SECOND DERIVATIVE MULTISTEP METHOD WITH NESTED HYBRID EVALUATION

Abstract

This paper considers second derivative multistep methods with nested hybrid evaluation (MMNHE). The methods derived are A-stable for step number $k = 1(1)8$. The schemes have been implemented on some stiff problems, the results obtained are compared with a second derivative linear multistep method for stiff ordinary differential equations in Enright (1974).

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1 Introduction

Several problems in science and engineering are often modeled as ordinary differential equations (ODEs), some of these ODEs are stiff problems arising in areas such as chemical kinetics, nuclear reactor, control theory, quantum mechanics and electrical circuit theory. Considered in this paper, is the numerical integration of a system of initial value problem (IVP) for stiff ODEs of the form

$$y'(x) = f(y(x)); \qquad y(x_0) = y_0 \in R^m, \qquad x \in [x_0, X] \tag{1}$$

where $f : R \times R^m \to R^m$ is a sufficiently differentiable function with $y(x)$ being the unique solution of the IVP in (1) in the interval $[x_0, X]$.

A potentially good numerical method for solving stiff systems of ODEs must have good accuracy and an infinite region of absolute stability, (see [2], [14]), hence, A-stable methods are the good choice for obtaining solution for stiff problems. However, the requirement of A-stability puts a severe limitation on the choice of suitable linear multistep methods. This is articulated in the Dahlquist order barrier, (see [2]) in the case of linear multistep methods (LMMs) and the Daniel-Moore conjecture (see [1]) in the case of general multiderivative LMM. In developing schemes that possess High order and A–stability, [5] highlighted that it is traditional to turn to Runge-Kutta methods (RKMs) or LMM in order to obtain high order A − stable methods. Fatunla [13] highlighted unconventional numerical integrator adopted in order to circumvent the Dahlquist order barrier. Some authors have developed schemes for the numerical integration of stiff problems of which include: the nonlinear multistep schemes of [6], the multiderivative multistep method of [14], [7]; Higher derivative methods of [1], [10, 11, 12], High order A-stable methods of [9]. Kulikov and Shindin [2, 3] presented nested implicit Runge-Kutta (IRK) formulas based on the Gauss quadrature formula with high order and good stability properties.

We present the multistep method with nested hybrid evaluation (MMNHE) defined as,

$$y_{n+k} = \sum_{j=0}^{k-1} \alpha_j^{(m)} y_{n+j} + h\left(\gamma_k^{(m)} f_{n+k} + \beta_{v_m}^{(m)} f_{n+v_m}\right) + h^2\left(\Omega_k^{(m)} f'_{n+k} + \Omega_{v_m}^{(m)} f'_{n+v_m}\right) \tag{2}$$

with the recursively nested hybrid solution,

$$y_{n+v_{l+1}} = \sum_{j=0}^{k} \alpha_j^{(l)} y_{n+j} + h\left(\beta_{v_l}^{(l)} f_{n+v_l} + \beta_{v_{l-1}}^{(l-1)} f_{n+v_{l-1}} + \beta_k^{(l)} f_{n+k}\right) \qquad l = 0(1)m-1 \tag{3}$$

where

$$y_{n+v_1} = \sum_{j=0}^{k} \alpha_j^{(0)} y_{n+j} + h\left(\beta_{v_0}^{(0)} f_{n+v_0} + \beta_k^{(0)} f_{n+k}\right) \tag{4}$$

with the hybrid predictor y_{n+v_0} given by

$$y_{n+v_0} = \begin{cases} \sum_{j=0}^{k} \alpha_j^{(-1)} y_{n+j} + h\beta_k^{(-1)} f_{n+k} & (M_1) \\ \sum_{j=0}^{k} \alpha_j^{(-1)} y_{n+j} + h\beta_k^{(-1)} f_{n+k} + h^2\lambda_k^{(-1)} f'_{n+k} & (M_2) \end{cases} \tag{5}$$

to obtain the solution of the IVP (1) from x_n to $x_{n+j} = x_n + jh$ (h being the step size), where $k \geq 1$ is the step number and $m = k-1$. Two case of hybrid predictors are considered and denoted as M_1 and M_2. The hybrid values v is chosen as

$$v_m = k - \frac{1}{2}, \quad v_{t-1} = \frac{(v_t + k)}{2}, \quad \alpha_{-j}^{(l)} = 0,\ j = 1(1)k, \quad t = 1(1)m \tag{6}$$

The y_{n+k} is the numerical approximation to the exact solution $y(x_{n+k})$. The advantage of the nested hybrid methods is that implicitness is on the output solution reducing computational cost compared to that of the Runge-kutta method (RKM), in which the implicitness is on the stages making the resolution of the implicitness of the RKM computational intensive, compared to the nested implicit methods. We exploit this advantage of recursively nested methods to present a new family of hybrid methods employing this approach.

2 Local truncation error and Order

The general form of the local truncation error of the MMNHE (2), (3), (4), (5) and (6) are:

$$LTE_a = y(x_{n+k}) - \Bigg(\sum_{j=0}^{k-1} \alpha_j^{(m)} y(x_{n+j}) + \left(\gamma_k^{(m)} y'(x_{n+k}) + \beta_{v_m}^{(m)} y'(x_{n+v_m})\right) + h^2\left(\Omega_k^{(m)} y''(x_{n+k}) + \Omega_{v_m}^{(m)} y''(x_{n+v_m})\right)\Bigg) \tag{7}$$

$$LTE_b = y(x_{n+v_{l+1}}) - \Bigg(\sum_{j=0}^{k} \alpha_j^{(l)} y(x_{n+j})) + h\Big(\beta_{v_l}^{(l)} y'(x_{n+v_l}) + \beta_{v_{l-1}}^{(l-1)} y'(x_{n+v_{l-1}}) + \beta_k^{(l)} y'(x_{n+k})\Big)\Bigg) \tag{8}$$

$$LTE_c = y(x_{n+v_1}) - \left(\sum_{j=0}^{k} \alpha_j^{(0)} y(x_{n+j})) + h\left(\beta_{v_0}^{(0)} y'(x_{n+v_0}) + \beta_k^{(0)} y'(x_{n+k})\right)\right) \tag{9}$$

$$LTE_d = y(x_{n+v_0}) - \left(\sum_{j=0}^{k} \alpha_j^{(-1)} y(x_{n+j}) + h\beta_k^{(-1)} y'(x_{n+k}) \right) \tag{10}$$

$$LTE_e = y(x_{n+v_0}) - \left(\sum_{j=0}^{k} \alpha_j^{(-1)} y(x_{n+j}) + h\beta_k^{(-1)} f(y(x_{n+k})) + h^2\lambda_k^{(-1)} f'(y(x_{n+k})) \right) \tag{11}$$

respectively. The Taylor's series expansion of (7), (8), (9), (10) and (11) about x_n gives the error constants of the MMNHE in (2), (3), (4) and (5) as

$$y_{n+k} - y(x_{n+k}) = C_{p+1}^{(a)} h^{p+1} y^{p+1}(x_n) + O(h^{p+2}) \tag{12}$$

$$y_{n+v_{l+1}} - y(x_{n+v_{l+1}}) = C_{q+1}^{(b)} h^{q+1} y^{q+1}(x_n) + O(h^{q+2}) \tag{13}$$

$$y_{n+v_1} - y(x_{n+v_1}) = C_{r+1}^{(c)} h^{r+1} y^{r+1}(x_n) + O(h^{r+2}) \tag{14}$$

$$y_{n+v_0} - y(x_{n+v_0}) = \begin{cases} C_{s+1}^{(d)} h^{s+1} y^{s+1}(x_n) + O(h^{s+2}) & (M_1) \\ \\ C_{t+1}^{(e)} h^{t+1} y^{t+1}(x_n) + O(h^{t+2}) & (M_2) \end{cases} \tag{15}$$

respectively, where $C_{p+1}^{(a)}$, $C_{q+1}^{(b)}$, $C_{r+1}^{(c)}$, $C_{s+1}^{(d)}$ and $C_{t+1}^{(e)}$ are the principal error constants of (2), (3), (4) and (5) respectively, with orders p, q, r, s and t given as $p = k+3$, $q = k+3$, $r = k+2$, $s = k+1$ and $t = k+2$ respectively.

Theorem 1. [6] *Given $C_0^{(a)} = 0,\ C_1^{(a)} = 0,\ C_2^{(a)} = 0,\ \cdots,\ C_p^{(a)} = 0$ if $C_{p+1}^{(a)} \neq 0$ the principal error constant $C_{p+1}^{(a)}$ of (2) is given as*

$$C_{p+1}^{(a)} = \frac{1}{(p+1)!} \Bigg(k^{p+1} - (p+1)v_m^p \beta_{v_m}^{(m)} - (p+1)k^p \gamma_k^{(m)} - p(p+1)k^{p-1}\Omega_k^{(m)} \\ - p(p+1)v_m^{p-1}\Omega_{v_m}^{(m)} - \sum_{j=0}^{k-1} j^{p+1}\alpha_j^{(m)} \Bigg) \tag{16}$$

and the method is of order p.

Proof. Expanding (7) using the Taylor's series expansion about x_n gives

$$L[y(x_n), h] = C_0^{(a)} y(x_n) + C_1^{(a)} h y'(x_n) + C_2^{(a)} h^2 y''(x_n) + \cdots + C_p^{(a)} h^p y^p(x_n) \\ + C_{p+1}^{(a)} h^{p+1} y^{p+1}(x_n) + O(h^{p+2}) \tag{17}$$

where the constants $C_p^{(a)}$ are given as

$$C_0^{(a)} = 1 - \sum_{j=0}^{k-1} \alpha_j^{(m)} \tag{18}$$

$$C_1^{(a)} = k - \beta_{v_m}^{(m)} - \gamma_k^{(m)} - \sum_{j=0}^{k-1} j\alpha_j^{(m)} \tag{19}$$

$$C_2^{(a)} = \frac{1}{2}k^2 - v_m\beta_{v_m}^{(m)} - k\gamma_k^{(m)} - \Omega_k^{(m)} - \Omega_{v_m}^{(m)} - \sum_{j=0}^{k-1} \frac{1}{2} j^2 \alpha_j^{(m)} \tag{20}$$

$$C_3^{(a)} = \frac{1}{3!} \left(k^3 - 3v_m^2\beta_{v_m}^{(m)} - 3k^2\gamma_k^{(m)} - 6k\Omega_k^{(m)} - 6v_m\Omega_{v_m}^{(m)} - \sum_{j=0}^{k-1} \frac{1}{2} j^2\alpha_j^{(m)} - \sum_{j=0}^{k-1} \frac{1}{2} j^3 \alpha_j^{(m)} \right) \tag{21}$$

$$\vdots$$

$$C_p^{(a)} = \frac{1}{p!}\Bigg(k^p - (p)v_m^{p-1}\beta_{v_m}^{(m)} - (p)k^{p-1}\gamma_k^{(m)} - p(p-1)k^{p-2}\Omega_k^{(m)} - p(p-1)v_m^{p-2}\Omega_{v_m}^{(m)} - \sum_{j=0}^{k-1} j^p\alpha_j^{(m)}\Bigg) \tag{22}$$

replacing p with $p+1$ in (21) gives (15). □

Theorem 2. [6] *Given $C_0^{(b)} = 0,\ C_1^{(b)} = 0,\ C_2^{(b)} = 0,\ \cdots,\ C_q^{(b)} = 0$, if $C_{q+1}^{(b)} \neq 0$. The principal error constant $C_{q+1}^{(b)}$ of (3) is given as*

$$C_{q+1}^{(b)} = \frac{1}{(q+1)!}\Bigg(v_{l+1}^{q+1} - (q+1)k^q\beta_k^{(l)} - (q+1)v_{l-1}^q\beta_{v_{l-1}}^{(l)} - (q+1)v_l^q\beta_{v_l}^{(l)} - \sum_{j=0}^{k} j^{q+1}\alpha_j^{(l)}\Bigg) \tag{23}$$

and the nested hybrid method is of order q.

Theorem 3. [6] *Given $C_0^{(c)} = 0,\ C_1^{(c)} = 0,\ C_2^{(c)} = 0,\ \cdots,\ C_r^{(c)} = 0$, if $C_{r+1}^{(c)} \neq 0$. The principal error constant $C_{r+1}^{(c)}$ of (4) is given as*

$$C_{r+1}^{(c)} = \frac{1}{(r+1)!}\left(v_1^{r+1} - (r+1)k^r\beta_k^{(l)} - (r+1)v_0^r\beta_0^{(l)} - \sum_{j=0}^{k} j^{r+1}\alpha_j^{(l)}\right) \tag{24}$$

and the hybrid method is of order r.

Theorem 4. [6] *Given $C_0^{(d)} = 0,\ C_1^{(d)} = 0,\ C_2^{(d)} = 0,\ \cdots,\ C_s^{(d)} = 0$, if $C_{s+1}^{(d)} \neq 0$. The principal error constant $C_{s+1}^{(d)}$ of (5) is given as*

$$C_{s+1}^{(d)} = \frac{1}{(s+1)!}\Bigg(v_0^{s+1} - (s+1)k^s\beta_k^{(-1)} - \sum_{j=0}^{k} j^{s+1}\alpha_j^{(-1)}\Bigg) \tag{25}$$

and the hybrid predictor is of order s.

Theorem 5. [6] *Given $C_0^{(e)} = 0,\ C_1^{(e)} = 0,\ C_2^{(e)} = 0,\ \cdots,\ C_r^{(e)} = 0$, if $C_{r+1}^{(e)} \neq 0$. The principal error constant $C_{r+1}^{(e)}$ of (5) is given as*

$$C_{t+1}^{(e)} = \frac{1}{(t+1)!}\Bigg(v_0^{t+1} - (t+1)k^t\beta_k^{(-1)} - t(t+1)k^{t-1}\lambda_k^{(-1)} - \sum_{j=0}^{k} j^{t+1}\alpha_j^{(-1)}\Bigg) \tag{26}$$

and the hybrid predictor is of order t.

3 The Derivation of the MMNHE

For a fixed step number $k \geq 1$ and with the hybrid points v as defined in (6), then setting up the order conditions in (16), (23), (24), (25) and (26) gives appropriately the respective methods for a varying k. For each $k = 1(1)9$, the $v = (v_0, v_1, v_2, \cdots, v_m)$ is computed from (6), whose results is given in table 1.

Table 1: Given values for v at each k.

k	$v = (v_0, v_1, v_2, \cdots, v_m)$
1	$\left(\frac{1}{2}\right)$
2	$\left(\frac{7}{4}, \frac{3}{2}\right)$
3	$\left(\frac{23}{8}, \frac{11}{4}, \frac{5}{2}\right)$
4	$\left(\frac{63}{16}, \frac{31}{8}, \frac{15}{4}, \frac{7}{2}\right)$
5	$\left(\frac{159}{32}, \frac{79}{16}, \frac{39}{8}, \frac{19}{4}, \frac{9}{2}\right)$
6	$\left(\frac{383}{64}, \frac{191}{32}, \frac{95}{16}, \frac{47}{8}, \frac{23}{4}, \frac{11}{2}\right)$
7	$\left(\frac{895}{128}, \frac{447}{64}, \frac{223}{32}, \frac{111}{16}, \frac{55}{8}, \frac{27}{4}, \frac{13}{2}\right)$
8	$\left(\frac{2047}{256}, \frac{1023}{128}, \frac{511}{64}, \frac{255}{32}, \frac{127}{16}, \frac{63}{8}, \frac{31}{4}, \frac{15}{2}\right)$
9	$\left(\frac{4607}{512}, \frac{2303}{256}, \frac{1151}{128}, \frac{575}{64}, \frac{287}{32}, \frac{143}{16}, \frac{71}{8}, \frac{35}{4}, \frac{17}{2}\right)$

3.1 Method of order p=4, s=2, t=3; k=1

Setting $k = 1$ in (16), (25) and (26), the method is derived as;

$$y_{n+1} = y_n + hf_{n+1} + h^2\left(-\frac{1}{3}f'_{n+\frac{1}{2}} - \frac{1}{6}f'_{n+1}\right) \qquad C_5 = \frac{1}{720} \tag{27}$$

with the hybrid predictor given as

$$y_{n+\frac{1}{2}} = \begin{cases} \frac{1}{4}y_n + \frac{3}{4}y_{n+1} - \frac{1}{4}hf_{n+1} & C_3 = \frac{1}{48} \quad (M_1) \\ \frac{1}{8}y_n + \frac{7}{8}y_{n+1} - \frac{3}{8}hf_{n+1} + \frac{1}{16}h^2 f'_{n+1} & C_4 = -\frac{1}{384} \quad (M_2) \end{cases} \tag{28}$$

3.2 Method of order p=5, r=4, s=3, t=4; k=2

Setting $k = 2$ in (16), (24),(25) and (26), the method is derived as;

$$y_{n+2} = -\frac{1}{91}y_n + \frac{92}{91}y_{n+1} + h\left(\frac{32}{91}f_{n+\frac{3}{2}} + \frac{58}{91}f_{n+2}\right) + h^2\left(-\frac{20}{91}f'_{n+\frac{3}{2}} - \frac{8}{91}f'_{n+2}\right) \quad C_6 = \frac{31}{131040} \tag{29}$$

with the hybrid method

$$y_{n+\frac{3}{2}} = -\frac{1}{512}y_n + \frac{9}{128}y_{n+1} + \frac{477}{512}y_{n+2} + h\left(-\frac{3}{8}f_{n+\frac{7}{4}} - \frac{15}{256}f_{n+2}\right) \quad C_5 = \frac{11}{81920} \tag{30}$$

where the hybrid predictor is given as

$$y_{n+\frac{7}{4}} = \begin{cases} -\frac{3}{256}y_n + \frac{7}{64}y_{n+1} + \frac{231}{256}y_{n+2} - \frac{21}{128}hf_{n+2} \quad C_4 = \frac{7}{2048} & (M_1) \\ -\frac{3}{2048}y_n + \frac{7}{256}y_{n+1} + \frac{1995}{2048}y_{n+2} - \frac{231}{1024}hf_{n+2} + \frac{21}{1024}h^2 f'_{n+2} \quad C_5 = -\frac{7}{40960} & (M_2) \end{cases} \tag{31}$$

3.3 Method of Order p=6, q=6, r=5, s=4, t=5; k=3

Setting $k = 3$ in (16), (23), (24), (25) and (26), the method is derived as;

$$\begin{aligned} y_{n+3} = \frac{124}{109879}y_n - \frac{351}{15697}y_{n+1} + \frac{112212}{109879}y_{n+2} + h\left(\frac{51840}{109879}f_{n+\frac{5}{2}} + \frac{55830}{109879}f_{n+3}\right) \\ + h^2\left(-\frac{1728}{9989}f'_{n+\frac{5}{2}} - \frac{6822}{109879}f'_{n+3}\right) \quad C_7 = \frac{2127}{30766120} \end{aligned} \tag{32}$$

with the recursive hybrid

$$\begin{aligned} y_{n+\frac{5}{2}} = \frac{3477}{40740832}y_n - \frac{128995}{81481664}y_{n+1} + \frac{2115585}{40740832}y_{n+2} + \frac{77372535}{81481664}y_{n+3} \\ + h\left(-\frac{614520}{1273151}f_{n+\frac{11}{4}} + \frac{192000}{1273151}f_{n+\frac{23}{8}} - \frac{4852755}{40740832}f_{n+3}\right) \quad C_7 = \frac{104823}{18251892736} \end{aligned} \tag{33}$$

$$y_{n+\frac{11}{4}} = \frac{581}{6480384}y_n - \frac{4323}{4320256}y_{n+1} + \frac{23639}{2160128}y_{n+2} + \frac{12830741}{12960768}y_{n+3} - h\left(\frac{924}{4219}f_{n+\frac{23}{8}} + \frac{47047}{2160128}f_{n+3}\right) \quad C_6 = -\frac{34727}{2073722880} \tag{34}$$

and the hybrid predictor $y_{n+\frac{23}{8}}$ defined as

$$y_{n+\frac{23}{8}} = \frac{35}{24576}y_n - \frac{161}{16384}y_{n+1} + \frac{345}{8192}y_{n+2} + \frac{47495}{49152}y_{n+3} - \frac{805}{8192}hf_{n+3} \quad C_5 = \frac{161}{262144} \tag{35}$$

for the case M_1, and

$$y_{n+\frac{23}{8}} = \frac{35}{589824}y_n - \frac{161}{262144}y_{n+1} + \frac{345}{65536}y_{n+2} + \frac{2348185}{2359296}y_{n+3} - \frac{47495}{393216}hf_{n+3} + \frac{805}{131072}h^2 f'_{n+3} \quad C_6 = -\frac{161}{12582912} \tag{36}$$

for the case M_2. The higher order methods are obtained similarly.

4 Stability of the method (2)

The stability of the MMNHE (2) is investigated using the scalar test problem

$$y'(x) = \lambda y(x) \qquad x \geq 0, \qquad Re(\lambda) < 0 \tag{37}$$

The resultant stability polynomial of the MMNHE (2) for using the first case of hybrid predictor M_1 is given by

$$\Pi_1(w,z) = w^k - \sum_{j=0}^{k-1} \alpha_j^{(m)} w^j - z\left[\gamma_k^{(m)} w^k + \beta_{v_m}^{(m)}(R_1(w,z))\right] - z^2\left[\Omega_k^{(m)} w^k + \Omega_{v_m}^{(m)}(R_1(w,z))\right] \tag{38}$$

where

$$\begin{aligned} R_1(w,z) = & \sum_{j=0}^{k} \alpha_j^{(m-1)} w^j + z\beta_k^{(m-1)} w^k \\ & + z\beta_{v_{m-1}}^{(m-1)}\left(\cdots\left(\left(\sum_{j=0}^{k} \alpha_j^{(0)} w^j + z\beta_k^{(0)} w^k + z\beta_{v_0}^{(0)}\left(\sum_{j=0}^{k} \alpha_j^{(-1)} w^j + z\beta_k^{(-1)} w^k\right)\right)\right)\right) \\ & + z\beta_{v_{m-2}}^{(m-2)}\left(\cdots\left(\left(\sum_{j=0}^{k} \alpha_j^{(-1)} w^j + z\beta_k^{(0)} w^k + z\beta_{v_0}^{(0)}\left(\sum_{j=0}^{k} \alpha_j^{(-1)} w^j + z\beta_k^{(-1)} w^k\right)\right)\right)\right) \end{aligned} \tag{39}$$

while the resultant stability polynomial of the MMNHE (2) for the second hybrid predictor M_2 is given by

$$\Pi_2(w,z) = w^k - \sum_{j=0}^{k-1} \alpha_j^{(m)} w^j - z\left[\gamma_k^{(m)} w^k + \beta_{v_m}^{(m)}(R_2(w,z))\right] - z^2\left[\Omega_k^{(m)} w^k + \Omega_{v_m}^{(m)}(R_2(w,z))\right] \tag{40}$$

where

$$\begin{aligned} R_2(w,z) = & \sum_{j=0}^{k} \alpha_j^{(m-1)} w^j + z\beta_k^{(m-1)} w^k \\ & + z\beta_{v_{m-1}}^{(m-1)}\left(\cdots\left(\left(\sum_{j=0}^{k} \alpha_j^{(0)} w^j + z\beta_k^{(0)} w^k + z\beta_{v_0}^{(0)}\left(\sum_{j=0}^{k} \alpha_j^{(-1)} w^j + z\beta_k^{(-1)} w^k + z^2\lambda_k^{(-1)} w^k\right)\right)\right)\right) \\ & + z\beta_{v_{m-2}}^{(m-2)}\left(\cdots\left(\left(\sum_{j=0}^{k} \alpha_j^{(0)} w^j + z\beta_k^{(0)} w^k + z\beta_{v_0}^{(0)}\left(\sum_{j=0}^{k} \alpha_j^{(-1)} w^j + z\beta_k^{(-1)} w^k + z^2\lambda_k^{(-1)} w^k\right)\right)\right)\right) \end{aligned} \tag{41}$$

Definition 1. [13] The MMNHE (2) is zero stable if for a fixed value k, the roots $(w_j,\ j = 1(1)k)$ of the first characteristics polynomial $\rho(k, w)$ defined as

$$\rho(k, w) = w^k - \sum_{j=0}^{k-1} \alpha_j^{(m)} w^j \tag{42}$$

satisfies that $|w_j| \leq 1$, with the roots $|w_j| = 1$ being simple.

Definition 2. [13] The region of absolute stability of the MMNHE (2) is the set

$$\Psi = \{z \in C : |w_j| \leq 1, j = 1(1)k\}$$

that is; if the root of $w_j, j = 0(1)k$ of (38) are less or equal to one in absolute value, such that those of magnitude one are not repeated.

Definition 3. [13] The MMNHE (2) is A–stable if the region of absolute stability includes the entire left half of the z–plane $(i.e. z \in C^-)$.

Definition 4. [13] The MMNHE (2) is A(α)-stable for some $\alpha \in \left[0, \frac{\pi}{2}\right)$ if the wedge

$$S_\alpha = \{z : |Arg(-z)| < \alpha, z \neq 0\}$$

is contained in its region of absolute stability.

We are interested on the A-stable methods, we investigate the stability of MMNHE (2) whose stability polynomial is stated in (38) and (40) by the boundary locus. Using the first case of hybrid predictor (M_1), the MMNHE (2) is A–stable for $1 \leq k \leq 8$ and $A(89.5^0)$-stable for $k = 9$, but A-stable for $2 \leq k \leq 6$ when investigated with the second case of hybrid predictor (M_2) as shown in table 2. Due to the intensive computations involved, we are unable to proceed beyond $k = 9$, and therefore unable to ascertain at which k instability sets in in the method (2).

Table 2: Angle of absolute stability of the MMNHE

k	MMNHE case M_1	MMNHE case M_2
1	90^0	89^0
2	90^0	90^0
3	90^0	90^0
4	90^0	90^0
5	90^0	90^0
6	90^0	90^0
7	90^0	80^0
8	90^0	89.2^0
9	89.5^0	89.5^0

5 Implementation and Numerical Results

The implementation of the MMNHE derived is considered. In implementing the MMNHE, we are faced with solving a system of non-linear equations in y_{n+k}, in which we shall resolve by applying the Newton-Raphson scheme;

$$y_{n+k}^{[s+1]} = y_{n+k}^{[s]} - J(y_{n+k}^{[s]})^{-1} F(y_{n+k}^{[s]}) \tag{43}$$

where

$$F(y_{n+k}^{[s]}) = y_{n+k}^{[s]} - \left(\sum_{j=0}^{k-1} \alpha_j^{(m)} y_{n+j}^{[s]} + h\left(\gamma_k^{(m)} f_{n+k}^{[s]} + \beta_{v_m}^{(m)} f_{n+v_m}^{[s]}\right) + h^2\left(\Omega_k^{(m)} f_{n+k}^{'[s]} + \Omega_{v_m}^{(m)} f_{n+v_m}^{'[s]}\right)\right) \quad (44)$$

and $J(y_{n+k}^{[s]})$ is the Jacobian matrix obtained from (45), which is given as

$$J(y_{n+k}^{[s]}) = \frac{\partial}{\partial y} F(y_{n+k}^{[s]}) \quad (45)$$

Our starting values for (44) is obtained from the second derivative explicit Euler scheme [6]

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2} f'_n \quad (46)$$

The MMNHE of order $p = 4$ and the second derivative linear multistep method (SDLMM)[14] is implemented and compared with the results of the BDF (MATLAB ode15s) and exact solution where available on the following problems.
Problem 1 van der Pol equation [1].
The van der pol equation which describes oscillations in an electrical circuit.

$$\begin{aligned} y_1'(x) &= y_2(x) \qquad y_1(0) = 2 \\ y_2'(x) &= a(1 - y_1^2(x))y_2(x) - y_1(x) \qquad y_2(0) = 0 \\ x &\in [0, 20], \qquad h = 10^{-4}, \quad a = 1 \end{aligned} \quad (47)$$

Problem 2 Non-linear chemical problem [14].

$$\begin{aligned} y_1'(x) &= -0.04y_1(x) + 10^4 y_2(x)y_3(x), \qquad y_1(0) = 1 \\ y_2'(x) &= 0.04y_1(x) - 10^4 y_2(x)y_3(x) - 3 \times 10^7 y_2^2(x), \qquad y_2(0) = 0 \\ y_3'(x) &= 3 \times 10^7 y_2^2(x), \qquad y_3(0) = 0 \\ x &\in [0, 40], \qquad h = 10^{-4} \end{aligned} \quad (48)$$

Problem 3 Singularly perturbed equation [1]

$$\begin{aligned} y_1'(x) &= -(2 + \varepsilon^{-1})y_1(x) + \varepsilon^{-1} y_2^2(x), \qquad y_1(0) = 1; \qquad y_1(x) = e^{-2x} \\ y_2'(x) &= y_1(x) - y_2(x) - y_2^2(x) \qquad y_2(0) = 1; \qquad y_2(x) = e^{-x} \\ x &\in [0, 10], \qquad h = 10^{-4} \end{aligned} \quad (49)$$

For problem 3, we imbibe the idea in [13], to compute the error using

$$Error = \| y(x_n) - y_n(x_n) \|_\infty \quad (50)$$

where $y_n(x_n)$ is the numerical solution obtained from the numerical scheme and $y(x_n)$ the numerical solution obtained from the exact solution .

5.1 Discussion of Results

Tables 3 and 4 shows the approximate numerical solution from the MMNHE, SDLMM [14] and that of the MATLAB Ode15s, while table 5 shows the error in the numerical solution from the MMNHE and that of the SDLMM compared with the results from the exact solution.

Table 3: Numerical results of Problem 1

x		MMNHE (2)	SDLMM [14]	MATLAB ode15s
0.2	$y_1(x)$	1.966922636527705	1.966937033212862	1.966954166032711
	$y_2(x)$	-0.300829185414409	-0.300876321668260	-0.300727448286640
2.0	$y_1(x)$	0.323358626938811	0.323203828018920	0.323312913693448
	$y_2(x)$	-1.832721119550892	-1.833147369972204	-1.832662038505209
20	$y_1(x)$	2.008385577874732	2.008388075022751	2.008072699875731
	$y_2(x)$	-0.038632274297246	-0.041047755836553	-0.043863123302697

Table 4: Numerical results of Problem 2

x		MMNHE (2)	SDLMM [14]	MATLAB ode15s
0.4	$y_1(x)$	0.985168920970488	0.972298116295858	0.985171821837282
	$y_2(x)$	0.000033863360308	0.000031690250848	0.000033864951839
	$y_3(x)$	0.014797464322566	0.027670031451090	0.014794313210879
4.0	$y_1(x)$	0.905518114838754	0.858546586351834	0.905526382166127
	$y_2(x)$	0.000022404594026	0.000017663612186	0.000022405644091
	$y_3(x)$	0.094460479505148	0.141435324360984	0.094451212189781
40	$y_1(x)$	0.715827588832913	0.642274129390961	0.715871511601004
	$y_2(x)$	0.000009185527822	0.000006794711821	0.000009187066500
	$y_3(x)$	0.284164228672376	0.357718768279810	0.284119301332496

Table 5: Numerical results of Problem 3 at $x = 10$

ε	Error in MMNHE (2)	Error in SDLMM [14]
10^{-1}	1.9997999999999e-004	9.99754620069238e-001
10^{-2}	1.9997999999999e-004	9.99754620069238e-001
10^{-3}	1.9997999999999e-004	9.99754620069238e-001
10^{-4}	1.9997999999999e-004	9.99754620069238e-001

The result above, shows that the MMNHE has comparable accuracy with that of the SDLMM [14] for problem 1, but the MMNHE performs better than the SDLMM [14] for problem 2 and 3, however, the MMNHE has comparable accuracy with that of the MATLAB ode15s for problem 2 and 3.

6 CONCLUSION

Conclusively, in this paper, a family of second derivative multistep methods with nested hybrid evaluation is proposed. The stability of the method is investigated using the boundary locus and the results shows that the method is A-stable for $1 \leq k \leq 8$ using the first case of hybrid predictor and $2 \leq k \leq 6$ using the second case of hybrid predictor. The numerical schemes constructed was used to implement non-linear stiff problems alongside the SDLMM discussed in [14] and the MATLAB ode15s for Problems 1 and 2, and also compared with the exact solution of Problem 3. The results of the MMNHE shows that the method is comparable in accuracy with the exact solution and MATLAB ode15s.

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