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One-Step Block Hybrid Integrator for the Numerical Solution of Semi-Explicit Index-1 DAEs Systems

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Abstract

In this study, the derivation, stability analysis and the application of a one-step Hybrid method for solving systems of semi-explicit Index-1 Differential-Algebraic Equations (DAEs) were discussed. A semi-explicit differential-algebraic equation consists of a system of ordinary differential equations and algebraic equations. Interpolation and collocation technique was employed for the derivation of the Continuous form of the proposed method (CHM). The discrete schemes were computed by evaluating CHM at specific grid and off-grid points and were implemented as a block Integrator (BHI). The numerical results of BHI obtained showed its efficiency when compared with the exact solutions and some existing methods.

Keywords: Block, Hybrid Integrator, Differential-Algebraic Equations, Stability, Collocation.
MSC2010:65L05, 65L06

1 Introduction

Most processing mathematical models consist of differential and algebraic equations which results in Differential-Algebraic Equations systems (DAEs). DAEs can be deduced from chemical process simulations, mechanical systems, electrical networks, incompressible fluids dynamics and so on.
Semi-explicit Index-1 Differential-Algebraic Equation is written in the form

$$\begin{aligned} y' &= f(y,z), \quad y(t_0) = y_0 \\ 0 &= g(y,z), \quad z(t_0) = z_0 \end{aligned} \tag{1}$$

Where $\frac{\partial g}{\partial z} = g_z$ is non-singular in a neighbourhood of solution and the unknown y and z are the differential and algebraic variables respectively. DAEs are characterized by a differential index which is the minimum number of times that all or part of the DAE must be differentiated with respect to time in order to convert the DAE (1) to a system of ODEs. Hence the algebraic part of the Index-1 DAEs will be differentiated once to convert it to an ordinary differential equation.
In Literature, several numerical methods have been proposed for the solution of semi-explicit Index-1 Differential-Algebraic Equations such as the idea of using numerical methods for ODEs to solve DAEs introduced by Gear [1], Chebyshev spectral procedure method by Khateb and Hussien [2],

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Backward Differentiation Formula [3,4], Implicit Runge-Kutta methods by Ascher and Petzold [5], L-stable extended Block Backward Differentiation Formula by Akinfenwa and Okunuga [6], 2-points and 3-points BBDF by Abasi et al. [7], Block method of Runge-Kutta type by Khoo Kai Wen et al [8] to mention a few.
In this paper, a one-step Block Hybrid Integrator of order five (BHI5) was developed via Interpolation and collocation techniques [9]. The method incorporate off-grid points to produce the discrete hybrid schemes which were implemented as a block method to simultaneously produce approximation at nodal points for the numerical solution of Index-1 DAE of the form (1). Block method was first introduced by Milne [10], then used by other scholars (see [1,11–13]). This method preserves the Runge-Kutta traditional advantage of being self-starting and efficient.

2 Derivation of BHI5

This section describes the derivation of the one-step Hybrid Integrator of the form

$$y_{n+1} = y_n + h\sum_{j=0}^{1}\beta_j f_{n+j} + h\sum_{j=1}^{2}\beta_{v_j} f_{n+v_j} + h^2\phi_1 g_{n+1} \tag{2}$$

where h, n, $v_1 = \frac{1}{6}$ and $v_2 = \frac{1}{2}$ are the step size, grid index and off-step points respectively while $\beta_j, j = 0, 1$, $\beta_{v_j}, j = 1, 2$ and ϕ_1 are parameters to be determined uniquely. An approximate solution to (1) by the interpolating function

$$y(t) = \sum_{j=0}^{r+s-1} b_j t^j \tag{3}$$

where b_j in (3) are the unknown coefficients to be determined while r and s are the number of interpoation and collocation points respectively. The imposing conditions for the construction of the proposed Method are:

$$y(t_{n+r}) = y_{n+r}, \quad r = 0 \tag{4}$$

$$y'(t_{n+r}) = f_{n+r}, \quad r = 0, \frac{1}{6}, \frac{1}{2}, 1 \tag{5}$$

$$y''(t_{n+r}) = g_{n+r}, \quad r = 1 \tag{6}$$

Equations (4)-(6) generate six equations which were solved simultaneously to obtain b_j and the values of b_j were substituted into equation (3) to form the Continuous Hybrid Method (CHM) which is second derivative in nature and expressed in the form

$$y(x) = y_n + h\sum_{j=0}^{1}\beta_j(x) f_{n+j} + h\sum_{j=1}^{2}\beta_{v_j}(x) f_{n+v_j} + h^2\phi_1(x) g_{n+1} \tag{7}$$

where $x = \frac{t-t_n}{h}$ and $\beta_j, j = 0, \frac{1}{6}, \frac{1}{2}, 1$ and $\phi_1(x)$ are written in matrix form as follows:

$$\begin{bmatrix} \beta_0(x) \\ \beta_{\frac{1}{6}}(x) \\ \beta_{\frac{1}{2}}(x) \\ \beta_1(x) \end{bmatrix} = \begin{bmatrix} 0 & 1 & -5 & \frac{29}{3} & -8 & \frac{12}{5} \\ 0 & 0 & \frac{162}{25} & -\frac{432}{25} & \frac{81}{5} & -\frac{648}{125} \\ 0 & 0 & -2 & \frac{32}{3} & -13 & \frac{24}{5} \\ 0 & 0 & \frac{13}{25} & -\frac{229}{75} & \frac{24}{5} & -\frac{252}{125} \end{bmatrix} \begin{bmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \\ x^4 \\ x^5 \end{bmatrix}$$

$$\left[\ \phi_1(x)\ \right] = \left[\begin{array}{cccccc} 0 & 0 & -\frac{1}{10} & \frac{3}{5} & -1 & \frac{12}{25} \end{array}\right] \left[\begin{array}{c} x^0 \\ x^1 \\ x^2 \\ x^3 \\ x^4 \\ x^5 \end{array}\right]$$

The main scheme was generated from interpolating CHM (7) at $t = t_{n+1}$ as

$$y_{n+1} = y_n + \frac{1}{15}hf_n + \frac{27}{125}hf_{n+\frac{1}{6}} + \frac{7}{15}hf_{n+\frac{1}{2}} + \frac{94}{375}hf_{n+1} - \frac{1}{50}h^2 g_{n+1} \tag{8a}$$

The additional methods were generated from interpolating CHM (7) at $t = t_{n+\frac{1}{2}}$ and $t = t_{n+\frac{1}{6}}$ as

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{30}hf_n + \frac{621}{2000}hf_{n+\frac{1}{6}} + \frac{41}{240}hf_{n+\frac{1}{2}} - \frac{11}{750}hf_{n+1} + \frac{1}{400}h^2 g_{n+1} \tag{8b}$$

and

$$y_{n+\frac{1}{6}} = y_n + \frac{1}{15}hf_n + \frac{671}{6000}hf_{n+\frac{1}{6}} - \frac{101}{6480}hf_{n+\frac{1}{2}} + \frac{38}{10125}hf_{n+1} - \frac{23}{32400}h^2 g_{n+1} \tag{8c}$$

The discrete hybrid methods (8a, 8b, 8c) together forms the One-step Block Hybrid Integrator of order five (BHI5). Equations (8a), (8b) and (8c) are denoted as equation (8) written together as:

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{15}hf_n + \frac{27}{125}hf_{n+\frac{1}{6}} + \frac{7}{15}hf_{n+\frac{1}{2}} + \frac{94}{375}hf_{n+1} - \frac{1}{50}h^2 g_{n+1} \\ y_{n+\frac{1}{2}} &= y_n + \frac{1}{30}hf_n + \frac{621}{2000}hf_{n+\frac{1}{6}} + \frac{41}{240}hf_{n+\frac{1}{2}} - \frac{11}{750}hf_{n+1} + \frac{1}{400}h^2 g_{n+1} \\ y_{n+\frac{1}{6}} &= y_n + \frac{1}{15}hf_n + \frac{671}{6000}hf_{n+\frac{1}{6}} - \frac{101}{6480}hf_{n+\frac{1}{2}} + \frac{38}{10125}hf_{n+1} - \frac{23}{32400}h^2 g_{n+1} \end{aligned} \tag{8}$$

The method (8) can be presented in a matrix block form as

$$A_{(1)}Y_{\varpi} = A_{(0)}Y_{\varpi-1} + hB_{(1)}F_{\varpi} + hB_{(0)}F_{\varpi-1} + h^2C_{(1)}G_{\varpi} \tag{9}$$

where

$$Y_{\varpi} = \left[\begin{array}{c} y_{n+\frac{1}{6}} \\ y_{n+\frac{1}{2}} \\ y_{n+1} \end{array}\right]; Y_{\varpi-1} = \left[\begin{array}{c} y_{n-\frac{1}{2}} \\ y_{n-\frac{1}{6}} \\ y_n \end{array}\right]; F_{\varpi} = \left[\begin{array}{c} f_{n+\frac{1}{6}} \\ f_{n+\frac{1}{2}} \\ f_{n+1} \end{array}\right]; F_{\varpi-1} = \left[\begin{array}{c} f_{n-\frac{1}{2}} \\ f_{n-\frac{1}{6}} \\ f_n \end{array}\right]; G_{\varpi} = \left[\begin{array}{c} g_{n+\frac{1}{6}} \\ g_{n+\frac{1}{2}} \\ g_{n+1} \end{array}\right]$$

The 3 by 3 matrices $A_{(0)}, A_{(1)}, B_{(0)}, B_{(1)}, C_{(1)}$ of the BHI5 (8) are defined as follows

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$$A_{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$A_{(0)} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$B_{(1)} = \begin{bmatrix} \frac{671}{6000} & -\frac{101}{6480} & \frac{38}{10125} \\ \frac{621}{2000} & \frac{41}{240} & -\frac{11}{750} \\ \frac{27}{125} & \frac{7}{15} & \frac{94}{375} \end{bmatrix}$$

$$B_{(0)} = \begin{bmatrix} 0 & 0 & \frac{1}{15} \\ 0 & 0 & \frac{1}{30} \\ 0 & 0 & \frac{1}{15} \end{bmatrix}$$

$$C_{(1)} = \begin{bmatrix} 0 & 0 & -\frac{23}{32400} \\ 0 & 0 & \frac{1}{400} \\ 0 & 0 & -\frac{1}{50} \end{bmatrix}$$

3 Analysis of BHI5

3.1 Order and Error Constant of the Method

Following Fatunla [14] and Lambert [15], a method was proposed for finding the order m and error constant C_{m+1} of the block hybrid method (8) by first expanding y function, f functions and g functions of the method (8) using Taylors series expansion about t and then comparing the coefficients of h . Using the above procedure, one-step Block Hybrid Integrator have order and error constants as $m = (5, 5, 5)^T$ and $C_{m+1} = (\frac{763}{335923200}, -\frac{7}{1382400}, \frac{1}{86400})^T$ respectively where T is transpose.

3.2 Zero Stability

A numerical method is said to be zero-stable if the roots R_j, $j = 1, 2, \ldots, N$ of the first characteristic polynomial $\rho(R)$ satisfies $|R_j| \leq 1, j = 1, \ldots, N$ and those roots with $|R_j| = 1$ is simple (see Lambert [15]). Applying the above conditions to the derived block method, the first characteristic polynomial $\rho(R) = 0$ is calculated as

$$\rho(R) = \det(RA_{(1)} - A_{(0)}) = R^2(R - 1)$$

The BHI5 is found to be zero-stable since $\rho(R) = 0$ satisfies $|R_j| \leq 1, j = 1, 2, 3$.

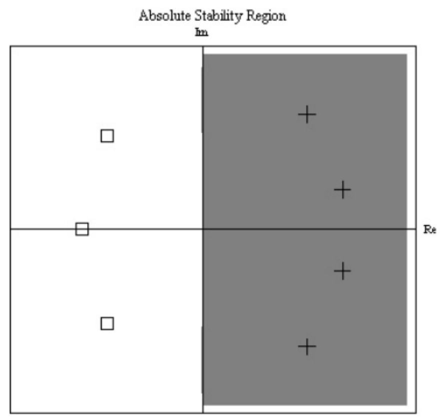

Figure 1: Stability Region of Block Hybrid Integrator of order 5

3.3 Consistency and Convergence

A numerical method converges if it is consistent and zero-stable (see Henrici [16]). Since BHI5 (8) is of order $m = 5 > 1$, then it is consistent and we have established earlier that the method satisfies the conditions of zero-stability. Therefore, the block hybrid Integrator (8) converges.

3.4 Stability of BHI5

Applying the BHI5 to the test equation

$$y' = \lambda y, \quad \lambda < 0$$

to obtain

$Y_{\varpi} = Q(z)Y_{\varpi-1}, \quad z = \lambda h$

where $Q(z)$ is the amplification matrix given by

$$Q(z) = \frac{A_{(0)} + zB_{(0)}}{A_{(1)} + zB_{(1)} + z^2C_{(1)}}$$

$Q(z)$ has eigenvalues $(\zeta_1, \zeta_2, \zeta_3) = (0, 0, \zeta_3)$. The dominant eigenvalue ζ_3 is the stability function with real coefficient as

$$\zeta_3 = \frac{1 + 0.466667z + 0.0875z^2 + 0.0069z^3}{1 - 0.533333z + 0.120833z^2 - 0.01388889z^3 + 0.00069444z^4}$$

The stability function is used to plot the Region of Absolute Stability (RAS) of the BHI5 (see Figure 1) which reveals that the method is L-stable in nature since the RAS covers the entire left plane of the graph (A-stable) and the limit of the stability function ζ_3 is zero as $z \to \infty$.

4 Numerical Results

The following test problems were considered in order to examine the accuracy and computational efficiency of BHI5. The numerical results with constant step size were compared with existing methods. All computations were carried out using MATHEMATICA 9.0.

Test Problem 4.1:

$$y'(t) = z, \quad y(0) = 1$$

$$z^3 - y^2 = 0, \quad z(0) = 1$$
$$0 \leq t \leq 10$$

Exact solution as

$$y(t) = \left(1 + \frac{t}{3}\right)^3, \quad z(t) = \left(1 + \frac{t}{3}\right)^2$$

Test Problem 4.2:

$$y'(t) = t\ cos\ t - y + (1 + t)z, \quad y(0) = 1$$
$$sin\ t - z = 0, \quad z(0) = 0$$

Exact solution is

$$y(t) = e^{-t} + t\ sin\ t, \quad z(t) = sin\ t$$

The results for the two test problems are tabulated for $h = 0.1$ and $h = 0.01$ and compared with some existing methods in [7] and [8].

Notations used in the result tables are as follows:

h	step size
$1BDF$	1-Point sequential BDF in Abasi et al. [7]
$2BDF$	2-Point blockl BDF in Abasi et al. [7]
$3BDF$	3-Point blockl BDF in Abasi et al. [7]
$2Bdae$	2-Point block one-step method in Khoo Kai Wen et al. [8]
$BHI5$	Block Hybrid Integrator of order 5
$MAXE$	Maximum Error of the computed solution

Maximum Error is

$$MAXE = Max_{1 \leq i \leq N}(error^{(i)})$$

where

$$error^{(i)} = |y^{(i)}_{exact} - y^{(i)}_{appro}|, |z^{(i)}_{exact} - z^{(i)}_{appro}|$$

Table 1: Numerical Results for Test Problem 4.1

t	i	Exact $y(t)$ $z(t)$	BHI5 y_i z_i	Error $h = 0.1$ $y(t) - y_i$ $z(t) - z_i$	i	Error$h = 0.01$ $y(t) - y_i$ $z(t) - z_i$
2	20	4.62962962	4.62962962	3.55271×10^{-15}	200	3.55271×10^{-15}
		2.77777777	2.77777777	3.10862×10^{-15}		3.55271×10^{-15}
4	40	12.7037037	12.7037037	1.42109×10^{-14}	400	2.18492×10^{-13}
		5.44444444	5.44444444	5.32907×10^{-15}		6.03961×10^{-14}
6	60	26.9999999	26.9999999	3.55271×10^{-14}	600	7.06999×10^{-13}
		8.99999999	8.99999999	5.32907×10^{-15}		1.33227×10^{-13}
8	80	49.2962962	49.2962962	1.35003×10^{-13}	800	1.63425×10^{-12}
		13.4444444	13.4444444	2.48690×10^{-14}		2.70006×10^{-13}
10	100	81.3703703	81.3703703	3.55271×10^{-13}	1000	3.01270×10^{-12}
		18.7777777	18.7777777	5.32907×10^{-14}		5.00933×10^{-13}

Table 2: Comparison of Results for Test Problem 4.1

h	Methods	MAXE
0.01	$1BDF$	$2.7469E-1$
	$2BDF$	$1.9608E-3$
	$3BDF$	$2.0417E-3$
	$2Bdae$	$3.2685E-12$
	$BHI5$	$3.0127E-12$
0.001	$1BDF$	$2.7528E-2$
	$2BDF$	$1.9799E-5$
	$3BDF$	$2.0631E-5$
	$2Bdae$	$1.0301E-11$
	$BHI5$	$1.2079E-12$

Table 3: Comparison of Results for Test Problem 4.1

h	$3BDF$[7]	h	$BHI5$
0.01	2.04173×10^{-3}	0.5	2.84217×10^{-14}
0.001	2.06314×10^{-5}	0.1	3.55271×10^{-13}
0.0001	2.06367×10^{-7}	0.05	3.12639×10^{-13}
0.00001	1.01275×10^{-9}	0.01	3.01270×10^{-12}
0.000001	1.04160×10^{-8}	0.005	3.33955×10^{-12}

Table 4: Numerical Results for Test Problem 4.2

t	i	Error $h = 0.1$	i	Error$h = 0.01$
		$y(t) - y_i$		$y(t) - y_i$
		$z(t) - z_i$		$z(t) - z_i$
2	20	1.69271×10^{-10}	200	5.77316×10^{-15}
		1.64869×10^{-10}		1.22125×10^{-15}
4	40	1.27069×10^{-9}	400	1.15019×10^{-13}
		1.90682×10^{-10}		3.43059×10^{-14}
6	60	2.22245×10^{-10}	600	1.00808×10^{-13}
		4.33142×10^{-12}		2.55351×10^{-14}
8	80	7.64584×10^{-10}	800	1.95399×10^{-14}
		1.33624×10^{-10}		2.22045×10^{-15}
10	100	2.62416×10^{-9}	1000	2.93099×10^{-13}
		2.12364×10^{-10}		3.00870×10^{-14}

Table 5: Comparison of Results for Test Problem 4.2

h	Methods	MAXE
0.01	$1BDF$	$2.51240E-1$
	$2BDF$	$7.38080E-4$
	$3BDF$	$6.60560E-4$
	$2Bdae$	$1.85820E-9$
	$BHI5$	$2.93099E-13$
0.001	$1BDF$	$2.509508E-2$
	$2BDF$	$6.43480E-6$
	$3BDF$	$6.60000E-6$
	$2Bdae$	$3.92310E-12$
	$BHI5$	$1.61782E-12$

The numerical results of the test problems shown in tables (1-5) reveal that the new method BHI5 is superior to the methods of Abasi et al. [7] and it compares favourably with the block method of Khoo Kai Wen et al. [8].

5 Conclusion

A one-step L-stable Block Hybrid Integrator of order five (BHI5) had been developed for the numerical solution of semi-explicit Index-1 Differential Algebraic Equations. The block method is self-starting and satisfies the zero-stability, consistency and convergence conditions. BHI5 possesses high accuracy as shown in tables $(1)-(5)$ where it was compared with some existing methods. The method had proved efficient and suitable for the solution of the class of problems under consideration.

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Competing financial interests

The author declares no competing financial interests.

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