

Implicit One-Step Legendre Polynomial Hybrid Block Method for the Solution of First-Order Stiff Differential Equations

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Abstract: We formulate an implicit hybrid block method for the numerical solution of stiff first-order Ordinary Differential Equations (ODEs) using the Legendre polynomial as our basis function via interpolation and collocation techniques. The paper further investigates the basic properties of the implicit hybrid block method and found it to be zero-stable, consistent and convergent. The method was also tested on some sampled stiff problems and found to perform better than some existing ones with which we compared our results.

Keywords: Hybrid, Implicit, Legendre, One-step, Stiff

AMS Subject Classification (2010): 65L05, 65L06, 65D30

1. Introduction

In this paper, we are concerned with the solution of stiff first-order differential equations of the form,

$$y' = f(x, y), \quad y(a) = \eta, \quad x \in [a, b] \quad (1)$$

where f is assumed to be Lipchitz continuous in y and η is a given initial value.

Different methods have been proposed for the solution of (1) ranging from predictor-corrector methods to hybrid methods. Despite the success recorded by the predictor-corrector methods, its major setback is that the predictors are in reducing order of accuracy especially when the value of the step-length is high and moreover the results are at overlapping interval [2]. Hybrid methods have advantage of incorporating function evaluation at off-step points which affords the opportunity of circumventing the ‘the Dahlquist zero stability barrier’ and it is actually possible to obtain convergent k-step methods with order $2k + 1$ up

to $k = 7$, [4]. The method is also useful in reducing the step number of a method and still remains zero-stable, [1].

Stiff differential equations were first encountered in the study of the motion of springs varying stiffness, from which the problem derives its name. Stiffness occurs when some components of the solution decay much more rapidly than others. These problems are of frequent occurrence in the mathematical formulation of physical situations in control theory and mass action kinetics, where processes with widely varying time constants are usually encountered. Historically, two chemical engineers, Curtis and Hirschfelder in 1952 proposed the first set of numerical integration formulas (both implicit backward differentiation formulas) that are well suited for stiff differential equations. Stiff equations pose stability problems for most numerical integrators, [6].

Definition 1 [7]: Legendre polynomials $y_n(x)$ defined on $[-1,1]$ are given by,

$$y_n(x) = \sum_{m=0}^M (-1)^m \frac{(2n-2m)! x^{n-2m}}{2^n m!(n-m)!(n-2m)!} \quad (2)$$

where $M = n/2$ or $(n-1)/2$ whichever is an integer.

In particular, $y_0(x) = 1$, $y_1(x) = x$, $y_2(x) = (3x^2 - 1)/2, \dots$ The polynomials satisfy the following properties;

- $y_n(x)$ is an even polynomial if n is even and an odd polynomial if n is odd,
- $y_n(x)$ are orthogonal polynomials and satisfy

$$\int_{-1}^1 y_m(x) y_n(x) dx = \begin{cases} 0, & m \neq n \\ \frac{2}{2n+1}, & m = n \end{cases}$$

- $y_n(-x) = (-1)^n y_n(x)$

Definition 2 [9]: A differential equation is said to be stiff if $\text{Re}(\lambda_i) < 0, i = 1(1)m$, where λ is the eigen value of the differential equation.

Many scholars have proposed various forms of methods for the solution of (1) by adopting power series, Chebyshev and Lagrange polynomials as basis functions. In this paper, we develop an implicit hybrid block method that gives better stability condition by using Legendre polynomial as our basis function.

2. Formulation of the Implicit One-Step Hybrid Block Method

We consider the first six terms of the Legendre polynomial as our basis function. This is given by,

$$(n+1)y_{n+1}(x) = y_0(x) + y_1(x) + \sum_{n=1}^4 [(2n+1)xy_n(x) - ny_{n-1}(x)] \quad (3)$$

Interpolating (3) at point x_{n+s} , $s = 0$ and collocating its first derivative at points x_{n+r} , $r = 0\left(\frac{1}{4}\right)1$, where s and r are the numbers of interpolation and collocation points respectively, leads to the following system of equations,

$$XA = U \quad (4)$$

where

$$A = [a_0 \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5]^T$$

$$U = [y_n \quad f_n \quad f_{n+\frac{1}{4}} \quad f_{n+\frac{1}{2}} \quad f_{n+\frac{3}{4}} \quad f_{n+1}]^T$$

and

$$X = \begin{bmatrix} 7 & 11x_n & -18x_n^2 & -50x_n^3 & 35x_n^4 & 63x_n^5 \\ 0 & 11 & -36x_n & -150x_n^2 & 140x_n^3 & 315x_n^4 \\ 0 & 11 & -36x_{n+\frac{1}{4}} & -150x_{n+\frac{1}{4}}^2 & 140x_{n+\frac{1}{4}}^3 & 315x_{n+\frac{1}{4}}^4 \\ 0 & 11 & -36x_{n+\frac{1}{2}} & -150x_{n+\frac{1}{2}}^2 & 140x_{n+\frac{1}{2}}^3 & 315x_{n+\frac{1}{2}}^4 \\ 0 & 11 & -36x_{n+\frac{3}{4}} & -150x_{n+\frac{3}{4}}^2 & 140x_{n+\frac{3}{4}}^3 & 315x_{n+\frac{3}{4}}^4 \\ 0 & 11 & -36x_{n+1} & -150x_{n+1}^2 & 140x_{n+1}^3 & 315x_{n+1}^4 \end{bmatrix}$$

Solving (4), for a_j 's, $j = 0(1)5$ and substituting back into (3) gives a continuous linear multistep method of the form,

$$y(x) = \alpha_0(x)y_n + h \sum_{j=0}^1 \beta_j(x) f_{n+j}, \quad j = 0\left(\frac{1}{4}\right)1 \quad (5)$$

where the coefficients of y_n and f_{n+j} are given by,

$$\begin{aligned}
& \left. \begin{aligned}
& \alpha_0(t) = 1 \\
& \beta_0(t) = -\frac{1}{90}(192t^5 - 600t^4 + 700t^3 - 375t^2 + 90t) \\
& \beta_{\frac{1}{4}}(t) = \frac{1}{45}(-384t^5 + 1080t^4 - 1040t^3 + 360t^2) \\
& \beta_{\frac{1}{2}}(t) = -\frac{1}{15}(192t^5 - 480t^4 + 380t^3 - 90t^2) \\
& \beta_{\frac{3}{4}}(t) = \frac{1}{45}(-384t^5 + 840t^4 - 560t^3 + 120t^2) \\
& \beta_1(t) = -\frac{1}{90}(192t^5 - 360t^4 + 220t^3 - 45t^2)
\end{aligned} \right\} \quad (6)
\end{aligned}$$

and $t = (x - x_n)/h$. Evaluating (5) at $t = \left(\frac{1}{4}\right)\left(\frac{1}{4}\right)1$ gives a discrete hybrid block method of the form,

$$A^{(0)}\mathbf{Y}_m = E\mathbf{y}_n + h\mathbf{d}\mathbf{f}(\mathbf{y}_n) + hb\mathbf{F}(\mathbf{Y}_m) \quad (7)$$

where

$$\mathbf{Y}_m = \begin{bmatrix} y_{n+\frac{1}{4}} & y_{n+\frac{1}{2}} & y_{n+\frac{3}{4}} & y_{n+1} \end{bmatrix}^T, \mathbf{y}_n = \begin{bmatrix} y_{n-\frac{3}{4}} & y_{n-\frac{1}{2}} & y_{n-\frac{1}{4}} & y_n \end{bmatrix}^T,$$

$$\mathbf{F}(\mathbf{Y}_m) = \begin{bmatrix} f_{n+\frac{1}{4}} & f_{n+\frac{1}{2}} & f_{n+\frac{3}{4}} & f_{n+1} \end{bmatrix}^T, \mathbf{f}(\mathbf{y}_n) = \begin{bmatrix} f_{n-\frac{3}{4}} & f_{n-\frac{1}{2}} & f_{n-\frac{1}{4}} & f_n \end{bmatrix}^T$$

$$A^{(0)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, E = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}, d = \begin{bmatrix} 0 & 0 & 0 & \frac{251}{2880} \\ 0 & 0 & 0 & \frac{29}{360} \\ 0 & 0 & 0 & \frac{-2997}{80} \\ 0 & 0 & 0 & \frac{7}{90} \end{bmatrix}$$

$$b = \begin{bmatrix} \frac{323}{1440} & \frac{-11}{120} & \frac{53}{1440} & \frac{-19}{2880} \\ \frac{31}{90} & \frac{1}{15} & \frac{1}{90} & \frac{-1}{360} \\ \frac{51}{160} & \frac{90}{40} & \frac{21}{160} & \frac{-3}{320} \\ \frac{16}{45} & \frac{2}{15} & \frac{16}{45} & \frac{7}{90} \end{bmatrix}$$

3. Analysis of Basic Properties of the Implicit One-Step Hybrid Block Method

3.1 Order of the Implicit One-step Hybrid Block Method

Let the linear operator $L\{y(x); h\}$ associated with the block (8) be defined as,

$$L\{y(x); h\} = A^{(0)}Y_m - Ey_n - hdf(y_n) - hbF(Y_m) \quad (8)$$

Expanding (8) using Taylor series and comparing the coefficients of h gives,

$$L\{y(x); h\} = c_0y(x) + c_1hy'(x) + c_2h^2y''(x) + \dots + c_ph^py^{(p)}(x) + c_{p+1}h^{p+1}y^{(p+1)}(x) + \dots \quad (9)$$

Definition 3 [6]: The linear operator L and the associated continuous linear multistep method (5) are said to be of order p if $c_0 = c_1 = c_2 = \dots = c_p = 0$ and $c_{p+1} \neq 0$.

c_{p+1} is called the error constant and the local truncation error is given by,

$$t_{n+k} = c_{p+1}h^{(p+1)}y^{(p+1)}(x_n) + O(h^{p+2}) \quad (10)$$

For implicit one-step hybrid block method,

$$L\{y(x);h\} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_{n+\frac{1}{4}} \\ y_{n+\frac{1}{2}} \\ y_{n+\frac{3}{4}} \\ y_{n+1} \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_{n-\frac{3}{4}} \\ y_{n-\frac{1}{2}} \\ y_{n-\frac{1}{4}} \\ y_n \end{bmatrix}$$

90

$$-h \begin{bmatrix} \frac{251}{2800} & \frac{323}{1440} & \frac{-11}{120} & \frac{53}{1440} & \frac{-19}{2880} \\ \frac{29}{360} & \frac{31}{90} & \frac{1}{15} & \frac{1}{90} & \frac{-1}{360} \\ \frac{-2997}{80} & \frac{51}{160} & \frac{90}{40} & \frac{21}{160} & \frac{-3}{320} \\ \frac{7}{90} & \frac{16}{45} & \frac{2}{15} & \frac{16}{45} & \frac{7}{90} \end{bmatrix} \begin{bmatrix} f_n \\ f_{n+\frac{1}{4}} \\ f_{n+\frac{1}{2}} \\ f_{n+\frac{3}{4}} \\ f_{n+1} \end{bmatrix} \quad (11)$$

91 Expanding (11) in Taylor series gives,

$$\begin{aligned}
 & \left[\begin{aligned}
 & \sum_{j=0}^{\infty} \frac{\left(\frac{1}{4}h\right)^j}{j!} y_n^j - y_n - \frac{251h}{2880} y_n' - \sum_{j=0}^{\infty} \frac{h^{j+1}}{j!} y_n^{j+1} \left\{ \frac{323}{1440} \left(\frac{1}{4}\right)^j - \frac{11}{120} \left(\frac{1}{2}\right)^j + \frac{53}{1440} \left(\frac{3}{4}\right)^j - \frac{19}{2880} (1)^j \right\} \\
 & \sum_{j=0}^{\infty} \frac{\left(\frac{1}{2}h\right)^j}{j!} y_n^j - y_n - \frac{29h}{360} y_n' - \sum_{j=0}^{\infty} \frac{h^{j+1}}{j!} y_n^{j+1} \left\{ \frac{31}{90} \left(\frac{1}{4}\right)^j + \frac{1}{15} \left(\frac{1}{2}\right)^j + \frac{7}{45} \left(\frac{3}{4}\right)^j - \frac{1}{360} (1)^j \right\} \\
 & \sum_{j=0}^{\infty} \frac{\left(\frac{3}{4}h\right)^j}{j!} y_n^j - y_n - \frac{-2997h}{80} y_n' - \sum_{j=0}^{\infty} \frac{h^{j+1}}{j!} y_n^{j+1} \left\{ \frac{51}{160} \left(\frac{1}{4}\right)^j + \frac{9}{40} \left(\frac{1}{2}\right)^j + \frac{21}{160} \left(\frac{3}{4}\right)^j - \frac{3}{320} (1)^j \right\} \\
 & \sum_{j=0}^{\infty} \frac{(h)^j}{j!} y_n^j - y_n - \frac{7h}{90} y_n' - \sum_{j=0}^{\infty} \frac{h^{j+1}}{j!} y_n^{j+1} \left\{ \frac{16}{45} \left(\frac{1}{4}\right)^j + \frac{2}{15} \left(\frac{1}{2}\right)^j + \frac{16}{45} \left(\frac{3}{4}\right)^j + \frac{7}{90} (1)^j \right\}
 \end{aligned} \right] = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\
 & \hspace{15em} (12)
 \end{aligned}$$

95 Equating the coefficients of the Taylor series expansion to zero yields,
 96 $\bar{c}_0 = \bar{c}_1 = \bar{c}_2 = \bar{c}_3 = \bar{c}_4 = \bar{c}_5 = 0$, $\bar{c}_6 = [4.5776(-06) \quad 1.2418(-11) \quad 4.5776(-06) \quad -5.1670(-07)]^T$.

97 Therefore, the implicit one-step hybrid block method is of uniform order five.

99 3.2 Zero Stability of the Implicit One-Step Hybrid Block Method

100 **Definition 4** [6]: The implicit one-step hybrid block method (7) is said to be zero-stable, if the roots
 101 $z_s, s=1,2,...,k$ of the first characteristic polynomial $\rho(z)$ defined by $\rho(z) = \det(z\mathbf{A}^{(0)} - \mathbf{E})$ satisfies
 102 $|z_s| \leq 1$ and every root satisfying $|z_s| = 1$ have multiplicity not exceeding the order of the differential
 103 equation. Moreover, as $h \rightarrow 0$, $\rho(z) = z^{r-\mu}(z-1)^\mu$ where μ is the order of the differential equation, r
 104 is the order of the matrices $\mathbf{A}^{(0)}$ and $\mathbf{E}$, see [3] for details.

105 For our method,

$$\rho(z) = \left| z \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right| = 0 \quad (13)$$

$\rho(z) = z^4 - z^3 = z^3(z-1) = 0, \Rightarrow z_1 = z_2 = z_3 = 0, z_4 = 1$. Hence, the implicit one-step hybrid block method is zero-stable.

3.3 Consistency and Convergence of the Implicit One-Step Hybrid Block Method

The implicit one-step hybrid block method (7) is consistent since it has order $p = 5 \geq 1$ and it is also convergent by consequence of Dahlquist theorem stated below.

Theorem 2 [5]: The necessary and sufficient conditions that a continuous LMM be convergent are that it be consistent and zero-stable.

3.4 Convergence and Region of Absolute Stability of the Implicit One-Step Hybrid Block Method

Definition 5 [12]: Region of absolute stability is a region in the complex z plane, where $z = \lambda h$. It is defined as those values of z such that the numerical solutions of $y' = -\lambda y$ satisfy $y_j \rightarrow 0$ as $j \rightarrow \infty$ for any initial condition.

We shall adopt the boundary locus method to determine the region of absolute stability of the implicit one-step hybrid block method. This gives the stability polynomial below,

$$\begin{aligned} \bar{h}(w) = & h^4 \left(\frac{1}{1280} w^4 + \frac{5}{8} w^3 \right) - h^3 \left(\frac{5}{384} w^4 + \frac{6433}{1920} w^3 \right) \\ & + h^2 \left(\frac{7}{64} w^4 + \frac{4237}{320} w^3 \right) - h \left(\frac{1}{2} w^4 + \frac{1}{2} w^3 \right) + w^4 - w^3 \end{aligned} \quad (14)$$

The stability region is shown in the figure below.

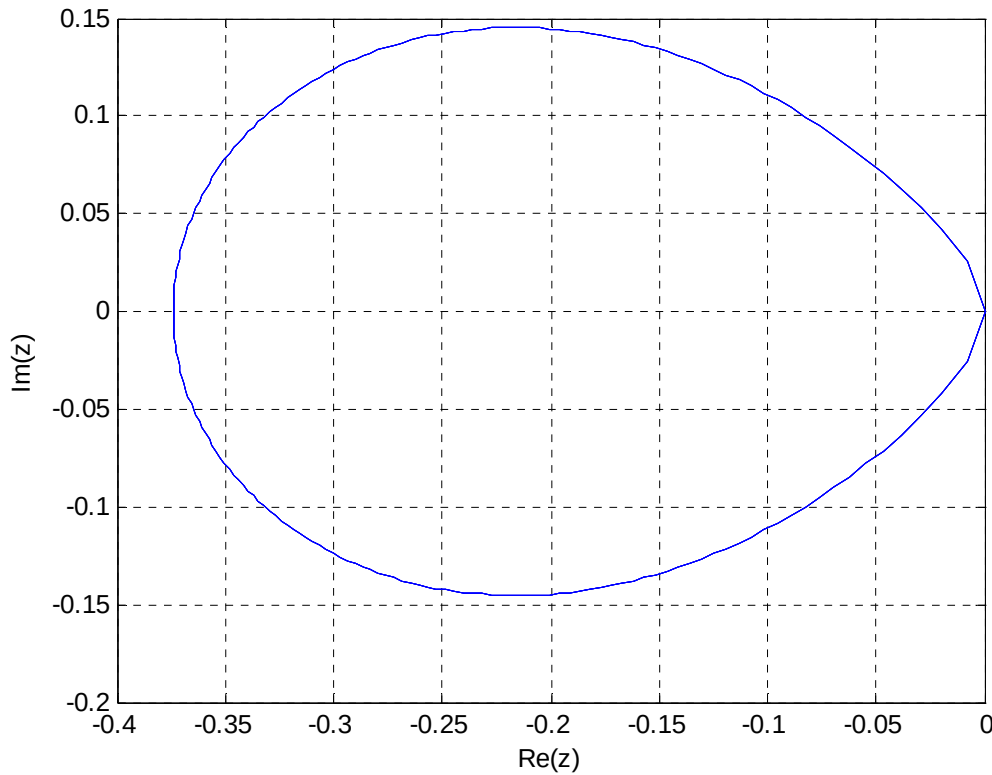


Figure 1: Stability Region of the Implicit One-Step Hybrid Block Method

The stability region obtained in Figure 1 above is A-Stable, since it contains the whole of the left-half complex plane, [9].

4. Numerical Experiments

The implicit one-step hybrid block method formulated shall be tested on some set of stiff differential equations and compare the results with solutions from some methods of similar derivation. The numerical results were obtained using MATLAB.

The following notations shall be used in the tables below;

ERR- |Exact Solution-Computed Solution|

EJA- Error in [8]

EOK- Error in [10]

Problem 1

A certain radioactive substance is known to decay at the rate proportional to the amount present. A block of this substance having a mass of $100g$ originally is observed. After 40hours, its mass reduced to $90g$. Test for the consistency of the implicit one-step hybrid block method on this problem for $t \in [0,1]$. This stiff problem is modeled by the differential equation,

$$\frac{dN}{dt} = \alpha N, \alpha = -0.0026, N(0) = 100, t \in [0,1] \quad (15)$$

where N represents the mass of the substance at any time t and α is a constant which specifies the rate at which this particular substance decays. The theoretical solution to (15) is given by;

$$N(t) = 100e^{-0.0026t} \quad (16)$$

Source: [11]

This problem was solved using Half-step hybrid method of order six.

Problem 2

Consider the highly stiff ODE

$$y' = -10(y-1)^2, y(0) = 2 \quad (17)$$

with the exact solution,

$$y(t) = 1 + \frac{1}{1+10t} \quad (18)$$

Source: [10].

This problem was earlier discussed by [9], he showed that many predictor-corrector and block methods become unstable with this problem, including the hybrid methods. However, the newly derived block method is used for the integration of this problem within the interval $0 \leq t \leq 0.1$. The authors in [10] solved this stiff problem by adopting a new 3-point block method with step size ratio at $r=1$ and of order five.

Table 1: Showing the results for stiff problem 1

t	Exact Solution	Computed Solution	ERR	EJA	t / sec
0.1000	99.9740033797070850	99.9740033797070850	0.000000e+000	0.000000e+000	0.0192
0.2000	99.9480135176568470	99.9480135176568470	0.000000e+000	1.421085e-014	0.0233
0.3000	99.9220304120923400	99.9220304120923400	0.000000e+000	0.000000e+000	0.0273
0.4000	99.8960540612571460	99.8960540612571460	0.000000e+000	0.000000e+000	0.0314
0.5000	99.8700844633952300	99.8700844633952300	0.000000e+000	1.421085e-014	0.0355
0.6000	99.8441216167510670	99.8441216167510670	0.000000e+000	1.421085e-014	0.0396
0.7000	99.8181655195695610	99.8181655195695610	0.000000e+000	1.421085e-014	0.0436
0.8000	99.7922161700960970	99.7922161700960970	0.000000e+000	0.000000e+000	0.0477
0.9000	99.7662735665764730	99.7662735665764730	0.000000e+000	0.000000e+000	0.0522
1.0000	99.7403377072569700	99.7403377072569700	0.000000e+000	0.000000e+000	0.0563

Table 2: Showing the result for stiff problem 2

t	Exact Solution	Computed Solution	ERR	EOK	t / sec
0.0100	1.9090909090909092	1.9090909331157688	2.402486e-008	1.07e-04	0.0637
0.0200	1.8333333333333335	1.8333333648932029	3.155987e-008	2.38e-04	0.0644
0.0300	1.7692307692307692	1.7692308018612271	3.263046e-008	4.51e-04	0.0649
0.0400	1.7142857142857144	1.7142857454780251	3.119231e-008	6.20e-04	0.0653
0.0500	1.6666666666666665	1.6666666955435152	2.887685e-008	8.84e-04	0.0657
0.0600	1.6250000000000000	1.6250000263694577	2.636946e-008	1.03e-03	0.0661
0.0700	1.5882352941176470	1.5882353180705253	2.395288e-008	1.27e-03	0.0665
0.0800	1.5555555555555556	1.5555555772891725	2.173362e-008	1.53e-03	0.0670
0.0900	1.5263157894736841	1.5263158092141216	1.974044e-008	1.75e-03	0.0674
0.1000	1.5000000000000000	1.5000000179685555	1.796856e-008	1.81e-03	0.0678

5. Conclusion

We formulated an A-stable implicit one-step hybrid block method for the solution of stiff first-order ordinary differential equations where we adopted Legendre polynomial as our basis function. The method developed was also found to be zero-stable, consistent and convergent. The hybrid block method was also found to perform better than some existing methods in view of the numerical results obtained.

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