Malaysian Journal of Mathematical Sciences 10(S) February: 243–251 (2016)
Special Issue: The 3rd International Conference on Mathematical Applications in Engineering 2014 (ICMAE'14)

MALAYSIAN JOURNAL OF MATHEMATICAL SCIENCES

Journal homepage: http://einspem.upm.edu.my/journal

Diagonally Implicit Hybrid Method for solving Special Second Order Ordinary Differential Equations

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ABSTRACT

This paper describes the derivation of a fifth-order diagonally implicit hybrid method. The method is zero dissipative and has phase-lag of order six. The method is compared with the existing hybrid method and the numerical comparisons carried out show that the new method improves the accuracy of the existing method for solving several special second order ordinary differential equations.

Keywords: Diagonally implicit hybrid method, zero dissipative, phase-lag, second order initial value problems.

1. Introduction

Much interests have been given on the development of numerical methods for solving special second order ordinary differential equations of the form

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

where the first derivative does not appear explicitly. The second order initial value problems often arise in science and engineering field such as celestial mechanics, molecular dynamics, semi-discretizations of wave equations and so on. To solve the initial value problems, many authors proposed Runge Kutta Nyström methods, block methods and multistep methods see for example (Fatunla, 1990, J. Dormand and Prince, 1987, Lambert and Watson, 1976). Authors such as (Cash, 1981, Hairer, 1979, M.M. Chawla and Neta, 1986, S.O. Fatunla and Otunta, 1999) and (Tsitouras, 2006) proposed hybrid methods which originate from the ideas between the Runge Kutta and multistep methods. In the derivation of a hybrid method, it is important to increase the algebraic order to achieve higher accuracy. In addition, if the solution of (1) is oscillatory in nature, then we have to consider the phase-lag and the dissipation errors. The study of phase-lag was introduced by (Brusa and Nigro, 1980) and has been given much attention by many authors in their derivations of numerical methods see for example (Chawla and Rao, 1987, Simos, 1992) and (S.Z. Ahmad and N. Senu, 2013).

In this paper, we are interested in the class of hybrid methods:

$$Y_i = (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), i = 1, \ldots, s, \tag{2a}$$

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \tag{2b}$$

for the numerical solution of Eq. (1).This class of methods has been investigated by (Coleman, 2003). Let $\mathbf{A}$ be $[a_{ij}]_{s\times s}$, $\mathbf{b}$ be $[b_i]_{s\times 1}$ and $\mathbf{c}$ be $[c_i]_{s\times 1}$. The hybrid methods can be represented by

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b^T} \end{array} \tag{3}$$

Choosing $c_1 = 0$, $c_2 = 1$, $a_{ij} = 0$ for $j > i$, $a_{ii} = \gamma$ and $s = 4$, we have the following form of hybrid methods:

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1 & a_{21} & \gamma & 0 & 0 \\ c_3 & a_{31} & a_{32} & \gamma & 0 \\ c_4 & a_{41} & a_{42} & a_{43} & \gamma \\ \hline & b_1 & b_2 & b_3 & b_4 \end{array} \tag{4}$$

These methods are diagonally implicit and have four function evaluations or stages at each step of integration. The leading term associated with the local truncation error of a pth-order hybrid method is given by

$$e_{p+1}(t_i) = \frac{\alpha(t_i)}{(p+2)}\left[1 + (-1)^{p+2} - \mathbf{b^T}\psi\prime\prime(t_i)\right], t_i \in T_2, \rho(t_i) = p+2 \qquad (5)$$

where T_2, $\alpha(t_i)$ and $\psi''(t_i)$ are as defined in (Coleman, 2003). The quantity $E = \sqrt{\sum_{i=1}^{n_{p+2}} {e_{p+1}}^2(t_i)}$ where n_{p+2} is the number of trees of order $p+2$, is called the error constant for the pth-order method.

In the following sections, we describe briefly the phase-lag and stability analysis of the class of methods given by Eq. (2). Then, the new method will be derived and applied to several special second order ordinary differential equations of the form Eq. (1) to provide numerical comparisons with the existing explicit hybrid method.

2. Phase-lag and Stability Analysis

Let us consider the standard test problem

$$y'' = -\lambda^2 y, \lambda > 0 \qquad (6)$$

Applying the hybrid methods as defined in Eq. (2) to the test problem gives us the following formula which is written in vector form:

$$\mathbf{Y} = (\mathbf{e} + \mathbf{c})\, y_n - \mathbf{c}y_{n-1} - H^2\mathbf{AY} y_{n+1} = 2y_n - y_{n-1} - H^2\mathbf{b}^T\mathbf{Y} \qquad (7)$$

where $\mathbf{e} = (1, 1, \cdots, 1)^T$ and $\mathbf{Y} = (Y_1, Y_2, \cdots, Y_s)^T$. This implies

$$y_{n+1} - S(H^2)y_n + P(H^2)y_{n-1} = 0 \qquad (8)$$

where $S(H^2) = 2 - H^2\mathbf{b^T}(\mathbf{I} + H^2\mathbf{A})^{-1}(\mathbf{e}+\mathbf{c})$ and $P(H^2) = 1 - H^2\mathbf{b^T}(\mathbf{I} + H^2\mathbf{A})^{-1}\mathbf{c}$. The characteristic equation that determines the numerical solution of Eq. (6) is

$$\zeta^2 - S(H^2)\zeta + P(H^2) = 0 \qquad (9)$$

According to (van der Houwen and Sommeijer, 1987), in the phase analysis, one compares the phase (or argument) of $\exp iH$ with the principal root of the characteristic equation. Thus, the phase-lag (or dispersion error) is given by

$$\phi(H) = H - \arccos\left(\frac{S(H^2)}{2\sqrt{P(H^2)}}\right) \qquad (10)$$

whereas the dissipation (or amplification) error is given by

$$d(H) = 1 - \sqrt{P(H^2)} \tag{11}$$

A hybrid method corresponding to the Eq. (9) is said to have the phase-lag of order n if $\phi(H) = c_\phi H^{n+1} + O(H^{n+3})$. If $d(H) = 0$ then the method is zero dissipative. If $d(H) = c_d H^{m+1} + O(H^{m+3})$, then the method is dissipative of order m. Here, c_ϕ and c_d are the phase-lag and the dissipation constants.

For the stability analysis, the hybrid methods corresponding to the Eq. (9) is said to have the interval of stability $(0, H_a)$ if $\left|P(H^2)\right| < 1$ and $\left|S(H^2)\right| < 1 + P(H^2)$ for all $H \in (0, H_a)$. If $P(H^2) = 1$ and $\left|S(H^2)\right| < 2$ for all $H \in (0, H_p)$, then the interval $(0, H_p)$ is called the interval of periodicity of the hybrid methods.

3. Derivation of the new method

The new method is diagonally implicit and has an algebraic order five. This method must satisfy 13 equations of order conditions for fifth order hybrid methods as listed in (Coleman, 2003):

$\sum_{i=1}^{s} b_i = 1$
$\sum_{i=1}^{s} b_i c_i = 0$
$\sum_{i=1}^{s} b_i {c_i}^2 = 1/6$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} = 1/12$
$\sum_{i=1}^{s} b_i {c_i}^3 = 0$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i c_i a_{ij} = 1/12$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} c_j = 0$
$\sum_{i=1}^{s} b_i {c_i}^4 = 1/15$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i {c_i}^2 a_{ij} = 1/30$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i c_i a_{ij} c_j = -1/60$
$\sum_{i=1}^{s} \sum_{j=1}^{s} \sum_{k=1}^{s} b_i a_{ij} a_{ik} = 7/120$
$\sum_{i=1}^{s} \sum_{j=1}^{s} b_i a_{ij} {c_j}^2 = 1/180$
$\sum_{i=1}^{s} \sum_{j=1}^{s} \sum_{k=1}^{s} b_i a_{ij} a_{jk} = 1/360$

Using Maple software, the following equations are obtained:

$$c_3 = -\frac{5c_4 + 2}{5(c_4 + 1)}, b_1 = \frac{25{c_4}^2 + 7c_4 - 3}{6c_4(5c_4 + 2)},$$
$$b_2 = \frac{5{c_4}^2 - 2}{6(c_4 - 1)(10c_4 + 7)}, b_3 = \frac{125(c_4 + 1)^4}{6(10c_4 + 7)(5c_4 + 2)(5{c_4}^2 + 10c_4 + 2)},$$
$$b_4 = -\frac{1}{2c_4(c_4 - 1)(5{c_4}^2 + 10c_4 + 2)},$$
$$a_{21} = -\gamma + 1,$$
$$a_{31} = -\frac{1}{250}\left[\frac{(250\gamma {c_4}^3 + 1250\gamma {c_4}^2 + 1300\gamma c_4 + 125{c_4}^2 + 390\gamma + 160c_4 + 44}{(c_4 + 1)^3}\right],$$
$$a_{32} = \frac{1}{250}\left[\frac{(10\gamma + 1)(10c_4 + 7)(5c_4 + 2)}{(c_4 + 1)^3}\right],$$
$$a_{41} = -\frac{1}{18(5c_4 + 2)}[150\gamma {c_4}^5 + 450\gamma {c_4}^4 - 5{c_4}^5 - 30\gamma {c_4}^3 + 5{c_4}^4$$
$$- 450\gamma {c_4}^2 - 36{c_4}^3 - 30\gamma c_4 - 68{c_4}^2 + 36\gamma - 22c_4],$$
$$a_{42} =$$
$$\frac{1}{18}\left[\frac{(c_4 + 1)c_4(150\gamma {c_4}^3 + 450\gamma {c_4}^2 - 5{c_4}^3 - 330\gamma c_4 + 25{c_4}^2 - 270\gamma - c_4 - 19)}{(10c_4 + 7)}\right],$$
$$a_{43} = \frac{5}{18}\left[\frac{(c_4 + 1)^2 c_4(150\gamma {c_4}^3 + 150\gamma {c_4}^2 - 5{c_4}^3 - 240\gamma c_4 - 5{c_4}^2 - 60\gamma + 8c_4 + 2)}{(10c_4 + 7)(5c_4 + 2)}\right].$$

It is noted that c_4 and γ are free parameters. To find c_4 and γ, the strategies that we use are
1) to nullify the dissipation errors, and 2) to minimize the error constant.
2) to nullify the dissipation error, we solve the following equation

$$\frac{-300\gamma^2 + 20\gamma - 1}{3600(c_4 + 1)} = 0$$

giving $\gamma = \frac{1}{30}$ and c_4 as the free parameter. Now we select c_4 so that the error constant E, is as small as possible. Using optimization package in Maple, we finally choose $c_4 = -63/100$. Thus, for this method, $E = 2.55 \times 10^{-2}$ while other coefficients are given by
$c_3 = \frac{23}{37}$, $a_{21} = \frac{29}{30}$, $a_{31} = \frac{281349}{506530}$, $a_{32} = -\frac{12880}{151959}$, $a_{41} = -\frac{87869}{375000}$, $a_{42} = \frac{42217}{500000}$, $a_{43} = 0$, $b_1 = \frac{1675}{2898}$, $b_2 = \frac{31}{13692}$, $b_3 = \frac{1874161}{8947092}$, $b_4 = \frac{10000000}{47555739}$.

The interval of periodicity is $(0, 4.47)$. The new method is zero dissipative and has phase-lag of order 6. The phase-lag quantity is given by $\phi(H) = (13/604800)H^7 + O(H^9)$.

4. Numerical examples and discussions

The new method has been coded in Microsoft Visual C++ and applied to several second-order problems with oscillating solutions to provide numerical comparisons with the results of the existing explicit hybrid method. In the implementation of the new method, $\mathbf{Y_j}$ is iterated until $\|\mathbf{Y_j} - \mathbf{Y_{j-1}}\| < \epsilon$ where ϵ is the chosen tolerance. Below are the abbreviations of the codes:

- DIHM: Fifth-order diagonally implicit hybrid method derived in this paper.
- ETSHM5: Fifth-order explicit hybrid method proposed by (Franco, 2006). This method has an interval of absolute stability $(0, 2.68)$ and is given by the following formula

$$
\begin{aligned}
&Y_1 = y_{n-1}, Y_2 = y_n \\
&Y_3 = (1 + c_3)y_n - c_3 y_{n-1} + h^2(a_{31} f_{n-1} + a_{32} f_n) \\
&Y_4 = (1 + c_4)y_n - c_4 y_{n-1} + h^2 \left[a_{41} f_{n-1} + a_{42} f_n + a_{43} f(x_n + c_3 h, Y_3)\right] \\
&y_{n+1} = 2y_n - y_{n-1} + h^2 \left[b_1 f_{n-1} + b_2 f_n + b_3 f(x_n + c_3 h, Y_3) + b_4 f(x_n + c_4 h, Y_4)\right]
\end{aligned}
$$

with
$c_3 = \frac{63}{100}$, $c_4 = -\frac{23}{37}$, $a_{31} = \frac{126651}{2000000}$,
$a_{32} = \frac{900249}{2000000}$,
$a_{41} = -\frac{43347640}{916464729}$,
$a_{42} = -\frac{4864523}{50602347}$, $a_{43} = \frac{213026000}{8248182561}$, $b_1 = \frac{31}{13692}$,
$b_2 = \frac{1675}{2898}$,
$b_3 = \frac{10000000}{47555739}$, $b_4 = \frac{1874161}{8947092}$.

The numerical comparisons are based on maximum global errors produced by each code when solving each problem. Formula for the maximum global error and the notation used are given by

Maximum global error=max($\|y(x_n) - y_n\|$)
Notation : For example 1.06226E−04 means 1.06226×10^{-4}

where $y(x_n)$ is the exact solution and y_n is the numerical solution. Table 1 to 3 display the maximum global errors for the following test problems:

Problem 1 (non-homogeneous linear problem)
$y'' = -100y + 99\sin x, y(0) = 1, y'(0) = 11, 0 \leqslant x \leqslant 100.$
Exact solution: $y(x) = \cos 10x + \sin 10x + \sin x.$

Problem 2 (almost periodic problem)
$z''(x) + z(x) = (1/1000)\exp ix, z(0) = 1, z' = 0.9995i, z \in \mathbf{C}, 0 \leqslant x \leqslant 100.$
Exact solution: $z(x) = (1 - 0.0005ix)\exp ix$. In this paper, we assume that $z(x) = y_1(x) + iy_2(x), y_1, y_2 \in \mathbf{R}$, then solve the following equivalent problem
$y_1'' = -y_1 + (1/1000)\cos x, y_1(0) = 1, y_1'(0) = 0$
$y_2'' = -y_2 + (1/1000)\sin x, y_2(0) = 0, y_2'(0) = 0.9995$
with the exact solution: $y_1(x) = \cos x + 0.0005x\sin x, y_2(x) = \sin x - 0.0005x\cos x.$

Problem 3 (nonlinear oscillatory problem)
$y_1'' = -4x^2 y_1 - \frac{2y_2}{\sqrt{{y_1}^2 + {y_2}^2}}, y_1(0) = 1, y_1'(0) = 0$
$y_2'' = -4x^2 y_2 + \frac{2y_1}{\sqrt{{y_1}^2 + {y_2}^2}}, y_2(0) = 0, y_2'(0) = 0, 0 \leqslant x \leqslant 10$
Exact solution: $y_1(x) = \cos x^2, y_2(x) = \sin x^2.$

Table 1: Maximum Global Errors for Problem 1

Step-size	DIHM	ETSHM5
0.1	1.06226E-04	2.80419E-01
0.05	1.99504E-06	7.70632E-03
0.025	5.19021E-08	2.36599E-04
0.0125	1.55025E-09	7.39372E-06
0.00625	4.81606E-11	2.30867E-07

From the numerical examples, DIHM gives smaller error compared to ETSHM5 code. This shows that the numerical solution by DIHM approximates the exact solutions better than the numerical solution by ETSHM5 code.

Table 2: Maximum Global Errors for Problem 2

Step-size	DIHM	ETSHM5
0.5	1.59350E-06	5.45857E-04
0.25	4.06247E-08	1.68505E-05
0.125	1.19357E-09	5.24871E-07
0.0625	3.66882E-11	1.63853E-08
0.03125	1.16941E-12	5.11886E-10

Table 3: Maximum Global Errors for Problem 3

Step-size	DIHM	ETSHM5
0.1	6.05791E-03	2.70440E-01
0.05	4.02130E-05	5.55132E-03
0.025	7.10976E-07	1.55348E-04
0.0125	1.77682E-08	4.64342E-06
0.00625	5.17788E-10	1.42237E-07

5. Conclusions

In this paper, we derive the new fifth-order diagonally implicit hybrid method with four stages. The performance of this method is evaluated based on its accuracy compared to the existing fifth-order explicit hybrid method derived by (Franco, 2006). Several special second order initial value problems with oscillating solutions are used for the numerical comparisons. We conclude that the new method improves the accuracy of the existing explicit hybrid method with the same algebraic order.

Acknowledgments

We acknowledge the financial support for this research given by Ministry of Higher Education Malaysia through grant Research Acculturation and Collaboration Effort (RACE).

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