^6 - 1698278400v^4 - 6270566400v^2$$
$$+26127360000)(\sin(v))^2 - 939(v^2 - \tfrac{6900}{313})((v^4 + \tfrac{56}{3}v^2$$
$$+200)\cos(v) - 200 + \tfrac{244}{3}v^2)v^9\sin(v) + (-156v^{14} + 290696v^{12}$$
$$-11468640v^{10} + 52704000v^8 + 241274880v^6 + 2728857600v^4$$
$$-17069875200v^2 + 34836480000)\cos(v) + 3756v^{14} - 66776v^{12}$$
$$-2139360v^{10} - 41817600v^8 + 847365120v^6 - 2728857600v^4$$
$$+17069875200v^2 - 34836480000)v^{-4}(((v^8 + \tfrac{112}{3}v^6 + 640v^4$$
$$+960v^2 + 960)(v^4 + \tfrac{56}{3}v^2 + 200)\cos(v) + \tfrac{206080}{3}v^6 - 149760v^4$$
$$-341760v^2 + \tfrac{49256}{9}v^8 - 576000 + 244v^{10})(\sin(v))^2$$
$$+\tfrac{122}{3}v^7((v^4 + \tfrac{56}{3}v^2 + 200)\cos(v) - 200 + \tfrac{244}{3}v^2)\sin(v)$$
$$+(-768000 - 263680v^2 - 56v^{10} - \tfrac{132904}{9}v^8 - 149760v^4$$
$$-v^{12} + \tfrac{134080}{3}v^6)\cos(v) + 768000 + 263680v^2 + 149760v^4$$
$$-244v^{10} - \tfrac{206080}{3}v^6 - \tfrac{49256}{9}v^8)^{-1} + \tfrac{1}{756}((26v^8 + 2640v^6$$
$$+110160v^4 + 1128960v^2 + 6048000)(\sin(v))^2 - 313\sin(v)v^9$$
$$+(626v^8 - 27600v^6 - 404640v^4 - 3790080v^2$$
$$+12096000)\cos(v) - 26v^8 - 2640v^6 - 1107360v^4$$
$$+3790080v^2 - 12096000)((v^8 + \tfrac{112}{3}v^6 + 640v^4 + 960v^2$$
$$+960)(\sin(v))^2 + \tfrac{122}{3}\sin(v)v^7 + (1920 + 960v^2$$
$$+400v^4 - \tfrac{488}{3}v^6)\cos(v) - 640v^4 - v^8 - 1920 - 960v^2$$
$$-\tfrac{112}{3}v^6)^{-1}v^{-4} - \tfrac{13}{15120},$$

$$\beta_1 = \tfrac{1}{181440}(((-156v^{14} - 14792v^{12} - 615840v^{10} - 9028800v^8$$
$$-63060480v^6 + 203212800v^4 + 2264371200v^2$$
$$+8709120000)\cos(v) + 3756v^{14} - 66776v^{12} - 2139360v^{10}$$
$$-41817600v^8 + 247242240v^6 + 1698278400v^4 + 6270566400v^2$$
$$-26127360000)(\sin(v))^2 + 939(v^2 - \tfrac{6900}{313})((v^4 + \tfrac{56}{3}v^2$$
$$+200)\cos(v) - 200 + \tfrac{244}{3}v^2)v^9\sin(v) + (156v^{14} - 290696v^{12}$$
$$+11468640v^{10} - 52704000v^8 - 241274880v^6 - 2728857600v^4$$
$$+17069875200v^2 - 34836480000)\cos(v) - 3756v^{14} + 66776v^{12}$$

$$+2139360v^{10} + 41817600v^8 - 847365120v^6 + 2728857600v^4$$
$$-17069875200v^2 + 34836480000)v^{-4}(((v^8 + \frac{112}{3}v^6 + 640v^4$$
$$+960v^2 + 960)(v^4 + \frac{56}{3}v^2 + 200)\cos(v) + \frac{206080}{3}v^6$$
$$-149760v^4 - 341760v^2 + \frac{49256}{9}v^8 - 576000$$
$$+244v^{10})(\sin(v))^2 + \frac{122}{3}v^7((v^4 + \frac{56}{3}v^2 + 200)\cos(v)$$
$$-200 + \frac{244}{3}v^2)\sin(v) + (-768000 - 263680v^2 - 56v^{10}$$
$$-\frac{132904}{9}v^8 - 149760v^4 - v^{12} + \frac{134080}{3}v^6)\cos(v)$$
$$+768000 + 263680v^2 + 149760v^4 - 244v^{10} - \frac{206080}{3}v^6 - \frac{49256}{9}v^8)^{-1},$$

$$\beta_2 = \frac{1}{60480}((-26v^8 - 2640v^6 - 110160v^4 - 1128960v^2$$
$$-6048000)(\sin(v))^2 + 313\sin(v)v^9 + (-626v^8$$
$$+27600v^6 + 404640v^4 + 3790080v^2 - 12096000)\cos(v)$$
$$+26v^8 + 2640v^6 + 1107360v^4 - 3790080v^2$$
$$+12096000)((v^8 + \frac{112}{3}v^6 + 640v^4 + 960v^2$$
$$+960)(\sin(v))^2 + \frac{122}{3}\sin(v)v^7 + (1920 + 960v^2$$
$$+400v^4 - \frac{488}{3}v^6)\cos(v) - 640v^4 - v^8 - 1920 - 960v^2 - \frac{112}{3}v^6)^{-1}v^{-4}.$$