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Hybrid Extended Backward Differentiation Formulas for Stiff Systems

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Abstract: In this paper we present details of a new class of hybrid methods which are based on backward differentiation formula (BDF) for the numerical solution of ordinary differential equations. In these methods, the first derivative of the solution in one super future point as well as in one off-step point is used to improve the absolute stability regions. The constructed methods are A(α)–stable up to order 9 so that, as it is shown in the numerical experiments, they are superior for stiff systems.

Keywords: stiff ODEs; multistep methods; hybrid methods; stability aspects

1 Introduction

The numerical integration of ordinary differential equations has been one of the principal concerns of numerical analysis. Many applications modeled by system of ordinary differential equations exhibit a behavior known as stiffness. Although there has been much controversy about the mathematical definition, simply we can say that the problem

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

on the finite interval $I = [x_0, x_N]$ where $y : [x_0, x_N] \to \mathbb{R}^m$ and $f : [x_0, x_N] \times \mathbb{R}^m \to \mathbb{R}^m$, is stiff if its Jacobian (in the neighborhood of the solution) has eigenvalues that verify $\frac{\max|Re\lambda_i|}{\min|Re\lambda_i|} >> 1$ (usually it is considered that $Re\lambda_i < 0$). A potentially good numerical method for the solution of stiff systems of ODEs must has good accuracy and some reasonably wide region of absolute stability [3]. The search for higher order A-stable multistep methods is carried out in the two main directions:

- use higher derivatives of the solutions,
- throw in additional stages, off-step points, super-future points and like.

This leads into the large field general linear methods [6].
Backward differentiation formulas (BDFs)

$$y_{n+k} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} = h\beta_k f_{n+k},$$

of order k are A-stable up to order 2.
Adaptive BDFs [5], blended methods of implicit and explicit BDF,

$$\sum_{j=0}^{k} (\alpha_j - t\bar{\alpha}_j) y_{n+j} = h\beta_k f_{n+k} - ht\bar{\beta}_k f_{n+k-1},$$

of order k, are A-stable up to order 3.
Extended backward differentiation formulas (EBDFs) [1]

$$y_{n+k} + \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} = h\hat{\beta}_k f_{n+k} + h\hat{\beta}_{k+1}\bar{f}_{n+k+1},$$

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of order $k+1$, which are A-stable up to order 4.
Hybrid BDF [4], where additional stage point (or off-step point) has been used in the first derivative of the solution to improve the absolute stability regions

$$y_{n+1}+\sum_{j=1}^{k}\alpha_{n+1-j}y_{n+1-j}=h\beta_s\bar{f}_{n+s}.$$

These methods are of order k and A-stable up to order 4.

Also numerous works have focused on more advanced methods like multistep methods which use second derivative of solution. For more details see [2, 6, 8, 9].

In this paper we introduce a modification of BDF which applies both off-step and one super-future point techniques. These methods, which we say Hybrid EBDF (HEBDF), have good stability properties so that they are effective and efficient for stiff ODEs.

This paper is organized as follows: Section 2 is devoted to the construction and the order of truncation error of presented methods. In section 3 stability analysis of the methods are discussed. In section 4 we give some numerical experiments to confirm the theoretical results.

2 Hybrid EBDF

Extended backward differentiation formulas (EBDFs) take the following general form

$$y_{n+k}+\sum_{j=0}^{k-1}\hat{\alpha}_j y_{n+j}=h\hat{\beta}_k f_{n+k}+h\hat{\beta}_{k+1}f_{n+k+1}, \tag{2}$$

where

$$f_{n+k}=f(x_{n+k},y_{n+k}),\quad f_{n+k+1}=f(x_{n+k+1},y_{n+k+1}),$$

and the coefficients are chosen so that (2) is of order $k+1$. For the coefficients of (2), see [1].

We are going to introduce HEBDFs. These methods are of the form of EBDF, where we reform its stages by adding a stage in which the first derivative of the solution in one off-step point $t_{n+k+s},\ \ 0<s<1$ is used. Also in the prediction of the solution in the super future point, we use the obtained first derivative of the solution in off-step point to improve stability region. Then EBDF is used to correct the value of y_{n+k}.

In practice for using (2), we need predictors for solution in the step point and off-step point. For prediction in the step point, we apply BDF [10] and for prediction of y_{n+k+s}, we introduce the k-step hybrid BDF (HBDF) as follows

$$y_{n+k+s}=h\mu f_{n+k}-\sum_{j=0}^{k-1}\eta_j y_{n+j}-\eta_k y_{n+k}, \tag{3}$$

where the coefficients are chosen so that (3) has order $k+1$. The coefficients of k-step methods of class (3) for some values of k are given in Table 1. We get the parameter $s\in(0,1)$ as a free parameter to find methods with largest absolute stability region.

Assuming that the solution values $y_n, y_{n+1},\dots,y_{n+k-1}$ are available, the way in which (2) is used in practice is by carry out the following computations:

Stage 1. Compute $\bar{y}_{n+k}$ as the solution of the k-step BDF

$$y_{n+k}=h\beta_k f_{n+k}-\sum_{j=0}^{k-1}\alpha_j y_{n+j}, \tag{4}$$

$$\text{Evaluate}\quad \bar{f}_{n+k}=f(x_{n+k},\bar{y}_{n+k}).$$

Stage 2. Compute $\bar{y}_{n+k+s}$ as the solution of k-step HBDF

$$y_{n+k+s}=h\mu\bar{f}_{n+k}-\sum_{j=0}^{k-1}\eta_j y_{n+j}-\eta_k\bar{y}_{n+k}, \tag{5}$$

$$\text{Evaluate}\quad \bar{f}_{n+k+s}=f(x_{n+k+s},\bar{y}_{n+k+s}).$$

Stage 3. Compute $\bar{y}_{n+k+1}$ (future point) as the solution of

$$y_{n+k+1} = h\bar{\beta}_k f_{n+k+1} + h\bar{\beta}_s f_{n+k+s} - \sum_{j=1}^{k} \bar{\alpha}_j y_{n+j}, \tag{6}$$

$$\text{Evaluate} \quad \bar{f}_{n+k+1} = f(x_{n+k+1}, \bar{y}_{n+k+1}).$$

The coefficients are chosen so that (6) has order $k+1$. These coefficients for some values of k are given in Table 2.

Stage 4. Correct y_{n+k} as the solution of

$$y_{n+k} + \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} = h\hat{\beta}_k f_{n+k} + h\hat{\beta}_{k+1} \bar{f}_{n+k+1}. \tag{7}$$

We note that in implementing stages 1, 3 and 4 to integrate a nonlinear initial value problem, it is necessary to solve a system of nonlinear algebraic equations for each of the required solutions $\bar{y}_{n+k}, \bar{y}_{n+k+1}$ and y_{n+k}. In each case, these algebraic equations are solved using a modified form of Newton *iterated to convergence*.

Table 1: Coefficients in HBDF (3)

k	4	6	8
μ	$\frac{2655739781}{2500000000}$	$\frac{78180547347}{102400000000}$	$\frac{83379706047}{640000000000}$
η_0	$\frac{273910381}{10000000000}$	$\frac{1436388009}{204800000000}$	$\frac{1029379087}{5120000000000}$
η_1	$-\frac{353075231}{1875000000}$	$-\frac{15343845741}{256000000000}$	$-\frac{1174362057}{560000000000}$
η_2	$\frac{1489805243}{2500000000}$	$\frac{18871166601}{81920000000}$	$\frac{3189387663}{320000000000}$
η_3	$-\frac{836739931}{625000000}$	$-\frac{2722705629}{5120000000}$	$-\frac{11444273379}{400000000000}$
η_4	$-\frac{115466947}{1200000000}$	$\frac{34931733921}{40960000000}$	$\frac{14235559569}{256000000000}$
η_5		$-\frac{60807092381}{51200000000}$	$-\frac{6275891853}{80000000000}$
η_6		$-\frac{636613028397}{2048000000000}$	$\frac{27793235349}{320000000000}$
η_7			$-\frac{7579973277}{80000000000}$
η_8			$-\frac{170011220629833}{179200000000000}$

Lemma 1 *Given that*
(i) formula (2) is of order $k+1$*,*
(ii) formula (4) is of order k*,*
(iii) formula (5) is of order $k+1$*,*
(iv) formula (6) is of order $k+1$*,*
the implicit algebraic equations defining $\bar{y}_{n+k}, \bar{y}_{n+k+1}$ *and* $\bar{y}_{n+k+s}$ *are solved exactly, then scheme (7) has order* $k+1$.

Proof. Suppose that the values $y_n, y_{n+1}, \cdots, y_{n+k-1}$ be exact. From (4) we have

$$y(x_{n+k}) - \bar{y}_{n+k} = C_1 h^{k+1} y^{(k+1)}(x_{n+k}) + O(h^{k+2}).$$

Also from (5) and if we suppose that $y(x_{n+k}) = y_{n+k}$, we have

$$y(x_{n+k+s}) - y_{n+k+s} = C_2 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}).$$

Table 2: Coefficients in HEBDF (6)

k	4	6	8
$\bar{\beta}_s$	$\frac{8000000}{10422303}$	$\frac{307200000000}{363267763651}$	$\frac{125440000000000}{81096283271999}$
$\bar{\beta}_k$	$\frac{8759012}{52111515}$	$\frac{76832537980}{363267763651}$	$\frac{20594196436520}{81096283271999}$
$\bar{\alpha}_1$	$\frac{29331}{17370505}$	$-\frac{165464170}{83831022381}$	$-\frac{290295371835}{81096283271999}$
$\bar{\alpha}_2$	$-\frac{278992}{17370505}$	$\frac{474175448}{27943674127}$	$\frac{3082162720320}{81096283271999}$
$\bar{\alpha}_3$	$\frac{1587492}{17370505}$	$-\frac{1831915275}{27943674127}$	$-\frac{15005174771440}{81096283271999}$
$\bar{\alpha}_4$	$-\frac{18708336}{17370505}$	$\frac{12630038800}{83831022381}$	$\frac{44582437037376}{81096283271999}$
$\bar{\alpha}_5$		$-\frac{6142498550}{27943674127}$	$-\frac{91405193688900}{81096283271999}$
$\bar{\alpha}_6$		$-\frac{24598293960}{27943674127}$	$\frac{141695479943360}{81096283271999}$
$\bar{\alpha}_7$			$-\frac{193878074995920}{81096283271999}$
$\bar{\alpha}_8$			$\frac{30122375855040}{81096283271999}$

But since in (5) we apply $\bar{y}_{n+k}$, we must add the errors of $y(x_{n+k}) - \bar{y}_{n+k}$ and $f(x_{n+k}, y(x_{n+k}) - f(x_{n+k}, \bar{y}_{n+k})$ to the above expression. Hence

$$\begin{aligned} y(x_{n+k+s}) - \bar{y}_{n+k+s} &= C_2 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}) + h\mu(f(x_{n+k}, y(x_{n+k}) - f(x_{n+k}, \bar{y}_{n+k})) \\ &\quad -\eta_k (y(x_{n+k}) - \bar{y}_{n+k}) \\ &= (h\mu \frac{\partial f}{\partial y}(\theta) - \eta_k)(C_1 h^{k+1} y^{(k+1)}(x_{n+k}) + O(h^{k+2})) \\ &\quad + C_2 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}) \\ &= -\eta_k C_1 h^{k+1} y^{(k+1)}(x_{n+k}) + O(h^{k+2}). \end{aligned}$$

Similarly, from (6) and if we suppose that $y(x_{n+k}) = y_{n+k}$ and $y(x_{n+k+s}) = y_{n+k+s}$, we have

$$y(x_{n+k+1}) - y_{n+k+1} = C_3 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}).$$

But considering the errors of $y(x_{n+k}) - \bar{y}_{n+k}$ and $f(x_{n+k+s}, y(x_{n+k+s}) - f(x_{n+k+s}, \bar{y}_{n+k+s})$ to the above expression, it leads to

$$y(x_{n+k+1}) - \bar{y}_{n+k+1} = -\bar{\alpha}_k C_1 h^{k+1} y^{(k+1)}(x_{n+k}) + O(h^{k+2}). \tag{8}$$

If now $C_4 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3})$ is the defect of formula (2), replacing $f(x_{n+k+1}, y(x_{n+k+1}))$ by $f(x_{n+k+1}, \bar{y}_{n+k+1})$ adds the expression obtained in (8) to this error and we obtain

$$\begin{aligned} y(x_{n+k}) - \bar{y}_{n+k} &= C_4 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}) + h\hat{\beta}_{k+1}(f(x_{n+k+1}, y(x_{n+k+1}) - f(x_{n+k+1}, \bar{y}_{n+k+1})) \\ &= C_4 h^{k+2} y^{(k+2)}(x_{n+k}) + O(h^{k+3}) + h\hat{\beta}_{k+1} \frac{\partial f}{\partial y}(\tau)(y(x_{n+k+1}) - \bar{y}_{n+k+1}) \\ &= h^{k+2}\big(C_4 y^{(k+2)}(x_{n+k}) - \bar{\alpha}_k \hat{\beta}_{k+1} C_1 \frac{\partial f}{\partial y}(\tau) y^{(k+1)}(x_{n+k})\big) + O(h^{k+3}), \end{aligned}$$

where τ is in $(y(x_{n+k+1}), \bar{y}_{n+k+1}))$. So the order of scheme (7) is $k+1$. ■

Table 3: The optimal values of s in HEBDF

k	1	2	3	4	5	6	7	8
s_{opt}	0.4	0.47	0.47	0.46	0.41	0.35	0.2	0.1

3 Stability Analysis

We now examine the stability behavior of our approach and determine the restrictions which we need to impose on the free parameter s to obtain highly stable methods. Applying (4) to Dalqusit's test equation $y' = \lambda y$, we get

$$y_{n+k} = -\sum_{j=0}^{k-1} \frac{\alpha_j}{z} y_{n+j}, \tag{9}$$

where $z = (1 - \bar{h}\beta_k), r = (1 - \bar{h}\bar{\beta}_k)$ and $\bar{h} = \lambda h$. From (5) and by substituting from (9), we obtain

$$y_{n+k+s} = \sum_{j=0}^{k-1} \frac{(\eta_k - \bar{h}\mu)\alpha_j - z\eta_j}{z} y_{n+j}. \tag{10}$$

Also if we apply (6) to the same scalar test equation and insert from (9) and (10), we get

$$y_{n+k+1} = \frac{\bar{h}\bar{\beta}_s((\eta_k - \bar{h}\mu)\alpha_0 - z\eta_0) + \bar{\alpha}_k\alpha_0}{zr} y_n - \sum_{j=1}^{k-1} \frac{\bar{h}\bar{\beta}_s((\eta_k - \bar{h}\mu)\alpha_j - z\eta_j) + \bar{\alpha}_k\alpha_j - \bar{\alpha}_j z}{zr} y_{n+j}. \tag{11}$$

Finally from (7) and by substituting (9), (10) and (11) we have

$$\sum_{j=0}^{k} C_j(\bar{h}) y_{n+j} = 0, \tag{12}$$

where

$$\begin{aligned}
C_0 &= \hat{\alpha}_0 zr - \bar{h}\hat{\beta}_{k+1}(\bar{h}\bar{\beta}_s((\eta_k - \bar{h}\mu)\alpha_0 - z\eta_0) + \bar{\alpha}_k\alpha_0), \\
C_j &= \hat{\alpha}_j zr - \bar{h}\hat{\beta}_{k+1}(\bar{h}\bar{\beta}_s((\eta_k - \bar{h}\mu)\alpha_j - z\eta_j) + \bar{\alpha}_k\alpha_j - \bar{\alpha}_j z), \quad j = 1, \cdots, k-1, \\
C_k &= (1 - \bar{h}\hat{\beta}_k) zr.
\end{aligned}$$

Therefore, corresponding characteristic equation of the k'th order difference equation of the HEBDF is

$$\pi(\xi, \bar{h}) = \sum_{j=0}^{k} C_j \xi^j = 0. \tag{13}$$

If in (13) we put $\bar{h} = \lambda h = 0$, then by a theorem of Schur [10], we conclude that HEBDF for some values of s, in the interval $0 < s < 1$, satisfies the root condition and so the method is zero-stable.

To obtain the region of absolute stability we use the boundary locus method [11]. By collecting coefficients of powers of $\bar{h}$ in (13), we have

$$A\bar{h}^3 + B\bar{h}^2 + C\bar{h} + D = 0, \tag{14}$$

where A, B, C, D are functions of ξ. Inserting $\xi = e^{i\theta}$, equation (14) gives us three roots $\bar{h}_i(\theta), i = 1, 2, 3$, which describe the stability domain.

The optimal values of s that conserve zero stability and give the largest absolute stability region are listed in Table 3. For these values of s, HEBDF is A-stable up to order 4 and A(α)–stable up to order 9. In Table 4 we tabulate a comparison in regions between HEBDF and the mentioned methods. It is seen that regions of A(α)-stability for our new methods are larger than those of the other mentioned methods.

Table 4: The comparison of A(α)-stability of HEBDF with other mentioned methods

k	BDF		EBDF		A-EBDF[7]		HBDF[4]		HEBDF	
	p	α	p	α	p	α_{max}	p	α_{max}	p	α_{max}
1	1	90	2	90	2	90	-	-	2	90
2	2	90	3	90	3	90	2	90	3	90
3	3	88	4	90	4	90	3	90	4	90
4	4	73	5	87.61	5	88.85	4	90	5	89.013
5	5	51	6	80.2	6	84.2	5	89.77	6	85.2
6	6	18	7	67.7	7	75	6	88.46	7	77.195
7	-	-	8	48.82	8	60.4	7	85.97	8	60.686
8	-	-	9	19.96	9	30.50	8	82.42	9	36.51

4 Numerical computations

In this section, we present some numerical results to compare the performance of our new methods HEBDF with that of EBDF [1] and HBDF [4].

Example 1 *Consider the stiff system:*

$$\begin{aligned} y_1' &= -y_1 - 30y_2 + 30e^{-x}, \\ y_2' &= 30y_1 - y_2 - 30e^{-x}, \end{aligned}$$

with initial value $y(0) = (1,1)^T$. *Its exact solution is* $y_1(x) = y_2(x) = e^{-x}$. *This system has eigenvalues of large modulus lying close to the imaginary axis* $-1 \pm 30i$. *We solve this problem by* 6*-step EBDF and HEBDF of order* 7, *and* 7*-step HBDF of order* 7, *with* $h = 0.002$. *We tabulate the results in Table 5. Also in Table 6, we compare the results of EBDF and HEBDF for* $k = 4$, $p = 5$ *with* $h = 0.01$.

Table 5: Absolute error of EBDF, HBDF and HEBDF for $h = 0.002$, $p = 7$ in Example 1.

x	y_i	Error in HEBDF ($k = 6, p = 7$)	Error in HBDF ($k = 7, p = 7$)	Error in EBDF $k = 6, p = 7$
0.04	y_1	4E-20	1.16E-14	4E-20
	y_2	1.81E-18	5.52E-15	1.81E-18
0.2	y_1	2.5E-19	2.77E-17	4.8E-19
	y_2	6.2E-19	5.55E-17	1.3E-19
2.0	y_1	2E-20	2.77E-17	4.3E-19
	y_2	3.8E-19	2.77E-17	4.7E-19

Table 6: Absolute error of EBDF and HEBDF for $h = 0.01$ with $k = 4$, $p = 5$ in Example 1.

x	y_i	Error in HEBDF	Error in EBDF
1.0	y_1	8.15E-15	1.71E-13
	y_2	8.48E-13	2.60E-12
10.0	y_1	9.83E-18	5.03E-17
	y_2	7.71E-17	3.36E-16
20.0	y_1	1.29E-21	1.17E-20
	y_2	2.79E-21	7.83E-21

Example 2 *Consider the nonlinear system*

$$\begin{aligned} y_1' &= -1002y_1 - 1000y_2^2, \\ y_2' &= y_1 - y_2(1 + y_2), \end{aligned}$$

with initial value $y(0) = (1, 1)^T$. The theoretical solution is $y_1(x) = e^{-2x}, y_2(x) = e^{-x}$. We integrate this system in $x \in [0, 5]$ by 6-step HEBDF and 7-step HBDF with $h = 0.005$, and report the results in Table 7. Also we integrate this system in $x \in [0, 30]$ by 8-step HEBDF with $h = 0.01$ and report the results in Table 8.

Table 7: Absolute error for 6-step HEBDF and 7-step HBDF with $h = 0.005$ in Example 2.

x	y_i	Error in HBDF	Error in HEBDF
0.4	y_1	1.30E-14	5.46E-17
	y_2	1.72E-12	4.05E-17
5.0	y_1	4.06E-20	7.08E-20
	y_2	8.67E-18	5.25E-18

Table 8: Absolute error for 8-step HEBDF with $h = 0.01$ in Example 2.

x	y_i	Exact Solution	Error in HEBDF
10.0	y_1	2.0611536224385578280E-9	3.88E-25
	y_2	4.5399929762484851536E-5	4.28E-21
20.0	y_1	4.2483542552915889953E-18	1.50E-33
	y_2	2.0611536224385578280E-9	3.65E-25
30.0	y_1	8.7565107626965203385E-27	6.78E-32
	y_2	9.3576229688401746049E-14	2.46E-29

Example 3 *Consider the system of differential equations:*

$$\begin{aligned} y_1' &= -20y_1 - 0.25y_2 - 19.75y_3, \\ y_2' &= 20y_1 - 20.25y_2 + 0.25y_3, \\ y_3' &= 20y_1 - 19.75y_2 - 0.25y_3, \end{aligned}$$

with initial value $y(0) = (1, 0, -1)^T$. *The theoretical solution is:*

$$\begin{aligned} y_1 &= \frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x)), \\ y_2 &= \frac{1}{2}(e^{-0.5x} - e^{-20x}(\cos(20x) - \sin(20x)), \\ y_3 &= -\frac{1}{2}(e^{-0.5x} + e^{-20x}(\cos(20x) - \sin(20x)). \end{aligned}$$

We integrate this system by 6*-step HEBDF with* $h = 0.01$ *and report the results in Table 9.*

Table 9: Absolute error for 6-step HEBDF in Example 3.

x	y_i	Exact solution	Error in HEBDF
	y_1	3.3689734995E-3	1.10E-19
10.0	y_2	3.3689734995E-3	1.11E-19
	y_3	-3.368973499E-3	1.12E-19
	y_1	2.2699964881E-5	1.51E-21
20.0	y_2	2.2699964881E-5	1.52E-21
	y_3	-2.2699964881E-5	1.53E-21
	y_1	1.52951160251E-7	1.55E-23
30.0	y_2	1.52951160251E-7	1.56E-23
	y_3	-1.52951160251E-7	1.56E-23

Example 4 *The following stiff initial value problem arose from a chemistry problem:*

$$\begin{aligned} y_1' &= -0.013y_2 - 1000y_1y_2 - 2500y_1y_3, \\ y_2' &= -0.013y_2 - 1000y_1y_2, \\ y_3' &= -2500y_1y_3, \end{aligned}$$

with initial value $y(0) = (0, 1, 1)^T$. *We solve this problem at* $x = 2$. *The results are tabulated in Table 10.*

Table 10: Absolute error for 4-step HEBDF with $h = 0.001$ in Example 4.

x	y_i	Exact Solution	Error in HEBDF
	y_1	-0.3616933169289E-5	1.53E-19
2.0	y_2	0.9815029948230	2.23E-14
	y_3	1.018493388244	1.91E-13

5 Conclusion

The introduced HEBDF is an extension of BDF and EBDF. These new methods, which are based on using of super future point and off-step point techniques, have good stability properties so that for special values of off-step parameter s, they are A(α)–stable up to order 9 and A-stable up to order 4. Although in comparison with the similar methods, the computational cost increases in HEBDFs, but they are often superior when high accuracy is requested for stiff systems.

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