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ON VARIABLE STEP L-STABLE GENERALIZED 5-STAGE DIRK SOLVERS OF ORDER 4 TO 9 FOR STIFF ODES

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Abstract. The ODE solvers HB of order 9 and 10 (T. Nguyen-Ba, T. Giordano and R. Vaillancourt, Variable-step 4-stage Hermite–Birkhoff solver of order 9 and 10 for stiff ODEs Acta Universitatis Apulensis (2015) 41:177–220) which combine k-step method and diagonally implicit Runge–Kutta method of order 3 is expanded into the variable-step (VS) L-stable 5-stage k-step Hermite–Birkhoff (HB) methods of order $p = (k+2)$, denoted by HB(p). These new methods are constructed as a combination of linear k-step methods of order $(p-3)$ and a two-step diagonally implicit 5-stage Runge–Kutta method of order 4 (TSDIRK4) for solving stiff ordinary differential equations. The main reason for considering this class of formulae is to obtain a set of methods which are L-stable and are suitable for the integration of stiff differential systems whose Jacobians have some large eigenvalues lying close to the imaginary axis. The approach, described in the present paper, allows us to develop L-stable methods of order up to 9 and $L(\alpha)$-stable methods of order up to 10 with $\alpha > 75°$. Selected L-stable HB(p) of order p, $p = 4, 5, \dots, 9$, compare favorably with existing Cash modified extended backward differentiation formulae, MEBDF(p), $p = 4, 5, \dots, 7$ in solving problems often used to test highly stable stiff ODE solvers.

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1. Introduction

Similar to Cash [4, 6], we expand the ODE solvers HB of order 9 and 10 developed in [22], which combine k-step method and diagonally implicit Runge–Kutta method of order 3, into the variable-step (VS) L-stable 5-stage k-step Hermite–Birkhoff (HB) methods of order $p = (k+2)$, denoted by HB(p), p, $p = 4, 5, \dots, 9$.

There is a variety of variable step (VS) methods designed to solve nonstiff and stiff systems of first-order differential equations (ODEs). Gear advocated a quasi-constant step size implementation in DIFSUB [14]. This software works with a constant step size until a change of step size is necessary or clearly advantageous. Then a continuous extension is used to get approximations to the solution at previous points in an equally spaced mesh. This was largely because constant mesh spacing is very helpful when solving stiff problems. Another possibility is fixed leading coefficient, which is seen in Petzold's popular code DASSL [24]. Finally, the actual mesh can be chosen by the code as done in MATLAB's `ode113`. This is the equivalent of a PECE Adams formula in contrast with the Adams–Moulton formula of DIFSUB and DASSL. In this paper, a fully variable step size implementation is used with actual mesh.

A more basic point about the implementation of a method is the choice of the form. The present method uses a generalized Lagrange form and much of the paper is devoted to computing the coefficients efficiently. Remark 2 in Subsection 6.4 connects the computation of coefficients for three well known forms: generalized Lagrange form, generalized Newton divided differences form (similar to Krogh's modified divided differences [19]) and Nordsieck form [23].

We shall be concerned with solving stiff systems of first-order ordinary differential equations of the form

$$y' = f(t,y), \qquad y(t_0) = y_0, \qquad \text{where} \quad {}' = \frac{d}{dt} \quad \text{and} \quad y \in \mathbb{R}^n. \tag{1}$$

A brief survey of methods for the numerical integration of (1) reveals that many of the advances in the class of general linear multistep methods for stiff ODEs, methods like extended backward differentiation formula (EBDF), modified extended backward differentiation formula (MEBDF), adaptive extended backward differentiation formula (AEBDF) and hybrid backward differentiation formula (HBDF) [4, 5, 8, 7, 17, 11], are based on backward differentiation formula (BDF). These methods are A-stable or $A(\alpha)$-stable. The first modification introduced by Cash [4] was the EBDF in which one superfuture point has been applied. D'Ambrosio, Izzo and Jackiewicz [10] further constructed recently perturbed modified extended backward differentiation formula (PMEBDF) and fully perturbed modified extended backward differentiation formula (FPMEBDF) methods which preserve the order of MEBDF methods and improve their stability property.

In this paper, methods with five off-step points are presented. A linear k-step method of order $p-3$ and a two-step diagonally implicit 5-stage Runge–Kutta method of order 4 (TSDIRK4) are cast into a k-step 5-stage Hermite–Birkhoff method of order $p = k+2$, named HB(p) because it uses Hermite–Birkhoff interpolation polynomials, for solving stiff ordinary differential equations (ODE) (1).

Here, the TSDIRK4 is defined in Section 2 with $p = 4$ and step number $k = 2$. This TSDIRK4 method is similar to the one-step diagonally implicit Runge–Kutta methods (DIRK) found in [1] except that the step number k equals 2 and, following the approach of Cash [4], the abscissae c_i are allowed to be $0 \leq c_i \leq 2$, $i = 3, 4, 5$.

Forcing a Taylor expansion of the numerical solution of HB(p) methods to agree with an expansion of the true solution leads to multistep and Runge–Kutta type order conditions which are reorganized into linear confluent Vandermonde-type systems. The solutions of these systems are obtained as generalized Lagrange basis functions by new fast algorithms. This approach allows us to develop L-stable methods of order up to 9 and $L(\alpha)$-stable methods of order up to 10 with $\alpha > 75°$. At the same time, we know well the difficulty of deriving multistep A-stable formulae of order greater than 2. A-stable linear multistep methods are limited to having maximum order 2 while high order, A-stable Runge-Kutta formulae can be very expensive to implement.

The extra stability of new L-stable HB(p), $p = 4, 5, \ldots, 9$ is particularly important when integrating an important class of stiff oscillatory problems, stiff differential systems whose Jacobians have some large eigenvalues lying close to the imaginary axis. Stiff oscillatory problems happen often in practice. In particular, they frequently develop when the method of lines technique is applied to a system of partial differential equations (PDE) that have some hyperbolic type of behaviour. Typical examples of such problems are the integro-differential equations describing the stiff beam problem [15], and advection-dominated PDE problems, as described, for example, in [16, 26]. A good description of the difficulties involved in integrating these hyperbolic type equations can be found in [15, pp. 12].

The selected L-stable HB(p), $p = 4, 5, \ldots, 9$ compare favorably with MEBDF(p), $p = 4, 5, \ldots, 7$, [4, 5] in solving stiff ODEs, representative of some problems mentioned above and often used to test highly stable stiff ODE solvers on the basis of the number of function evaluations (NFE) and the error at the endpoint of the interval of integration.

The paper is organized as follows: in Section 2, we introduce new general VS HB(p) methods of order p. Order conditions of general VS HB(p) are listed in Section 3. In Section 4, particular variable step HB(p) are defined by fixing a set of parameters and are represented in terms of Vandermonde-type systems. In Section 5, symbolic elementary matrices are constructed as functions of the parameters of the methods in view of factoring the coefficient matrices of Vandermonde-type systems. Fast solution of Vandermonde-type systems for particular variable step HB(p) is constructed in Section 6. Section 7 considers the regions of absolute stability of constant step HB(p), $p = 4, 5, \ldots, 10$. Section 8 deals with the step control. In Section 9, we compare the numerical performance of the methods considered in this paper. Appendix A lists the algorithms. Appendix B lists the coefficients of constant step HB(p) methods of order $p = 4, 5, \dots, 10$.

2. General variable step HB(p) of order p

Variable step 5-stage HB methods are constructed by the following formulae to perform integration from t_n to t_{n+1}.

Let h_{n+1} denote the step size. The abscissa vector $[c_1, c_2, \dots, c_6]^T$ defines the off-step points $t_n + c_j h_{n+1}$ with $c_1 = 0$ and $c_6 = 1$. Following the approach of Cash [4], c_i are allowed to be $0 \le c_i \le 2$, $i = 3, 4, 5$.

Let $F_1 = f_n$ and $F_j := f(t_n + c_j h_{n+1}, Y_j)$, $j = 2, 3, 4, 5$, denote the jth stage derivative.

With the initial stage value, $Y_1 = y_n$, HB polynomials of maximum degree $k+i-3$ are used as predictors P_i to obtain the stage values Y_i to at least order $p-3$,

$$Y_i = h_{n+1} a_{ii} f(t_n + c_i h_{n+1}, Y_i) + \sum_{j=0}^{p-3} \alpha_{ij} y_{n-j} + h_{n+1}\left[\sum_{j=2}^{i-1} a_{ij} F_j\right], \quad i = 2, 3, 4, 5. \tag{2}$$

An HB polynomial of degree $k+2$ is used as implicit integration formula IF to obtain y_{n+1} to order p,

$$y_{n+1} = h_{n+1} b_6 f(t_n + h_{n+1}, y_{n+1}) + \sum_{j=0}^{p-3} \alpha_j y_{n-j} + h_{n+1}\left[\sum_{j=3}^{5} b_j F_j\right]. \tag{3}$$

An HB polynomial of degree $k+2$ is used as implicit predictor P_6 to control the step size, h_{n+2}, and obtain $\widetilde{y}_{n+1}$ to order $p-1$,

$$\widetilde{y}_{n+1} = h_{n+1} a_{66} f(t_n + h_{n+1}, y_{n+1}) + \sum_{j=0}^{p-3} \alpha_{6j} y_{n-j} + h_{n+1}\left[\sum_{j=3}^{5} a_{6j} F_j\right]. \tag{4}$$

Here, the forms (2)–(3) are used by the implicit algebraic equations system defining Y_i, $i = 2, 3, 4, 5$ and y_{n+1} to handle implicitness in the context of stiffness.

The distinct implicit algebraic equations systems (2)–(3) defining Y_i, $i = 2, 3, 4, 5$ and y_{n+1} are solved sequentially (see Remark 1).

Remark 1. *Iteration schemes for formulae* (2)–(3)*:*

To obtain numerical results, for example, formulae (2) *are implemented with variable steps. The system of implicit algebraic equations* (2) *with a given i is solved* *iteratively by the modified Newton–Raphson method similar to the usual resolution of system of implicit algebraic equations of BDF method [20, p. 11–13]:*

$$J^0_{n+1}\left(Y_i^{l+1} - Y_i^l\right) = -Y_i^l + h_{n+1}a_{ii}f(t_n + c_ih, Y_i^l) + \sum_{j=0}^{p-3}\alpha_{ij}y_{n-j} + h_{n+1}\left[\sum_{j=2}^{i-1}a_{ij}F_j\right], \quad l = 0, 1, 2, \dots, \tag{5}$$

where the Jacobian J^0_{n+1} at iteration $l = 0$,

$$J^0_{n+1} = \left[I - ha_{22}\frac{\partial f(t_n + c_2h_{n+1}, Y_2^0)}{\partial y}\right], \tag{6}$$

computed at $t_n + c_2h_{n+1}$, generally, needs not to be updated for the whole step of integration from t_n to t_{n+1}. The iteration scheme for formula (3) *can be obtained similarly.*

The following terminology will be useful. An HB(p) method is said to be a *general* variable-step HB method if its backstep, off-step points and the coefficients

$$a_{22} = a_{33} = a_{44} = a_{55} = b_6, \tag{7}$$

in (2)–(3) are variable parameters. Hence, the general variable-step HB method has five degrees of freedom ($c_2, c_3, c_4, c_5, a_{22} = a_{33} = a_{44} = a_{55} = b_6$). If the off-step points and the coefficients in (7) are fixed, the method is said to be a *particular* variable-step method. If the step size is constant, and hence the backsteps, off-steps and the coefficients in (7) are fixed parameters, the method is said to be a *constant-step* method.

3. Order conditions of general HB(p)

To derive the order conditions of 5-stage ($p-2$)-step HB(p), we shall use the following expressions coming from the backsteps of the methods:

$$B_i(j) = \sum_{\ell=1}^{p-3}\alpha_{i\ell}\,\frac{\eta^j_{\ell+1}}{j!}, \qquad \begin{cases} i = 2, 3, 4, 5, \\ j = 1, 2, \dots, p, \end{cases} \tag{8}$$

and

$$\eta_j = -\frac{1}{h_{n+1}}\left(t_n - t_{n+1-j}\right) = -\frac{1}{h_{n+1}}\sum_{i=0}^{j-2}h_{n-i}, \qquad j = 2, 3, \dots, p-2. \tag{9}$$

In the sequel, η_j will be frequently used without explicit reference to (9).

Forcing an expansion of the numerical solution produced by formulae (2)–(3) to agree with the Taylor expansion of the true solution, we obtain multistep- and RK-type order conditions that must be satisfied by 5-stage HB(p) methods.

First, we need to satisfy the following set of multistep-type consistency conditions:

$$\sum_{j=0}^{p-3} \alpha_{ij} = 1, \qquad i = 2,3,4,5, \qquad \text{and} \qquad \sum_{j=0}^{p-3} \alpha_j = 1. \tag{10}$$

Second, to reduce a large number of RK-type order conditions (see [21]), we impose the following simplifying assumptions:

$$\sum_{j=2}^{i} a_{ij} c_j^k + k! B_i(k+1) = \frac{1}{k+1}\, c_i^{k+1}, \qquad \begin{cases} i = 2,3,4,5, \\ k = 0,1,\dots,p-4. \end{cases} \tag{11}$$

Thus, there remain only five sets of equations to be solved:

$$\sum_{i=2}^{6} b_i c_i^k + k! B(k+1) = \frac{1}{k+1}, \qquad k = 0,1,\dots,p-1, \tag{12}$$

$$\sum_{i=2}^{5} b_i \left[\sum_{j=2}^{i} a_{ij} \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + b_6 \frac{c_6^{p-2}}{(p-2)!} + B(p-1) = \frac{1}{(p-1)!}, \tag{13}$$

$$\sum_{i=2}^{5} b_i \frac{c_i}{p-1} \left[\sum_{j=2}^{i} a_{ij} \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + b_6 \frac{c_6^{p-1}}{(p-1)!} + B(p) = \frac{1}{p!}, \tag{14}$$

$$\sum_{i=2}^{5} b_i \left[\sum_{j=2}^{i} a_{ij} \frac{c_j^{p-2}}{(p-2)!} + B_i(p-1) \right] + b_6 \frac{c_6^{p-1}}{(p-1)!} + B(p) = \frac{1}{p!}, \tag{15}$$

$$\sum_{i=2}^{5} b_i \left[\sum_{j=2}^{i} a_{ij} \left(\sum_{k=2}^{j} a_{jk} \frac{c_k^{p-3}}{(p-3)!} + B_j(p-2) \right) + B_i(p-1) \right] + b_6 \frac{c_6^{p-1}}{(p-1)!} + B(p) = \frac{1}{p!}, \tag{16}$$

where the backstep parts, $B(j)$, are defined by

$$B(j) = \sum_{\ell=1}^{p-3} \alpha_\ell \frac{\eta_{\ell+1}^j}{j!}, \qquad j = 1,2,\dots,p+1. \tag{17}$$

These order conditions are simply RK order conditions with backstep parts $B_i(\cdot)$ and $B(\cdot)$.

4. Particular variable step HB(p)

4.1. Vandermonde-type formulation of particular L-stable HB(p)

The general HB(p) methods obtained in Section 3 contain free coefficients: c_i, $i = 2, 3, 4, 5$, coefficients in (7), and depend on h_{n+1} and the previous nodes, $t_n, t_{n-1}, \ldots, t_{n-(p-3)}$, which determine $\eta_2, \eta_3, \ldots, \eta_{p-2}$ in (9). To obtain A-stability of particular HB(p) methods, the coefficients listed in Table 1 were chosen. It is to be noted that, in Table 1, since $a_{22} = a_{33} = a_{44} = a_{55} = b_6$, only a_{22} values are listed.

Table 1: Coefficients c_i, $i = 2, 3, 4, 5$ and a_{22} of particular VS HB(p) $p = 4, 5, \ldots, 9$.

k	2	3	4
$c_i \backslash p$	4	5	6
c_2	1.0	1.0	1.0
c_3	9.509999999999998e-01	8.509999999999999e-01	9.509999999999998e-01
c_4	7.520000000000000e-01	9.520000000000000e-01	6.519999999999997e-01
c_5	9.030000000000004e-01	9.030000000000004e-01	8.530000000000003e-01
a_{22}	4.954545454545454554e-01	5.9545454545454557e-01	5.9545454545454546e-01
k	5	6	7
$c_i \backslash p$	7	8	9
c_2	1.0	9.500000000000000e-01	8.500000000000000e-01
c_3	1.201000000000000e+00	1.101000000000000e+00	1.751000000000000e+00
c_4	7.519999999999996e-01	1.652000000000000e+00	1.502000000000000e+00
c_5	9.530000000000004e-01	9.530000000000004e-01	9.530000000000004e-01
a_{22}	8.4545454545455279e-01	1.0954545454544657e+00	1.0454545454544011e+00

The remaining of this paper is concerned with particular VS HB(p) $p = 4, 5, \ldots, 9$, with coefficients c_i, $i = 2, 3, 4, 5$, and $a_{22} = a_{33} = a_{44} = a_{55} = b_6$ given in Table 1.

4.2. Integration formula IF

The $(p+1)$-vector of reordered coefficients of the integration formula IF in (3),

$$\boldsymbol{u}^1 = [\alpha_0, \alpha_1, \ldots, \alpha_{p-3}, b_5, b_4, b_3]^T,$$

is the solution of the Vandermonde-type system of order conditions

$$M^1 \boldsymbol{u}^1 = \boldsymbol{r}^1, \tag{18}$$

where

$$M^1 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 & 0 & 0 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 & 1 & 1 \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} & c_5 & c_4 & c_3 \\ \vdots & & & & & & & \vdots \\ 0 & \frac{\eta_2^p}{p!} & \frac{\eta_3^p}{p!} & \cdots & \frac{\eta_{p-2}^p}{p!} & \frac{c_5^{p-1}}{(p-1)!} & \frac{c_4^{p-1}}{(p-1)!} & \frac{c_3^{p-1}}{(p-1)!} \end{bmatrix}, \tag{19}$$

and $\boldsymbol{r}^1 = r_1(1 : p+1)$ has components

$$\begin{aligned} r_1(1) &= 1, \\ r_1(i) &= \frac{1}{(i-1)!} - b_6 \frac{c_6^{i-2}}{(i-2)!}, \qquad i = 2, 3, \ldots, p+1. \end{aligned}$$

The leading error term of IF is

$$\left[b_6 \frac{c_6^p}{p!} + \sum_{j=1}^{p-3} \alpha_j \frac{\eta_{j+1}^{p+1}}{(p+1)!} + \sum_{j=2}^{5} b_j \frac{c_j^p}{p!} - \frac{1}{(p+1)!} \right] h_{n+1}^{p+1} y_n^{p+1}.$$

4.3. Predictor P_2

The $(p-2)$-vector of reordered coefficients of the predictor P_2 in (2) with $i = 2$,

$$\boldsymbol{u}^2 = [\alpha_{20}, \alpha_{21}, \ldots, \alpha_{2,p-3}]^T,$$

is the solution of the Vandermonde-type system of order conditions

$$M^2 \boldsymbol{u}^2 = \boldsymbol{r}^2, \tag{20}$$

where

$$M^2 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} \\ \vdots & & & & \vdots \\ 0 & \frac{\eta_2^{p-3}}{(p-3)!} & \frac{\eta_3^{p-3}}{(p-3)!} & \cdots & \frac{\eta_{p-2}^{p-3}}{(p-3)!} \end{bmatrix}, \tag{21}$$

and $\boldsymbol{r}^2 = r_2(1 : p-2)$ has components

$$\begin{aligned} r_2(1) &= 1, \\ r_2(i) &= \frac{c_2^{i-1}}{(i-1)!} - a_{22} \frac{c_2^{i-2}}{(i-2)!}, \qquad i = 2, 3, \ldots, p-2. \end{aligned}$$

A truncated Taylor expansion of the right-hand side of (2) with $i = 2$ about t_n gives

$$\sum_{j=0}^{p+1} S(2,j) h_{n+1}^j y_n^{(j)}$$

with coefficients

$$\begin{aligned} S(2,j) &= a_{22} \frac{c_2^{j-1}}{(j-1)!} + M^2(j+1, 1:p-2)\boldsymbol{u}^2 \\ &= a_{22} \frac{c_2^{j-1}}{(j-1)!} + r_2(j+1) = \frac{c_2^j}{j!}, \qquad j = 1,2,\dots,p-3. \end{aligned}$$

We define

$$S(2,j) = a_{22} S(2,j-1) + \sum_{i=1}^{p-3} \alpha_{2i} \frac{\eta_{i+1}^j}{j!}, \qquad j = p-2, p-1, \tag{22}$$

$$S_{c^{p-2}}(2,p-1) = a_{22} c_2^{p-2} + \sum_{i=1}^{p-3} \alpha_{2i} \frac{\eta_{i+1}^{p-1}}{(p-1)!}. \tag{23}$$

Here, coefficient $S(2,j)$, $j = p-2, p-1$ and $S(i,j)$, $i = 3,4,5$, $j = p-2, p-1$, defined later, will be used in subsequent formulae to satisfy order conditions (13) and (16). Coefficient $S_{c^{p-2}}(2,p-1)$ and $S_{c^{p-2}}(i,p-1)$, $i = 3,4,5$, defined later, will be used to satisfy order condition (15). We note that P_2 is of order $p-3$ since it satisfies the order conditions

$$S(2,j) = c_2^j/j!, \qquad j = 0,1,\dots,p-3,$$

and its leading error term is

$$\left[S(2,p-2) - \frac{c_2^{p-2}}{(p-2)!} \right] h_{n+1}^{p-2} y_n^{(p-2)}.$$

4.4. Predictor P_3

We consider the $(p-1)$-vector of coefficients of the predictor P_3 in (2) with $i = 3$,

$$\boldsymbol{u}^3 = [\alpha_{30}, \alpha_{31}, \dots, \alpha_{3,p-3}, a_{32}]^T,$$

is the solution of the Vandermonde-type system of order conditions

$$M^3 \boldsymbol{u}^3 = \boldsymbol{r}^3, \tag{24}$$

where

$$M^3 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} & c_2 \\ 0 & \frac{\eta_2^3}{3!} & \frac{\eta_3^3}{3!} & \cdots & \frac{\eta_{p-2}^3}{3!} & \frac{c_2^2}{2!} \\ \vdots & & & & & \vdots \\ 0 & \frac{\eta_2^{p-2}}{(p-2)!} & \frac{\eta_3^{p-2}}{(p-2)!} & \cdots & \frac{\eta_{p-2}^{p-2}}{(p-2)!} & \frac{c_2^{p-3}}{(p-3)!} \end{bmatrix}. \tag{25}$$

The $(p-1)$ components of $\boldsymbol{r}^3 = r_3(1:p-1)$ are

$$\begin{aligned} r_3(1) &= 1, \\ r_3(i) &= \frac{c_3^{i-1}}{(i-1)!} - a_{33}\frac{c_3^{i-2}}{(i-2)!}, \qquad i = 2, 3, \dots, p-1. \end{aligned}$$

A truncated Taylor expansion of the right-hand side of (2), with $i = 3$, about t_n gives

$$\sum_{j=0}^{p+1} S(3,j) h_{n+1}^j y_n^{(j)}$$

with coefficients

$$\begin{aligned} S(3,j) &= a_{33}\frac{c_3^{j-1}}{(j-1)!} + M^3(j+1, 1:p-1)\boldsymbol{u}^3 \\ &= a_{33}\frac{c_3^{j-1}}{(j-1)!} + r_3(j+1) = \frac{c_3^j}{j!}, \qquad j = 1, 2, \dots, p-2. \end{aligned}$$

We define

$$\begin{aligned} S(3,j) &= a_{33}S(3,j-1) + a_{32}S(2,j-1) + \sum_{i=1}^{p-3} \alpha_{3i}\frac{\eta_{i+1}^j}{j!}, \qquad j = p-2, p-1, \\ S_{c^{p-2}}(3,p-1) &= a_{33}c_3^{p-2} + a_{32}c_2^{p-2} + \sum_{i=1}^{p-3} \alpha_{3i}\frac{\eta_{i+1}^{p-1}}{(p-1)!}, \end{aligned}$$

which will be used in subsequent formulae to satisfy order conditions (13), (15) and (16).

4.5. Predictor P_4

The $(p-1)$-vector of reordered coefficients of the predictor P_4 in (2) with $i=4$,

$$\boldsymbol{u}^4 = [\alpha_{40}, \alpha_{41}, \dots, \alpha_{4,p-3}, a_{43}]^T,$$

is the solution of the Vandermonde-type system of order conditions

$$M^4\boldsymbol{u}^4 = \boldsymbol{r}^4, \tag{26}$$

where

$$M^4 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} & c_3 \\ 0 & \frac{\eta_2^3}{3!} & \frac{\eta_3^3}{3!} & \cdots & \frac{\eta_{p-2}^3}{3!} & \frac{c_3^2}{2!} \\ \vdots & & & & & \vdots \\ 0 & \frac{\eta_2^{p-2}}{(p-2)!} & \frac{\eta_3^{p-2}}{(p-2)!} & \cdots & \frac{\eta_{p-2}^{p-2}}{(p-2)!} & \frac{c_3^{p-3}}{(p-3)!} \end{bmatrix}. \tag{27}$$

The $(p-1)$ components of $\boldsymbol{r}^4 = r_4(1:p-1)$ are

$$r_4(1) = 1,$$
$$r_4(i) = \frac{c_4^{i-1}}{(i-1)!} - a_{44}\frac{c_4^{i-2}}{(i-2)!}, \qquad i = 2, 3, \dots, p-1.$$

We define

$$S(4,j) = a_{44}\frac{c_4^{j-1}}{(j-1)!} + a_{43}\frac{c_3^{j-1}}{(j-1)!} + a_{42}\frac{c_2^{j-1}}{(j-1)!} + \sum_{i=1}^{p-3}\alpha_{4i}\frac{\eta_{i+1}^j}{j!} = \frac{c_4^j}{j!},$$
$$j = 1, 2, \dots, p-3,$$
$$S(4,j) = a_{44}S(4,j-1) + a_{43}S(3,j-1) + a_{42}S(2,j-1) + \sum_{i=1}^{p-3}\alpha_{4i}\frac{\eta_{i+1}^j}{j!},$$
$$j = p-2, p-1,$$
$$S_{c^{p-2}}(4,p-1) = a_{44}c_4^{p-2} + a_{43}c_3^{p-2} + a_{42}c_2^{p-2} + \sum_{i=1}^{p-3}\alpha_{4i}\frac{\eta_{i+1}^{p-1}}{(p-1)!},$$

which will be used in subsequent formulae.

4.6. Predictor P_5

The $(p+1)$-vector of reordered coefficients of the predictor P_5 in (2) with $i=5$,

$$\boldsymbol{u}^5 = [\alpha_{50}, \alpha_{51}, \dots, \alpha_{5,p-3}, a_{54}, a_{53}, a_{52}]^T,$$

is the solution of the Vandermonde-type system of order conditions

$$M^5 \boldsymbol{u}^5 = \boldsymbol{r}^5, \tag{28}$$

where

$$M^5 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 & 0 & 0 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 & 1 & 1 \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} & c_4 & c_3 & c_2 \\ 0 & \frac{\eta_2^3}{3!} & \frac{\eta_3^3}{3!} & \cdots & \frac{\eta_{p-2}^3}{3!} & \frac{c_4^2}{2!} & \frac{c_3^2}{2!} & \frac{c_2^2}{2!} \\ \vdots & & & & & & & \vdots \\ 0 & \frac{\eta_2^{p-1}}{(p-1)!} & \frac{\eta_3^{p-1}}{(p-1)!} & \cdots & \frac{\eta_{p-2}^{p-1}}{(p-1)!} & \frac{c_4^{p-2}}{(p-2)!} & \frac{c_3^{p-2}}{(p-2)!} & \frac{c_2^{p-2}}{(p-2)!} \\ 0 & \frac{\eta_2^{p-1}}{(p-1)!} & \frac{\eta_3^{p-1}}{(p-1)!} & \cdots & \frac{\eta_{p-2}^{p-1}}{(p-1)!} & S(4,p-2) & S(3,p-2) & S(2,p-2) \end{bmatrix}. \tag{29}$$

The first $(p-1)$ components of $\boldsymbol{r}^5 = r_5(1:p+1)$ are

$$r_5(1) = 1,$$
$$r_5(i) = \frac{c_5^{i-1}}{(i-1)!} - a_{55}\frac{c_5^{i-2}}{(i-2)!}, \qquad i = 2, 3, \ldots, p-1,$$

and the pth and $(p+1)$th component are

$$r_5(p) = S_{c^{p-2}}(5, p-1) - a_{55}\frac{c_5^{p-2}}{(p-2)!}, \tag{30}$$
$$r_5(p+1) = S(5, p-1) - a_{55}S(5, p-2), \tag{31}$$

where

$$S(5, j) = \frac{1}{b_5}\left[\frac{1}{(j+1)!} - b_2 S(2, j) - b_3 S(3, j) - b_4 S(4, j) - b_6\frac{c_6^j}{j!} - B(j+2)\right], \qquad j = p-2, p-1,$$

$$S_{c^{p-2}}(5, p-1) = \frac{1}{b_5}\left[\frac{1}{p!} - b_2 S_{c^{p-2}}(2, p-1) - b_3 S_{c^{p-2}}(3, p-1) - b_4 S_{c^{p-2}}(4, p-1) - b_6\frac{c_6^{p-1}}{(p-1)!} - B(p)\right].$$

Here $r_5(p)$ and $r_5(p+1)$ correspond to order conditions (15) and (16) respectively.

4.7. Step control predictor P_6

We consider the $(p+2)$-vector of the coefficients of predictor P_6 in (4),

$$\widetilde{\boldsymbol{u}}^6 = [a_{66}, \alpha_{60}, \alpha_{61}, \ldots, \alpha_{6,p-3}, a_{63}, a_{64}, a_{65}]^T.$$

By setting $a_{66} = b_6 + \omega_6$ and $a_{65} = b_5 + \omega_5$, $\widetilde{\boldsymbol{u}}^6$ reduces to the p-vector $\boldsymbol{u}^6$ which is the solution of the system of order conditions

$$M^6 \boldsymbol{u}^6 = \boldsymbol{r}^6, \tag{32}$$

where

$$M^6 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 & 0 \\ 0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 & 1 \\ 0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \cdots & \frac{\eta_{p-2}^2}{2!} & c_4 & c_3 \\ 0 & \frac{\eta_2^3}{3!} & \frac{\eta_3^3}{3!} & \cdots & \frac{\eta_{p-2}^3}{3!} & \frac{c_4^2}{2!} & \frac{c_3^2}{2!} \\ \vdots & & & & & & \vdots \\ 0 & \frac{\eta_2^{p-1}}{(p-1)!} & \frac{\eta_3^{p-1}}{(p-1)!} & \cdots & \frac{\eta_{p-2}^{p-1}}{(p-1)!} & \frac{c_4^{p-2}}{(p-2)!} & \frac{c_3^{p-2}}{(p-2)!} \end{bmatrix}, \tag{33}$$

and $\boldsymbol{r}^6 = r_6(1:p)$ has components

$$\begin{aligned} r_6(1) &= 1, \\ r_6(i) &= \frac{1}{(i-1)!} - (b_6+\omega_6)\frac{c_6^{i-2}}{(i-2)!} - (b_5+\omega_5)\frac{c_5^{i-2}}{(i-2)!}, \\ & \qquad\qquad\qquad\qquad\qquad\qquad i = 2, 3, \ldots, p. \end{aligned}$$

For arbitrary nonzero ω_5, P_6 yields $\widetilde{y}_{n+1}$ to order $(p-1)$. A good experimental choice is $\omega_6 = 0.025$ and $\omega_5 = 0.025$.

The solutions $\boldsymbol{u}^\ell$, $\ell = 1, 2, \ldots, 6$, form generalized Lagrange basis functions for representing the HB interpolation polynomials.

5. Symbolic construction of elementary matrix functions

Consider the matrices

$$M^\ell \in \mathbb{R}^{m_\ell \times m_\ell}, \qquad \ell = 1, 2, \ldots, 6, \tag{34}$$

of the Vandermonde-type systems (18), (20), (24), (26), (28) and (32), where

$$\begin{aligned} m_1 = p+1, \qquad m_2 = p-2, \qquad m_3 = p-1, \\ m_4 = p-1, \qquad m_5 = p+1, \qquad m_6 = p, \end{aligned} \tag{35}$$

and p is the order of the method.

The purpose of this section is to construct elementary lower and upper triangular matrices as symbolic functions of the parameters of HB(p). These matrices are most easily constructed by means of a symbolic software. These functions will be used in Section 6 to factor

- M^ℓ into a diagonal+last-3-column matrix, W_3^ℓ, $\ell = 1, 5$, which will be further diagonalized by a Gaussian elimination,
- M^2 into the identity matrix I^2,
- M^ℓ into a diagonal+last-1-column matrix, W_1^ℓ, $\ell = 3, 4$, which will be further diagonalized by a Gaussian elimination,
- M^6 into a diagonal+last-2-column matrix W_2^6, which will be further diagonalized by a Gaussian elimination.

This decomposition will lead to a fast solution of the systems $M^\ell \boldsymbol{u}^\ell = \boldsymbol{r}^\ell$, $\ell = 1, 2, \dots, 6$ in $\mathrm{O}(p^2)$ operations.

Since the Vandermonde-type matrices M^ℓ can be decomposed into the product of a diagonal matrix containing reciprocals of factorials and a confluent Vandermonde matrix, the factorizations used in this paper hold following the approach of Björck and Pereyra [3], Krogh [19], Galimberti and Pereyra [13] and Björck and Elfving [2]. Pivoting is not needed in this decomposition because of the special structure of Vandermonde-type matrices.

5.1. Symbolic construction of lower bidiagonal matrices for M^ℓ, $\ell = 1, 2, 3, 4, 6$

We first describe the zeroing process of a general vector $\boldsymbol{x} = [x_1, x_2, \dots, x_m]^T$ with no zero elements. The lower bidiagonal matrix

$$L_k = \begin{bmatrix} I_{k-1} & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & & 0 \\ 0 & -\tau_{k+1} & 1 & & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -\tau_m & 1 \end{bmatrix}, \tag{36}$$

defined by the multipliers $\tau_i = \frac{x_i}{x_{i-1}} = -L_k(i, i-1)$, $\quad i = k+1, k+2, \dots, m$, zeros the last $(m-k)$ components, $x_{k+1}, x_{k+2}, \dots, x_m$, of $\boldsymbol{x}$. This zeroing process will be applied recursively on M^ℓ, $\ell = 1, 2, 3, 4, 6$, as follows. For $k = 2, 3, \dots$, left multiplying $T_k^\ell = L_{k-1}^\ell L_{k-2}^\ell \cdots L_3^\ell L_2^\ell M^\ell$ by L_k^ℓ zeros the last $(m_\ell - k)$ components of the kth column of T_k^ℓ. Thus we obtain the upper triangular matrix

$$L^1 M^1 = L^1_{m_1-3} \cdots L^1_3 L^1_2 M^1, \tag{37}$$
$$L^\ell M^\ell = L^\ell_{m_\ell-1} \cdots L^\ell_3 L^\ell_2 M^\ell, \quad \ell = 2,3,4, \tag{38}$$
$$L^6 M^6 = L^6_{m_6-2} \cdots L^6_3 L^6_2 M^6, \tag{39}$$

in $(m_1 - 4)$, $(m_\ell - 2)$, $\ell = 2,3,4$ and $(m_6 - 3)$ steps respectively.

We note that L^ℓ does not change the first two rows of M^ℓ.

Process 1. At the kth step, starting with $k = 2$,

- $M^{\ell(k-1)} = L^\ell_{k-1} L^\ell_{k-2} \cdots L^\ell_2 M^\ell$ is an upper triangular matrix in columns 1 to $k-1$.
- The multipliers in L^ℓ_k are obtained from $M^{\ell(k-1)}(k+1 : m_\ell, k)$ since $M^\ell(i,k) \neq 0$ for $i = k+1, k+2, \dots, m_\ell$.

Algorithm 1 in Appendix A describes this process. The input is $M = M^\ell$; $m = m_\ell$. The output are $L_k = L^\ell_k$, $k = 2,3,\dots,k^\ell_{\text{end}}$, $\ell = 1,2,\dots,4,6$, where $k^1_{\text{end}} = m_1 - 3$, $k^\ell_{\text{end}} = m_\ell - 1$, $\ell = 2,3,4$ and $k^6_{\text{end}} = m_6 - 2$.

5.2. Symbolic construction of lower tridiagonal matrices for M^5

The symbolic construction of lower tridiagonal matrices for M^5 is as in Subsection 5.1 with the following changes. Since the column 2 to $p-2$ of M^5 have the following form, $\boldsymbol{x} = [x_1, x_2, \dots, x_{m-1}, x_m = x_{m-1}]^T$ with no zero elements and two last identical elements, the lower tridiagonal matrix L_k is as in (36) with the two last rows,

$$\begin{bmatrix} 0 & \cdots & 0 & -\tau_{m-1} & 1 & 0 \\ 0 & \cdots & 0 & -\tau_m & 0 & 1 \end{bmatrix}, \tag{40}$$

defined by the multipliers $\tau_{m-1} = \frac{x_{m-1}}{x_{m-2}} = -L_k(m-1, m-2)$ and $\tau_m = \frac{x_{m-1}}{x_{m-2}} = -L_k(m, m-2)$. The lower tridiagonal matrix L_k, so defined, zeros the last $(m-k)$ components, $x_{k+1}, x_{k+2}, \dots, x_m$, of $\boldsymbol{x}$.

We, thus, obtain the upper triangular matrix

$$L^5 M^5 = L^5_{m_5-3} \cdots L^5_3 L^5_2 M^5, \tag{41}$$

in $(m_5 - 4)$ steps.

Algorithm 2 in Appendix A describes this process. The input is $M = M^5$; $m = m_5$. The output are $L_k = L^5_k$, $k = 2,3,\dots,m_5 - 3$.

5.3. Symbolic construction of upper bidiagonal matrices for M^ℓ, $\ell = 1, 2, \dots, 6$

For matrix $L^\ell M^\ell$, $\ell = 1, 2, \dots, 6$, we construct recursively upper bidiagonal matrices $U_1^\ell, U_2^\ell \dots, U_{p-3}^\ell$ such that right multiplying $L^\ell M^\ell$ by the upper triangular matrix $U^\ell = U_1^\ell U_2^\ell \cdots U_{p-3}^\ell$ transforms $L^\ell M^\ell$ into a matrix $W_{\mathcal{C}_\ell}^\ell = L^\ell M^\ell U^\ell$ with nonzero diagonal elements, $W_{\mathcal{C}_\ell}^\ell(i,i) \neq 0$, $i = 1, 2, \dots, m_\ell$, the last $\mathcal{C}_\ell$ nonzero columns $W_{\mathcal{C}_\ell}^\ell(1 : m_\ell, j) \neq 0$, $j = m_\ell - \mathcal{C}_\ell + 1, m_\ell - \mathcal{C}_\ell + 2, \dots, m_\ell$, and zero elsewhere. We call such a matrix a "diagonal+last-$\mathcal{C}_\ell$-column matrix". Here

$$\mathcal{C}_\ell = 3, \text{ for } \ell = 1, 5, \qquad \mathcal{C}_2 = 0, \qquad \mathcal{C}_\ell = 1, \text{ for } \ell = 3, 4, \qquad \mathcal{C}_6 = 2. \tag{42}$$

We describe the zeroing process of the upper bidiagonal matrix U_k^ℓ on the two-row matrix $(L^\ell M^\ell)(k : k+1, 1 : m_\ell)$:

$$\begin{aligned}&(L^\ell M^\ell)(k : k+1, 1 : m_\ell) U_1^\ell U_2^\ell \cdots U_{k-1}^\ell \\ &= \begin{bmatrix} y_{k1} & \cdots & y_{k,k-1} & 1 & \cdots & 1 & y_{k,m_\ell-\mathcal{C}_\ell+1} & y_{k,m_\ell-\mathcal{C}_\ell+2} & \cdots & y_{k,m_\ell} \\ y_{k+1,1} & \cdots & y_{k+1,k-1} & y_{k+1,k} & \cdots & y_{k+1,m_\ell-\mathcal{C}_\ell} & y_{k+1,m_\ell-\mathcal{C}_\ell+1} & y_{k+1,m_\ell-\mathcal{C}_\ell+2} & \cdots & y_{k+1,m_\ell} \end{bmatrix}.\end{aligned} \tag{43}$$

The divisors $\sigma_i = \frac{1}{y_{k+1,i} - y_{k+1,i-1}} = U_k^\ell(i,i)$, $\quad i = k+1, k+2, \dots, m_\ell - \mathcal{C}_\ell$, define the upper bidiagonal matrix

$$U_k^\ell = \begin{bmatrix} I_{k-1} & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -\sigma_{k+1} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \sigma_{k+1} & -\sigma_{k+2} & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \ddots & \ddots & & \vdots & & & \vdots \\ 0 & 0 & 0 & \cdots & \sigma_{m_\ell-\mathcal{C}_\ell-1} & -\sigma_{m_\ell-\mathcal{C}_\ell} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & \sigma_{m_\ell-\mathcal{C}_\ell} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}. \tag{44}$$

Right multiplying (43) by U_k^ℓ zeros the 1's in position $k+1, k+2, \dots, m_\ell - \mathcal{C}_\ell$ in the first row and puts 1's in position $k+1, k+2, \dots, m_\ell - \mathcal{C}_\ell$ in the second row:

$$\begin{aligned}&(L^\ell M^\ell)(k : k+1, 1 : m_\ell) U_1^\ell U_2^\ell \cdots U_{k-1}^\ell U_k^\ell \\ &= \begin{bmatrix} y_{k1} & \cdots & y_{k,k-1} & 1 & 0 & \cdots & 0 & y_{k,m_\ell-\mathcal{C}_\ell+1} & y_{k,m_\ell-\mathcal{C}_\ell+2} & \cdots & y_{k,m_\ell} \\ y_{k+1,1} & \cdots & y_{k+1,k-1} & y_{k+1,k} & 1 & \cdots & 1 & y_{k+1,m_\ell-\mathcal{C}_\ell+1} & y_{k+1,m_\ell-\mathcal{C}_\ell+2} & \cdots & y_{k+1,m_\ell} \end{bmatrix}.\end{aligned} \tag{45}$$

Thus, $U^\ell = U_1^\ell U_2^\ell \cdots U_{p-3}^\ell$ transforms the upper triangular matrix $L^\ell M^\ell$ into the diagonal+last-$\mathcal{C}_\ell$-column matrix

$$W_{\mathcal{C}_\ell}^\ell = L^\ell M^\ell U_1^\ell U_2^\ell \cdots U_{p-3}^\ell, \tag{46}$$

in $(p-3)$ steps.

Process 2. At the kth step, starting with $k=1$,

- $M^{\ell(k)} = L^\ell M^\ell U_1^\ell U_2^\ell \cdots U_k^\ell$ is a diagonal+last-$\mathcal{C}_\ell$-column matrix in rows 1 to k.
- The divisors in U_k^ℓ are obtained from $M^{\ell(k-1)}(k+1, k : m_\ell - \mathcal{C}_\ell)$ since $M^{\ell(k-1)}(k+1, j) - M^{\ell(k-1)}(k+1, j-1) \neq 0$, $j = k+1, k+2, \dots, m_\ell - \mathcal{C}_\ell$.

Algorithm 3 in Appendix A describes this process for M^ℓ, $\ell = 1, 2, \dots, 6$. The input is $M = M^\ell$; $m = m_\ell$. The output is $U_k = U_k^\ell$, $k = 1, 2, \dots, p-3$.

6. Fast solution of Vandermonde-type systems for particular HB(p)

Symbolic elementary matrix functions L_k^ℓ and U_k^ℓ, $\ell = 1, 2, \dots, 6$, are constructed once as functions of η_j, for $j = 2, 3, \dots, p-2$, by Algorithms 1 to 3 in Appendix A to factor

- for $\ell = 1, 3, 4, 5, 6$, M^ℓ into a diagonal+last-$\mathcal{C}_\ell$-column matrix, $W_{\mathcal{C}_\ell}^\ell$ which will be further diagonalized by a Gaussian elimination,
- M^2 into the identity matrix I^2.

Here $\mathcal{C}_\ell$ is defined in (42).

These elementary matrix functions are used, first, to find the solution $\boldsymbol{u}^\ell$, $\ell = 1, 2, \dots, 6$ in elementary matrix functions form and, then, to construct fast Algorithms 4, 5, 6, 6, 4 and 7, in Appendix A, to solve systems (18), (20), (24), (26), (28), (32), respectively, at each integration step.

6.1. Solution of $M^\ell \boldsymbol{u}^\ell = \boldsymbol{r}^\ell$, $\ell = 1, 5$

We let $m_\ell = p+1$, $\ell = 1, 5$ as defined in (35).

(1) The elimination procedures of Subsections 5.1 and 5.2 are applied, respectively, to M^ℓ, $\ell = 1, 5$, to construct $m_\ell \times m_\ell$ lower tridiagonal matrices L_k^ℓ, $k = 2, 3, \dots, m_\ell - 3$, with multipliers
(1.a) for $\ell = 1$, $\tau_i = \frac{M^1(2,k)}{i-1} = -L_k^1(i, i-1)$, $\quad i = k+1, k+2, \dots, m_1$,
(1.b) for $\ell = 5$, $\tau_i = \frac{M^5(2,k)}{i-1} = -L_k^5(i, i-1)$, $\quad i = k+1, k+2, \dots, m_5 - 1$, and $\tau_{m_5} = \frac{M^5(2,k)}{m_5-2} = -L_k^5(m_5, m_5-2)$.
Left multiplying the coefficient matrix M^ℓ by the lower triangular matrix $L^\ell = L_{m_\ell-3}^\ell \cdots L_3^\ell L_2^\ell$ transforms M^ℓ into the upper triangular matrix $L^\ell M^\ell$ in column 1 to $m_\ell - 3$ of the form (37) and (41), respectively, for $\ell = 1, 5$.

(2) The elimination procedure of Subsection 5.3 is used to construct $m_\ell \times m_\ell$ upper bidiagonal matrices U_k^ℓ, $k = 1, 2, \dots, p-3$, with multipliers

$$\sigma_i = \frac{k}{M^\ell(2,i) - M^\ell(2,i-k)} = U_k^\ell(i,i), \qquad i = k+1, k+2, \dots, m_\ell - 3. \tag{47}$$

Right multiplying $L^\ell M^\ell$ by the upper triangular matrix $U^\ell = U_\ell^\ell U_2^\ell \cdots U_{p-3}^\ell$ transforms $L^\ell M^\ell$ into a diagonal+last-3-column matrix W_3^ℓ of the form (46).

(3) A factored Gaussian elimination, $L_{m_\ell-1}^\ell L_{m_\ell-2}^\ell$, will transform W_3^ℓ into a diagonal+last-2-column matrix $W_2^\ell = L_{m_\ell-1}^\ell L_{m_\ell-2}^\ell W_3^\ell$ as follows. First, $W_3^\ell(m_\ell - 2, m_\ell - 2)$ is set to 1 by the diagonal matrix $L_{m_\ell-2}^\ell$ whose entries are zeros, except for,

$$\begin{aligned} L_{m_\ell-2}^\ell(i,i) &= 1, \qquad i = 1, 2, \dots, m_\ell - 3, \\ L_{m_\ell-2}^\ell(m_\ell-2, m_\ell-2) &= 1/W_3^\ell(m_\ell-2, m_\ell-2), \\ L_{m_\ell-2}^\ell(i,i) &= 1, \qquad i = m_\ell - 1, m_\ell. \end{aligned}$$

Then the non-diagonal entries in the column $m_\ell - 2$ of $L_{m_\ell-2}^\ell W_3^\ell$ are zeroed by the unit diagonal+column-$(m_\ell - 2)$ matrix $L_{m_\ell-1}^\ell$ whose entries are zeros, except for,

$$\begin{aligned} L_{m_\ell-1}^\ell(i, m_\ell-2) &= -W_3^\ell(i, m_\ell-2), \qquad i = 1, 2, \dots, m_\ell - 3, \\ L_{m_\ell-1}^\ell(i,i) &= 1, \qquad i = 1, 2, \dots, m_\ell, \\ L_{m_\ell-1}^\ell(i, m_\ell-2) &= -W_3^\ell(i, m_\ell-2), \qquad i = m_\ell - 1, m_\ell. \end{aligned}$$

(4) Similarly, factored Gaussian eliminations, $L_{m_\ell+1}^\ell L_{m_\ell}^\ell$ and $L_{m_\ell+3}^\ell L_{m_\ell+2}^\ell$, will transform W_2^ℓ into the identity matrix

$$I^\ell = L_{m_\ell+3}^\ell L_{m_\ell+2}^\ell L_{m_\ell+1}^\ell L_{m_\ell}^\ell W_2^\ell,$$

where L_k^ℓ, $k = m_\ell, m_\ell+1, m_\ell+2, m_\ell+3$ have nonzero entries listed in Table 2 and zeros elsewhere. In Table 2, $W_2^\ell = L_{m_\ell-1}^\ell L_{m_\ell-2}^\ell W_3^\ell$, $W_\ell^\ell = L_{m_\ell+1}^\ell L_{m_\ell}^\ell W_2^\ell$.

We now obtain the following procedure which transforms M^ℓ into the identity matrix

$$I^\ell = L_{m_\ell+3}^\ell L_{m_\ell+2}^\ell \cdots L_2^\ell M^\ell U_\ell^\ell U_2^\ell \cdots U_{p-3}^\ell.$$

Thus we have the following factorization of M^ℓ into the product of elementary matrices:

$$M^\ell = \left(L_{m_\ell+3}^\ell L_{m_\ell+2}^\ell \cdots L_2^\ell\right)^{-1} \left(U_\ell^\ell U_2^\ell \cdots U_{p-3}^\ell\right)^{-1},$$

Table 2: The nonzero entries of Gaussian elimination matrices L^ℓ_k, $k = m_\ell - 2, m_\ell - 1, \dots, m_\ell + 3$ for $\ell = 1, 5$.

Gaussian elimination matrices	
$L^\ell_{m_\ell-2}$	$L^\ell_{m_\ell-1}$
$L^\ell_{m_\ell-2}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell - 3,$ $L^\ell_{m_\ell-2}(m_\ell - 2, m_\ell - 2) = 1/W^\ell_3(m_\ell - 2, m_\ell - 2),$ $L^\ell_{m_\ell-2}(i,i) = 1, \quad i = m_\ell - 1, m_\ell.$	$L^\ell_{m_\ell-1}(1 : m_\ell - 3, m_\ell - 2) = -W^\ell_3(1 : m_\ell - 3, m_\ell - 2),$ $L^\ell_{m_\ell-1}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell,$ $L^\ell_{m_\ell-1}(i, m_\ell - 2) = -W^\ell_3(i, m_\ell - 2), \quad i = m_\ell - 1, m_\ell.$
Gaussian elimination matrices	
$L^\ell_{m_\ell}$	$L^\ell_{m_\ell+1}$
$L^\ell_{m_\ell}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell - 2,$ $L^\ell_{m_\ell}(m_\ell - 1, m_\ell - 1) = 1/W^\ell_2(m_\ell - 1, m_\ell - 1),$ $L^\ell_{m_\ell}(m_\ell, m_\ell) = 1.$	$L^\ell_{m_\ell+1}(1 : m_\ell - 2, m_\ell - 1) = -W^\ell_2(1 : m_\ell - 2, m_\ell - 1),$ $L^\ell_{m_\ell+1}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell,$ $L^\ell_{m_\ell+1}(m_\ell, m_\ell - 1) = -W^\ell_2(m_\ell, m_\ell - 1).$
Gaussian elimination matrices	
$L^\ell_{m_\ell+2}$	$L^\ell_{m_\ell+3}$
$L^\ell_{m_\ell+2}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell - 1,$ $L^\ell_{m_\ell+2}(m_\ell, m_\ell) = 1/W^\ell_\ell(m_\ell, m_\ell).$	$L^\ell_{m_\ell+3}(i,i) = 1, \quad i = 1, 2, \dots, m_\ell,$ $L^\ell_{m_\ell+3}(1 : m_\ell - 1, m_\ell) = -W^\ell_\ell(1 : m_\ell - 1, m_\ell).$

and the solution is

$$\boldsymbol{u}^\ell = U^\ell_\ell U^\ell_2 \cdots U^\ell_{p-3} L^\ell_{m_\ell+3} L^\ell_{m_\ell+2} \cdots L^\ell_2 \, \boldsymbol{r}^\ell, \tag{48}$$

where fast computation goes from right to left.

Procedure (48) is implemented in Algorithm 4 in Appendix A in $O(m_\ell^2)$ operations. The input is $M = M^\ell$; $m = m_\ell$; $\boldsymbol{r} = \boldsymbol{r}^\ell$; $L_k = L^\ell_k$, $k = 2, 3, \dots, m_\ell + 3$; $U_k = U^\ell_k$, $k = 1, 2, \dots, p - 3$. The output is $\boldsymbol{u} = \boldsymbol{u}^\ell$, $\ell = 1, 5$.

It is to be noted that, by using Algorithm 3, the new $\sigma_i = \frac{k}{M^\ell(2,i) - M^\ell(2,i-k)} = U^\ell_k(i,i)$ in (47) is found for integration formula IF and P_5 instead of $\sigma_i = \frac{1}{M^\ell(2,i) - M^\ell(2,i-k)} = U^\ell_k(i,i)$ of the usual Newton divided differences. Similar result is found for predictor P_2, P_3, P_4 and P_6.

6.2. Solution of $M^2\boldsymbol{u}^2 = \boldsymbol{r}^2$

We let $m_2 = p - 2$ as defined in (35).

Similar to steps (1) and (2) of Subsection 6.1, the matrix $L^2 = L^2_{m_2-1}\cdots L^2_3 L^2_2$ transforms the coefficient matrix M^2 into the upper triangular matrix L^2M^2 in column 1 to $m_2 - 1$ of the form (38). Next, the right-product of the U^2_k, $k = 1, 2, \dots, p-3$, will transform L^2M^2 into the identity matrix I^2 of the form (46).

Thus we have the following factorization of M^2 into the product of elementary matrices:

$$M^2 = \left(L^2_{m_2-1}\cdots L^2_2\right)^{-1}\left(U^2_1U^2_2\cdots U^2_{p-3}\right)^{-1},$$

and the solution is

$$\boldsymbol{u}^2 = U^2_1U^2_2\cdots U^2_{p-3}L^2_{m_2-1}\cdots L^2_2\,\boldsymbol{r}^2, \tag{49}$$

where fast computation goes from right to left.

Procedure (49) is implemented in Algorithm 5 in Appendix A in $O(m_2^2)$ operations. The input is $M = M^2$; $m = m_2$; $\boldsymbol{r} = \boldsymbol{r}^2$; $L_k = L^2_k$, $k = 2, 3, \dots, m_2 - 1$; $U_k = U^2_k$, $k = 1, 2, \dots, p-3$. The output is $\boldsymbol{u} = \boldsymbol{u}^2$.

6.3. Solution of $M^\ell\boldsymbol{u}^\ell = \boldsymbol{r}^\ell$, $\ell = 3, 4$

We let $m_\ell = p - 1$, $\ell = 3, 4$ as defined in (35).

(1) Similar to steps (1) and (2) of Subsection 6.1, the matrix $L^\ell = L^\ell_{m_\ell-1}\cdots L^\ell_3L^\ell_2$ transforms the coefficient matrix M^ℓ into the upper triangular matrix $L^\ell M^\ell$ in column 1 to $m_\ell - 1$ of the form (38). Next, the right-product of the U^ℓ_k, $k = 1, 2, \dots, p-3$, will transform $L^\ell M^\ell$ into a diagonal+last-1-column matrix W^ℓ_1 of the form (46).

(3) Similar to steps (3) of Subsection 6.1, factored Gaussian eliminations, $L^\ell_{m_\ell+1}L^\ell_{m_\ell}$, will eliminate column m_ℓ of W^ℓ_1 and transform W^ℓ_1 into the identity matrix $I^\ell = L^\ell_{m_\ell+1}L^\ell_{m_\ell}W^\ell_1$ where L^ℓ_k, $k = m_\ell, m_\ell + 1$ have nonzero entries listed in Table 3 and zeros elsewhere.

This procedure transforms M^ℓ into the identity matrix

$$I^\ell = L^\ell_{m_\ell+1}L^\ell_{m_\ell}\cdots L^\ell_2M^\ell U^\ell_1U^\ell_2\cdots U^\ell_{p-3}.$$

Thus we have the following factorization of M^ℓ into the product of elementary matrices:

$$M^\ell = \left(L^\ell_{m_\ell+1}L^\ell_{m_\ell}\cdots L^\ell_2\right)^{-1}\left(U^\ell_1U^\ell_2\cdots U^\ell_{p-3}\right)^{-1},$$

Table 3: The nonzero entries of Gaussian elimination matrices L_k^ℓ, $k = m_\ell, m_\ell + 1$, $\ell = 3, 4$.

Gaussian elimination matrices	
$L_{m_\ell}^\ell$	$L_{m_\ell+1}^\ell$
$L_{m_\ell}^\ell(i,i) = 1, \quad i = 1, 2, \ldots, m_\ell - 1$ $L_{m_\ell}^\ell(m_\ell, m_\ell) = 1/W^\ell(m_\ell, m_\ell)$	$L_{m_\ell+1}^\ell(i,i) = 1, \quad i = 1, 2, \ldots, m_\ell$ $L_{m_\ell+1}^\ell(1 : m_\ell - 1, m_\ell) = -W^\ell(1 : m_\ell - 1, m_\ell)$

and the solution is

$$\boldsymbol{u}^\ell = U_1^\ell U_2^\ell \cdots U_{p-3}^\ell L_{m_\ell+1}^\ell L_{m_\ell}^\ell \cdots L_2^\ell \, \boldsymbol{r}^\ell, \tag{50}$$

where fast computation goes from right to left.

Procedure (50) is implemented in Algorithm 6 in Appendix A in $O(m_\ell^2)$ operations, $\ell = 3, 4$. The input is $M = M^\ell$; $m = m_\ell$; $\boldsymbol{r} = \boldsymbol{r}^\ell$; $L_k = L_k^\ell$, $k = 2, 3, \ldots, m_\ell+1$; $U_k = U_k^\ell$, $k = 1, 2, \ldots, p-3$. The output is $\boldsymbol{u} = \boldsymbol{u}^\ell$, $\ell = 3, 4$.

6.4. Solution of $M^6\boldsymbol{u}^6 = \boldsymbol{r}^6$

We let $m_6 = p + 1$ as defined in (35).

(1) Similar to steps (1) and (2) of Subsection 6.1, the matrix $L^6 = L_{m_6-2}^6 \cdots L_3^6 L_2^6$ transforms the coefficient matrix M^6 into an upper triangular matrix $L^6 M^6$ in columns 1 to $m_6 - 2$ of the form (39). Next, right multiplying $L^6 M^6$ by the upper triangular matrix $U_1^6 U_2^6 \cdots U_{p-3}^6$, will transform $L^6 M^6$ into a diagonal+last-2-column matrix W_2^6 of the form (46).

(3) Similar to steps (3) and (4) of Subsection 6.1, factored Gaussian eliminations, $L_{m_6}^6 L_{m_6-1}^6$, $L_{m_6+2}^6 L_{m_6+1}^6$ will eliminate columns (m_6-1) and (m_6) respectively of W_2^6 and transform W_2^6 into the identity matrix

$$I^6 = L_{m_6+2}^6 L_{m_6+1}^6 L_{m_6}^6 L_{m_6-1}^6 W_2^6,$$

where L_k^6, $k = m_6 - 1, m_6, m_6 + 1, m_6 + 2$ have nonzero entries listed in Table 4 and zeros elsewhere. In Table 4, $W_1^6 = L_{m_6}^6 L_{m_6-1}^6 W_2^6$.

We now obtain the following procedure which transforms M^6 into the identity matrix:

$$I^6 = L_{m_6+2}^6 L_{m_6+1}^6 \cdots L_2^6 M^6 U_1^6 U_2^6 \cdots U_{p-3}^6.$$

Table 4: The nonzero entries of Gaussian elimination matrices L_k^6, $k = m_6 - 1, m_6, m_6+1, m_6+2$.

Gaussian elimination matrices	
$L^6_{m_6-1}$	$L^6_{m_6}$
$L^6_{m_6-1}(i,i) = 1, \quad i = 1,2,\dots,m_6-2,$ $L^6_{m_6-1}(m_6-1,m_6-1) = 1/W^6_2(m_6-1,m_6-1),$ $L^6_{m_6-1}(m_6,m_6) = 1.$	$L^6_{m_6}(1:m_6-2,m_6-1) = -W^6_2(1:m_6-2,m_6-1),$ $L^6_{m_6}(i,i) = 1, \quad i = 1,2,\dots,m_6,$ $L^6_{m_6}(m_6,m_6-1) = -W^6_2(m_6,m_6-1).$
Gaussian elimination matrices	
$L^6_{m_6+1}$	$L^6_{m_6+2}$
$L^6_{m_6+1}(i,i) = 1, \quad i = 1,2,\dots,m_6-1,$ $L^6_{m_6+1}(m_6,m_6) = 1/W^6_1(m_6,m_6).$	$L^6_{m_6+2}(i,i) = 1, \quad i = 1,2,\dots,m_6,$ $L^6_{m_6+2}(1:m_6-1,m_6) = -W^6_1(1:m_6-1,m_6).$

Thus we have the following factorization of M^6 into the product of elementary matrices:

$$M^6 = \left(L^6_{m_6+2}L^6_{m_6+1}\cdots L^6_2\right)^{-1}\left(U^6_1U^6_2\cdots U^6_{p-3}\right)^{-1},$$

and the solution is

$$\boldsymbol{u}^6 = U^6_1U^6_2\cdots U^6_{p-3}L^6_{m_6+2}L^6_{m_6+1}\cdots L^6_2\,\boldsymbol{r}^6, \tag{51}$$

where fast computation goes from right to left.

Procedure (51) is implemented in Algorithm 7 in Appendix A in $O(m_6^2)$ operations. The input is $M = M^6$; $m = m_6$; $\boldsymbol{r} = \boldsymbol{r}^6$; $L_k = L^6_k$, $k = 2,3,\dots,m_6+2$; $U_k = U^6_k$, $k = 1,2,\dots,p-3$. The output is $\boldsymbol{u} = \boldsymbol{u}^6$.

Remark 2. *Formulae* (2)–(4) *can be put in matrix form. For instance,* (3) *can be written as*

$$y_{n+1} = F^1.\boldsymbol{u}^1 + G^1.\boldsymbol{v}^1$$

where

$$F^1 = \Big[y_n, y_{n-1},\dots,y_{n-(p-3)}, h_{n+1}F_5, h_{n+1}F_4, h_{n+1}F_3\Big],$$
$$G^1 = \Big[h_{n+1}f(t_n+h, y_{n+1})\Big],$$

$$\begin{aligned}\boldsymbol{u}^1 &= [\alpha_0, \alpha_1, \dots, \alpha_{p-3}, b_5, b_4, b_3]^T,\\ \boldsymbol{v}^1 &= [b_6].\end{aligned}$$

It is interesting to note the three decomposition forms of the system $F\boldsymbol{u}$:

$$\begin{aligned}&F(UL\boldsymbol{r}) && (\textit{generalized Lagrange interpolation}),\\ &(FU)L\boldsymbol{r} && (\textit{generalized divided differences}),\\ &(FUL)\boldsymbol{r} && (\textit{Nordsieck's formulation}).\end{aligned}$$

The first form is used in this paper, the form similar to the second form for Vandermonde systems is found in [19], and the third form is found in [23].

7. Regions of absolute stability

The regions $\mathcal{R}$ of constant step HB(p), $p = 4, 5, \dots, 10$, listed in Appendix B, are obtained by applying formulae (2)–(3) of the predictors P_i, $i = 2, 3, 4, 5$ and the integration formula IF with constant h to the linear test equation

$$y' = \lambda y, \qquad y_0 = 1.$$

This gives the following difference equation and corresponding characteristic equation

$$\sum_{j=0}^{k} \eta_j(z)\, y_{n+j} = 0, \qquad \sum_{j=0}^{k} \eta_j(z)\, r^j = 0, \tag{52}$$

respectively, where $k = p - 2$ is the number of steps of the method and $z = \lambda h$. A complex number z is in $\mathcal{R}$ if the k roots of the characteristic equation in (52) satisfy the root condition (see [20, pp. 70]).

The scanning method used to find $\mathcal{R}$ is similar to the one used for Runge–Kutta methods (see [20]).

The stability functions $\eta_j(z)$, $j = 0, 1, \dots, k$ in (52) are rational functions of the form

$$\eta_k(z) = 1, \qquad \eta_j(z) = \frac{\sum_{\ell=0}^{4} n_{j\ell} z^\ell}{\sum_{\ell=0}^{5} d_{j\ell} z^\ell}, \qquad j = 0, 1, \dots, k - 1.$$

Hence, in the difference equation of (52), $y_{n+k} \to 0$ as $z \to \infty$. This implies that HB(p), $p = 4, 5, \dots, 10$ are L-stable or $L(\alpha)$-stable according to whether these methods are A-stable or $A(\alpha)$-stable, respectively.

Table 5: For each given step number k, the table lists the order p, the α angles of $A(\alpha)$-stability for HB(p), FPMEBDF(p), PMEBDF(p), HBDF(p) and MEBDF(p), respectively.

HB(p)			FPMEBDF(p)			PMEBDF(p)			HBDF(p)			MEBDF(p)		
k	p	α	k	p	α	k	p	α	k	p	α	k	p	α
			1	2	90.00°	1	2	90.00°	2	2	90.00°	1	2	90.00°
			2	3	90.00°	2	3	90.00°	3	3	90.00°	2	3	90.00°
2	4	90.00°	3	4	90.00°	3	4	90.00°	4	4	90.00°	3	4	90.00°
3	5	90.00°	4	5	89.71°	4	5	89.32°	5	5	89.77°	4	5	88.36°
4	6	90.00°	5	6	88.01°	5	6	86.19°	6	6	88.46°	5	6	83.07°
5	7	90.00°	6	7	84.67°	6	7	80.60°	7	7	85.97°	6	7	74.48°
6	8	90.00°	7	8	78.70°	7	8	72.63°	8	8	82.42°	7	8	61.98°
7	9	90.00°	8	9	65.01°	8	9	60.60°	9	9	77.75°	8	9	42.87°
8	10	75.38°							10	10	70.18°			
									11	11	58.96°			
									12	12	46.12°			

Table 5 lists the α angles of $A(\alpha)$-stability of HB(4–10), FPMEBDF(2–9), PMEBDF(2–9) [10], HBDF(2–12) [11] and MEBDF(2–9) [15, p. 270], respectively. It is seen that, generally, α of HB methods compare favorably with α of the considered methods of the same order.

8. Controlling step size

The estimate $\|y_n - \widetilde{y}_n\|_\infty$ and the current step h_n are used to calculate the next step size h_{n+1} by means of formula [18]

$$h_{n+1} = \min\left\{ h_{\max}, \beta\, h_n \left[\frac{\text{tolerance}}{\|y_n - \widetilde{y}_n\|_\infty}\right]^{1/\kappa}, 4\, h_n \right\}, \tag{53}$$

with $\kappa = p$ and safety factor $\beta = 0.81$.

The procedure to advance integration from t_n to t_{n+1} is as follows.

(a) The step size, h_{n+1}, is obtained by formula (53).

(b) The numbers $\eta_2, \eta_3, \dots, \eta_{p-2}$, defined in (9), are calculated.

(c) The coefficients of integration formula IF, predictors P_2, P_3, P_4, P_5 and step control predictor P_6 are obtained successively as solutions of systems (18), (20), (24), (26), (28) and (32).

(d) The values Y_2, Y_3, Y_4, Y_5, y_{n+1}, and $\widetilde{y}_{n+1}$ are obtained by formulae (2)–(4).

(e) The step is accepted if $\|y_{n+1} - \widetilde{y}_{n+1}\|_\infty$ is smaller than the chosen tolerance and the program goes to (a) with n replaced by $n+1$. Otherwise the program returns to (a) and a new smaller step size h_{n+1} is computed.

9. Numerical results

The *error at the endpoint of the integration interval* (EPE, endpoint error) is taken in the uniform norm,

$$\mathrm{EPE} = \{\|y_{\mathrm{end}} - z_{\mathrm{end}}\|_\infty\},$$

where y_{end} is the numerical value obtained by the numerical method at the endpoint t_{end} of the integration interval and z_{end} is the "exact solution" obtained by MATLAB's `ode15s` with stringent tolerance 5×10^{-14}.

The necessary starting values at $t_1, t_2, \dots, t_{k-1}$ for HB(p) were obtained by MATLAB's `ode15s` with stringent tolerance 5×10^{-14}.

Computations were performed on a PC with the following characteristics: Memory: 5.8 GB, Processor 0,1,...,7: Intel(R) Core(TM) i7 CPU 920 @ 2.67GHz, Operating system: Ubuntu Release 11.04, Kernel Linux 2.6.38-12-generic, GNOME 2.32.1.

We consider the following test problems. Problem 1 is representative of some stiff oscillatory problems which arise frequently in practice. In particular, they often arise when the method of lines technique is applied to a system of partial differential equations that have some hyperbolic type of behaviour. We have chosen Problems 1 and 2 where the eigenvalues of the Jacobian matrix lie close to the imaginary axis, since it is problems of this type that cause major difficulties to many existing codes. And new L-stable HB(p), $p = 4, 5, \dots, 9$ are suitable for such problems.

(1) The stiff DETEST problem B5 [12].

Problem 1.

$$\begin{aligned} y_1' &= -10y_1 + \alpha y_2, & y_1(0) &= 1,\\ y_2' &= -\alpha y_1 - 10y_2 & y_2(0) &= 1,\\ y_3' &= -4y_3 & y_3(0) &= 1,\\ y_4' &= -y_4 & y_4(0) &= 1,\\ y_5' &= -0.5y_5 & y_5(0) &= 1,\\ y_6' &= -0.1y_6 & y_6(0) &= 1, \end{aligned} \tag{54}$$

with $\alpha = 500$ and $t_{\mathrm{end}} = 20$.

(2) As above with $\alpha = 1000$.

(3) A problem with large eigenvalues lying close to the imaginary axis [6].

Problem 2.

$$\begin{aligned} y_1' &= -\alpha y_1 - \beta y_2 + (\alpha+\beta-1)e^{-t} & y_1(0) &= 1, \\ y_2' &= \beta y_1 - \alpha y_2 + (\alpha-\beta-1)e^{-t} & y_2(0) &= 1, \\ y_3' &= 1 & y_3(0) &= 0, \end{aligned} \tag{55}$$

with $\alpha = 2.5$, $\beta = 60$, fixed step $h = 0.025$ and $t_{\text{end}} = 20$. The exact solution is

$$y_1(t) = y_2(t) = e^{-t}, \quad y_3(t) = t.$$

(4) As above with $\alpha = 0.5$ and $\beta = 60$.

9.1. Comparing NFE of L-stable HB(p), $p = 8, 9$ and MEBDF(p), $p = 4, 7$

In our first tests, we numerically compare our new methods with MEBDF(p), $p = 4, 7$, on the basis of the endpoint error (EPE) as a function of the number of function evaluations (NFE). These classical MEBDF(p) methods have been widely used in solving stiff ODEs. Their main merit is high efficiency. For this comparison, similar to Cash [9], we use Problem 1.

Table 6 and 7 list the number of function evaluations (NFE) as a function of endpoint errors (EPE) of HB(p), $p = 8, 9$ and MEBDF(p), $p = 4, 7$ for stiff DETEST problem B5 with $\alpha = 500$ and $\alpha = 1000$, respectively.

It is seen that, in general, HB(p), $p = 8, 9$, compare favorably with MEBDF(p), $p = 4, 7$, at all tolerances.

The *NFE percentage efficiency gain* (NFE PEG) is defined by the formula (cf. Sharp [25]),

$$(\text{NFE PEG})_i = 100 \left[\frac{\sum_j \text{NFE}_{2,ij}}{\sum_j \text{NFE}_{1,ij}} - 1 \right], \tag{56}$$

where $\text{NFE}_{1,ij}$ and $\text{NFE}_{2,ij}$ are the estimates of NFE of methods 1 and 2, respectively, associated with problem i, and estimate of EPE $= 10^{-j}$. To compute $\text{NFE}_{2,j}$ and $\text{NFE}_{1,j}$ appearing in (56), we approximate the data $(\log_{10}(\text{EPE}), \log_{10}(\text{NFE}))$ in a least-squares sense by MATLAB's `polyfit`. Then, for chosen integer values of the summation index j, we take $-\log_{10}(\text{EPE estimate}) = j$ and obtain $\log_{10}(\text{NFE estimate})$ from the approximating curve, and finally the estimate of NFE.

Table 8 lists the NFE PEG of HB(p), $p = 8, 9$, over MEBDF(p), $p = 4, 7$, for the listed problems. It is seen that HB(p), $p = 8, 9$, win.

Table 6: Number of function evaluations (NFE) as a function of endpoint errors (EPE) of HB(p), $p = 8, 9$ and MEBDF(p), $p = 4, 7$ for stiff DETEST problem B5 with $\alpha = 500$.

	NFE in		NFE in	
endpoint errors	HB(8)	HB(9)	MEBDF(4)	MEBDF(7)
4.87e-05	0.05e+05	0.07e+05	0.08e+05	1.05e+05
4.19e-06	0.14e+05	0.11e+05	0.17e+05	1.13e+05
3.80e-07	0.21e+05	0.17e+05	0.32e+05	1.21e+05
5.07e-08	0.30e+05	0.24e+05	0.55e+05	1.28e+05
5.92e-09	0.42e+05	0.34e+05	0.99e+05	1.36e+05
5.47e-10	0.58e+05	0.51e+05	1.89e+05	1.46e+05
5.68e-11	0.79e+05	0.75e+05	3.49e+05	1.56e+05

Table 7: Number of function evaluations (NFE) as a function of endpoint errors (EPE) of HB(p), $p = 8, 9$ and MEBDF(p), $p = 4, 7$ for stiff DETEST problem B5 with $\alpha = 1000$.

	NFE in		NFE in	
endpoint errors	HB(8)	HB(9)	MEBDF(4)	MEBDF(7)
6.21e-05	0.13e+05	0.18e+05	0.17e+05	2.23e+05
4.40e-06	0.27e+05	0.27e+05	0.34e+05	2.39e+05
4.14e-07	0.41e+05	0.39e+05	0.64e+05	2.55e+05
5.39e-08	0.59e+05	0.54e+05	1.11e+05	2.69e+05
5.66e-09	0.83e+05	0.78e+05	2.02e+05	2.86e+05
4.68e-10	1.14e+05	1.15e+05	3.91e+05	3.06e+05
5.01e-11	1.57e+05	1.65e+05	7.07e+05	3.24e+05

Table 8: NFE PEG of HB(p), $p = 8, 9$, over MEBDF(p), $p = 4, 7$, for the listed problems.

	NFE PEG of HB(8) over:		NFE PEG of HB(9) over:	
Problem	MEBDF(4)	MEBDF(7)	MEBDF(4)	MEBDF(7)
Prob. B5 with $\alpha = 500$	176%	322%	213%	380%
Prob. B5 with $\alpha = 1000$	181%	356%	180%	355%

9.2. Comparing errors of methods on problems with large eigenvalues lying close to the imaginary axis

Our second result is a comparison of the errors of HB(p), $p = 4, 5, \ldots, 9$ and MEBDF(p), $p = 4, 5, 6, 7$ on problems whose Jacobians have some large eigenvalues lying close to the imaginary axis. For this comparison, similar to Cash [6], we use Problem 2.

Table 9 presents error results obtained for the solution of Problem 2 (with $\alpha = 2.5$, $\beta = 60$, fixed step $h = 0.025$) as a function of step number k and t. It is seen that HB(p), $p = 4, 5, \ldots, 9$, and MEBDF(p), $p = 4, 5$ remain stable for the integration of this problem while there is instability for MEBDF(p), $p = 6, 7$.

Next, we present a numerical example which demonstrates the superior stability of the class of high order HB(p), $p = 5, 6, \ldots, 9$. The problem integrated was Problem 2 with large eigenvalues lying closer to the imaginary axis, for example, α reduced to 0.5, $\beta = 60$ and fixed step $h = 0.025$. Table 10 shows HB(p), $p = 4, 5, \ldots, 9$, remain stable while there is instability for MEBDF(p), $p = 5, 6, 7$.

10. Conclusion

Multistep 5-stage Hermite–Birkhoff (HB) methods of orders p, $p = 4, 5, \ldots, 10$ were considered. It is seen that HB(p) are L-stable up to order 9 and, generally, α angles of $L(\alpha)$-stability of HB(p), $p = 4, 5, \ldots, 10$ compare favorably with α of the considered methods of comparable order p.

Selected L-stable HB(p) of order p, $p = 4, 5, \ldots, 9$, compare favorably with existing Cash modified extended backward differentiation formulae, MEBDF(p), $p = 4, 5, \ldots, 7$ in solving problems often used to test highly stable stiff ODE solvers.

HB(p) of order p, $p = 4, 5, \ldots, 9$, are members of variable-step variable-order (VSVO) highly stable 5-stage k-step of order $p = k+2$ which appear to be promising highly stable stiff ODE solvers in the light of the numerical results obtained in this paper.

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Table 9: Error results obtained for the solution of Problem 2 (with $\alpha = 2.5$, $\beta = 60$, fixed step $h = 0.025$) as a function of order p and t.

		HB methods		MEBDF methods	
		$\lvert$Error in $y_1\rvert$	$\lvert$Error in $y_2\rvert$	$\lvert$Error in $y_1\rvert$	$\lvert$Error in $y_2\rvert$
$p = 4$					
	$t = 5.0$	0.791×10^{-7}	0.477×10^{-7}	0.467×10^{-10}	0.108×10^{-10}
	$t = 10.0$	0.533×10^{-9}	0.321×10^{-9}	0.314×10^{-12}	0.728×10^{-13}
	$t = 15.0$	0.359×10^{-11}	0.216×10^{-11}	0.212×10^{-14}	0.490×10^{-15}
	$t = 20.0$	0.242×10^{-13}	0.145×10^{-13}	0.142×10^{-16}	0.330×10^{-17}
$p = 5$					
	$t = 5.0$	0.161×10^{-8}	0.227×10^{-9}	0.401×10^{-11}	0.251×10^{-11}
	$t = 10.0$	0.108×10^{-10}	0.153×10^{-11}	0.683×10^{-13}	0.227×10^{-12}
	$t = 15.0$	0.731×10^{-13}	0.103×10^{-13}	0.391×10^{-14}	0.125×10^{-13}
	$t = 20.0$	0.492×10^{-15}	0.697×10^{-16}	0.555×10^{-15}	0.460×10^{-15}
$p = 6$					
	$t = 5.0$	0.255×10^{-10}	0.652×10^{-12}	0.299×10^{-7}	0.158×10^{-7}
	$t = 10.0$	0.171×10^{-12}	0.443×10^{-14}	0.112×10^{-2}	0.459×10^{-3}
	$t = 15.0$	0.115×10^{-14}	0.298×10^{-16}	$0.418 \times 10^{+2}$	$0.123 \times 10^{+2}$
	$t = 20.0$	0.779×10^{-17}	0.201×10^{-18}	$0.153 \times 10^{+7}$	$0.293 \times 10^{+6}$
$p = 7$					
	$t = 5.0$	0.484×10^{-11}	0.335×10^{-11}	0.675×10^{-5}	0.130×10^{-4}
	$t = 10.0$	0.326×10^{-13}	0.226×10^{-13}	$0.927 \times 10^{+4}$	$0.143 \times 10^{+5}$
	$t = 15.0$	0.220×10^{-15}	0.152×10^{-15}	$0.123 \times 10^{+14}$	$0.154 \times 10^{+14}$
	$t = 20.0$	0.148×10^{-17}	0.102×10^{-17}	$0.159 \times 10^{+23}$	$0.164 \times 10^{+23}$
$p = 8$					
	$t = 5.0$	0.194×10^{-12}	0.138×10^{-12}		
	$t = 10.0$	0.129×10^{-14}	0.929×10^{-15}		
	$t = 15.0$	0.872×10^{-17}	0.626×10^{-17}		
	$t = 20.0$	0.587×10^{-19}	0.422×10^{-19}		
$p = 9$					
	$t = 5.0$	0.351×10^{-14}	0.476×10^{-15}		
	$t = 10.0$	0.242×10^{-16}	0.271×10^{-17}		
	$t = 15.0$	0.166×10^{-18}	0.201×10^{-19}		
	$t = 20.0$	0.109×10^{-20}	0.130×10^{-21}		

Table 10: Error results obtained for the solution of Problem 2 (with $\alpha = 0.5$, $\beta = 60$, fixed step $h = 0.025$) as a function of step number k and t.

		HB methods		MEBDF methods	
		$\lvert$Error in $y_1\rvert$	$\lvert$Error in $y_2\rvert$	$\lvert$Error in $y_1\rvert$	$\lvert$Error in $y_2\rvert$
$p = 4$					
	$t = 5.0$	0.852×10^{-7}	0.109×10^{-6}	0.484×10^{-10}	0.111×10^{-10}
	$t = 10.0$	0.590×10^{-9}	0.106×10^{-9}	0.326×10^{-12}	0.749×10^{-13}
	$t = 15.0$	0.316×10^{-11}	0.333×10^{-11}	0.220×10^{-14}	0.505×10^{-15}
	$t = 20.0$	0.278×10^{-13}	0.125×10^{-13}	0.148×10^{-16}	0.340×10^{-17}
$p = 5$					
	$t = 5.0$	0.166×10^{-8}	0.274×10^{-9}	0.164×10^{-8}	0.108×10^{-8}
	$t = 10.0$	0.112×10^{-10}	0.184×10^{-11}	0.311×10^{-7}	0.508×10^{-7}
	$t = 15.0$	0.757×10^{-13}	0.124×10^{-13}	0.201×10^{-6}	0.179×10^{-5}
	$t = 20.0$	0.510×10^{-15}	0.839×10^{-16}	0.175×10^{-4}	0.519×10^{-4}
$p = 6$					
	$t = 5.0$	0.570×10^{-10}	0.138×10^{-11}	0.695×10^{-6}	0.139×10^{-4}
	$t = 10.0$	0.782×10^{-13}	0.140×10^{-12}	$0.203 \times 10^{+3}$	$0.145 \times 10^{+3}$
	$t = 15.0$	0.281×10^{-14}	0.237×10^{-14}	$0.417 \times 10^{+10}$	$0.166 \times 10^{+10}$
	$t = 20.0$	0.464×10^{-17}	0.273×10^{-16}	$0.154 \times 10^{+17}$	$0.791 \times 10^{+17}$
$p = 7$					
	$t = 5.0$	0.516×10^{-11}	0.357×10^{-11}	0.440×10^{-2}	0.105×10^{-2}
	$t = 10.0$	0.341×10^{-13}	0.237×10^{-13}	$0.155 \times 10^{+10}$	$0.105 \times 10^{+10}$
	$t = 15.0$	0.230×10^{-15}	0.159×10^{-15}	$0.115 \times 10^{+21}$	$0.772 \times 10^{+21}$
	$t = 20.0$	0.155×10^{-17}	0.107×10^{-17}	$0.204 \times 10^{+33}$	$0.252 \times 10^{+33}$
$p = 8$					
	$t = 5.0$	0.538×10^{-12}	0.310×10^{-12}		
	$t = 10.0$	0.380×10^{-14}	0.652×10^{-15}		
	$t = 15.0$	0.770×10^{-16}	0.161×10^{-16}		
	$t = 20.0$	0.688×10^{-18}	0.693×10^{-18}		
$p = 9$					
	$t = 5.0$	0.230×10^{-13}	0.122×10^{-13}		
	$t = 10.0$	0.144×10^{-14}	0.134×10^{-14}		
	$t = 15.0$	0.651×10^{-16}	0.118×10^{-15}		
	$t = 20.0$	0.162×10^{-17}	0.905×10^{-17}		

A. Algorithms

Definition 1. ***This algorithm constructs*** $L_k(i,i-1)$ ***entries of lower bidiagonal matrices*** L_k ***(applied to IF,*** P_i***,*** $i=2,3,4,6$***) as functions of*** η_j***,*** $j=2,3,\dots,p-2$***.***

For $k=2:k_{\text{end}}$, do the following iteration:

For $i=m:-1:k+1$, do the following two steps:

Step (1) $L_k(i,i-1)=-M(i,k)/M(i-1,k)$.

Step (2) For $j=k:m$, compute:

$$M(i,j)=M(i,j)+M(i-1,j)L_k(i,i-1),$$

where $k_{\text{end}}=m-3,m-1,m-1,m-1$ and $m-2$ for IF, P_i, $i=2,3,4,6$, respectively.

Definition 2. ***This algorithm constructs entries of lower tridiagonal matrices*** L_k ***(applied to*** P_5***) as functions of*** η_j***,*** $j=2,3,\dots,p-2$***.***

For $k=2:m-3$, do the following iteration:

Step (a) (for $i=m$) do the following two steps:

Step (1) $L_k(m,m-2)=-M(m,k)/M(m-2,k)$.

Step (2) For $j=k:m$, compute:

$$M(m,j)=M(m,j)+M(m-2,j)L_k(m,m-2).$$

Step (b) For $i=m-1:-1:k+1$, do the following two steps:

Step (1) $L_k(i,i-1)=-M(i,k)/M(i-1,k)$.

Step (2) For $j=k:m$, compute:

$$M(i,j)=M(i,j)+M(i-1,j)L_k(i,i-1).$$

Definition 3. ***This algorithm constructs diagonal entries*** $U_k(j,j)$ ***of upper bidiagonal matrices*** U_k ***(applied to IF,*** P_i***,*** $i=2,3,\dots,6$***) as functions of*** η_j***,*** $j=2,3,\dots,p-2$***.***

For $k=1:p-3$, do the following iteration:

For $j=p-2:-1:k+1$, do the following two steps:

Step (1) $U_k(j,j)=1/[M(k+1,j)-M(k+1,j-1)]$.

Step (2) for $i=k:j$, compute

$$M(i,j)=(M(i,j)-M(i,j-1))U_k(j,j).$$

Definition 4. ***This algorithm solves the systems for IF and*** P_5 ***in*** $O(m^2)$ ***operations.***

Given $[\eta_2,\eta_3,\dots,\eta_{p-2}]$ and $\boldsymbol{r}=r(1:m)$, the following algorithm overwrites $\boldsymbol{r}$ with the solution $\boldsymbol{u}=u(1:m)$ of the system $M\boldsymbol{u}=\boldsymbol{r}$.

Step (1) The following iteration overwrites $\boldsymbol{r}=r(1:m)$ with $L_{m-3}L_{m-4}\cdots L_2\boldsymbol{r}$:

for $k=2,3,\dots,m-3$, compute

$$r(i)=r(i)+r(i-1)L_k(i,i-1),\qquad i=m,m-1,\dots,k+1.$$

Step (2) This step forms the two matrices L_{m-2} and L_{m-1} which transform W_3^1 into a diagonal+last-2-column matrix $W_2^1 = L_{m-1}L_{m-2}W_3^1$ (Gaussian elimination of column $m-2$): it computes the transformed coefficients $G_{m-2}(i)$, $i = 1, 2, \ldots, m$ of column $m-2$ of M and $G_{m-2}(i)$, $i = 1, 2, \ldots, m$ are used to form the two matrices L_{m-2} and L_{m-1} by means of the formulae in Table 2 as follows.

First set $G_{m-2}(1 : m)$,

$$G_{m-2}(1 : m) = M(1 : m, m-2).$$

The following computation overwrites $G_{m-2}(1 : m)$ with $L_{m-3}L_{m-4}\cdots\ L_2G_{m-2}(1 : m)$:

for $k = 2, 3, \ldots, m-3$, compute

$$G_{m-2}(i) = G_{m-2}(i) + G_{m-2}(i-1)L_k(i, i-1), \quad i = m, m-1, \ldots, k+1.$$

Step (3) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_{m-1}L_{m-2}\boldsymbol{r}$:

$$r(m-2) = r(m-2)/G_{m-2}(m-2),$$

next, for $k = m, m-1, m-3, m-4, \ldots, 1$, $(k \neq m-2)$ compute

$$r(k) = r(k) - G_{m-2}(k)r(m-2).$$

Step (4) Similar to step (2) above, this step forms the two matrices L_m and L_{m+1} which transform W_2^1 into a diagonal+last-1-column matrix $W_1^1 = L_{m+1}L_mW_2^1$ (Gaussian elimination of column $m-1$): it computes the transformed coefficients $G_{m-1}(i)$, $i = 1, 2, \ldots, m$ of column $m-1$ of M and $G_{m-1}(i)$, $i = 1, 2, \ldots, m$ are used to form the two matrices L_m and L_{m+1} by means of the formulae in Table 2.

Step (5) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_{m+1}L_m\boldsymbol{r}$:

$$r(m-1) = r(m-1)/G_{m-1}(m-1),$$

next, for $k = m, m-2, m-3, \ldots, 1$, $(k \neq m-1)$ compute

$$r(k) = r(k) - G_{m-1}(k)r(m-1),$$

Step (6) Similar to step (2) above, this step forms the two matrices L_{m+2} and L_{m+3} which transform W_1^1 into the identity matrix $I^1 = L_{m+3}L_{m+2}W_1^1$ (Gaussian elimination of column m): it computes the transformed coefficients $G_m(i)$, $i = 1, 2, \ldots, m$ of column m of M and $G_m(i)$, $i = 1, 2, \ldots, m$ are used to form the two matrices L_{m+2} and L_{m+3} by means of the formulae in Table 2.

Step (7) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_{m+3}L_{m+2}\boldsymbol{r}$:

$$r(m) = r(m)/G_m(m),$$

next, for $k = m-1, m-2, \ldots, 1$, compute

$$r(k) = r(k) - G_m(k)r(m).$$

Step (8) The following iteration overwrites $\boldsymbol{r} = r(1 : m)$ with $U_1U_2\cdots U_{p-3}\boldsymbol{r}$:

For $k = p-3, p-4, \ldots, 1$, compute

$$\begin{aligned} r(i) &= r(i)U_k(i,i), \qquad i = k+1, k+2, \ldots, p-2, \\ r(i) &= r(i) - r(i+1), \qquad i = k, k+1, \ldots, p-3. \end{aligned}$$

Definition 5. ***This algorithm solves the systems for $\boldsymbol{P}_2$ in $O(m^2)$ operations.***

Given $[\eta_2, \eta_3, \ldots, \eta_{p-2}]$ and $\boldsymbol{r} = r(1:m)$, the following algorithm overwrites $\boldsymbol{r}$ with the solution $\boldsymbol{u} = u(1:m)$ of the system $M\boldsymbol{u} = \boldsymbol{r}$.

Step (1) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $L_{m-1}L_{m-2}\cdots, L_2\boldsymbol{r}$:

for $k = 2, 3, \ldots, m-1$, compute

$$r(i) = r(i) + r(i-1)L_k(i, i-1), \qquad i = m, m-1, \ldots, k+1.$$

Step (2) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $U_1U_2\cdots U_{m-2}\boldsymbol{r}$:

For $k = m-1, m-2, \ldots, 1$, compute

$$\begin{aligned} r(i) &= r(i)U_k(i,i), \qquad i = k+1, k+2, \ldots, m, \\ r(i) &= r(i) - r(i+1), \qquad i = k, k+1, \ldots, m-1. \end{aligned}$$

Definition 6. ***This algorithm solves the systems for $\boldsymbol{P}_\ell$, $\ell = 3, 4$ in $O(m^2)$ operations.***

Given $[\eta_2, \eta_3, \ldots, \eta_{p-2}]$ and $\boldsymbol{r} = r(1:m)$, the following algorithm overwrites $\boldsymbol{r}$ with the solution $\boldsymbol{u} = u(1:m)$ of the system $M\boldsymbol{u} = \boldsymbol{r}$.

Step (1) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $L_{m-1}L_{m-2}\cdots, L_2\boldsymbol{r}$:

for $k = 2, 3, \ldots, m-1$, compute

$$r(i) = r(i) + r(i-1)L_k(i, i-1), \qquad i = m, m-1, \ldots, k+1.$$

Step (2) Similar to Step (2) of Algorithm 4, this step forms the two matrices L_m and L_{m+1} which transform W_1^ℓ into the identity matrix $I^\ell = L_{m+1}L_mW_1^\ell$ (Gaussian elimination of column m): this step computes the transformed coefficients $G_m(i)$, $i = 1, 2, \ldots, m$ of column m of M and $G_m(i)$, $i = 1, 2, \ldots, m$ are used to form the two matrices L_m and L_{m+1} by means of the formulae in Table 3.

Step (3) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_{m+1}L_m\boldsymbol{r}$:

$$r(m) = r(m)/G_m(m),$$

next, for $k = m-1, m-2, \ldots, 1$, compute

$$r(k) = r(k) - G_m(k)r(m).$$

Step (4) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $U_1U_2\cdots U_{p-3}\boldsymbol{r}$:

For $k = p-3, p-4, \ldots, 1$, compute

$$\begin{aligned} r(i) &= r(i)U_k(i,i), \qquad i = k+1, k+2, \ldots, p-2, \\ r(i) &= r(i) - r(i+1), \qquad i = k, k+1, \ldots, p-3. \end{aligned}$$

Definition 7. ***This algorithm solves the systems for $\boldsymbol{P}_6$ in $O(m^2)$ operations.***

Given $[\eta_2, \eta_3, \ldots, \eta_{p-2}]$ and $\boldsymbol{r} = r(1:m)$, the following algorithm overwrites $\boldsymbol{r}$ with the solution $\boldsymbol{u} = u(1:m)$ of the system $M\boldsymbol{u} = \boldsymbol{r}$.

Step (1) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $L_{m-2}L_{m-3}\cdots L_3L_2\boldsymbol{r}$:

For $k = 2, 3, \dots, m-2$, compute

$$r(i) = r(i) + r(i-1)L_k(i, i-1), \quad i = m, m-1, \dots, k+1.$$

Step (2) Similar to Step (2) of Algorithm 4, this step forms the two matrices L_{m-1} and L_m which transform W_2^4 into a diagonal+last-1-column matrix $W_1^4 = L_mL_{m-1}W_2^4$ (Gaussian elimination of column $m-1$): it computes the transformed coefficients $G_{m-1}(i)$, $i = 1, 2, \dots, m$ of column $m-1$ of M and $G_{m-1}(i)$, $i = 1, 2, \dots, m$ are used to form the two matrices L_{m-1} and L_m by means of the formulae in Table 4.

Step (3) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_mL_{m-1}\boldsymbol{r}$:

$$r(m-1) = r(m-1)/G_{m-1}(m-1),$$

next, for $k = m, m-2, m-3, \dots, 1$, $(k \neq m-1)$ compute

$$r(k) = r(k) - G_{m-1}(k)r(m-1).$$

Step (4) Similar to Step (2) of Algorithm 4, this step forms the two matrices L_{m+1} and L_{m+2} which transform W_1^4 into the identity matrix $I^4 = L_{m+2}L_{m+1}W_1^4$ (Gaussian elimination of column m): this step computes the transformed coefficients $G_m(i)$, $i = 1, 2, \dots, m$ of column m of M and $G_m(i)$, $i = 1, 2, \dots, m$ are used to form the two matrices L_{m+1} and L_{m+2} by means of the formulae in Table 4.

Step (5) The following computation overwrites the newly obtained $\boldsymbol{r}$ with $L_{m+2}L_{m+1}\boldsymbol{r}$:

$$r(m) = r(m)/G_m(m),$$

next, for $k = m-1, m-2, \dots, 1$, compute

$$r(k) = r(k) - G_m(k)r(m).$$

Step (6) The following iteration overwrites $\boldsymbol{r} = r(1:m)$ with $U_1U_2U_3\cdots U_{p-3}\boldsymbol{r}$:

For $k = p-3, p-4, \dots, 1$, compute

$$\begin{aligned} r(i) &= r(i)U_k(i,i), &\quad i &= k+1, k+2, \dots, p-2, \\ r(i) &= r(i) - r(i+1), &\quad i &= k, k+1, \dots, p-3. \end{aligned}$$

B. Coefficients of HB(p), $p = 4, 5, \dots, 10$.

The appendix lists the coefficients of HB(p), of order $p = 4, 5, \dots, 10$, considered in this paper. It is to be noted that, in Tables 11–13, $a_{42} = b_2 = 0$ and, since $a_{22} = a_{33} = a_{44} = a_{55} = b_6$, only a_{22} values are listed.

Table 11: Coefficients of the implicit predictors P_i, $i = 2, 3, 4, 5$ and of the integration formulae of HB(p), $p = 4, 5$.

k	2	3
coeffs\\p	4	5
c_2	1.0	1.0
a_{22}	4.9545454545454554e-01	5.9545454545454557e-01
α_{20}	1.5045454545454544e+00	1.5113636363636362e+00
α_{21}	-5.0454545454545441e-01	-6.1818181818181783e-01
α_{22}		1.0681818181818170e-01
c_3	9.5099999999999998e-01	8.5099999999999999e-01
a_{32}	1.3919730303030287e-01	-9.4008025528925732e-02
α_{30}	1.3163481515151514e+00	1.4737069274586774e+00
α_{31}	-3.1634815151515144e-01	-5.9786037484297494e-01
α_{32}		1.2415344738429746e-01
c_4	7.5200000000000000e-01	9.5200000000000000e-01
a_{43}	2.6494079318338387e-02	-7.8182087932457622e-02
α_{40}	1.2300513752271161e+00	1.6049035432746619e+00
α_{41}	-2.3005137522711608e-01	-7.7507954407141211e-01
α_{42}		1.7017600079675005e-01
c_5	9.0300000000000001e-01	9.0300000000000004e-01
a_{54}	4.3387940883063157e-02	-3.3210993189336242e-02
a_{53}	-1.7026263951199987e-02	7.0635671109614264e-03
a_{52}	8.9643453156579428e-02	-5.4934233194668745e-02
α_{50}	1.2915403244570123e+00	1.5334897192817816e+00
α_{51}	-2.9154032445701222e-01	-6.7835232474506502e-01
α_{52}		1.4486260546328336e-01
b_5	-1.3783763845118045e+01	-3.5848221757165504e+01
b_4	5.3636001573953527e+00	1.5213952013055099e+01
b_3	8.8767825358096637e+00	2.0948153761791403e+01
α_0	1.0479266064584820e+00	1.1009206888496665e+00
α_1	-4.7926606458482027e-02	-1.1117994083487694e-01
α_2		1.0259251985210388e-02

References

[1] Alexander, R., *Diagonally implicit Runge–Kutta methods for stiff ODEs*, SIAM J. Numer. Anal. 14(1977), 1006–1021.

[2] Björck, A., Elfving, T., *Algorithms for confluent Vandermonde systems*, Numer. Math. 21(1973), 130–137.

[3] Björck, A., Pereyra, V., *Solution of Vandermonde systems of equations*, Math. Comp. 24(1970), 893–903.

[4] Cash, J. R., *On the integration of stiff systems of ODEs using extended backward differentiation formula*, Numer. Math. 34(1980), 235–246.

[5] Cash, J. R., *The integration of stiff initial value problems in ODEs using modified extended backward differentiation formula*, Comput. Math. Appl. 9(1983), 645–657.

[6] Cash, J. R., *Second derivative extended backward differentiation formulas for the numerical integration of stiff systems*, SIAM J. Numer. Anal. 18 (2) (1981), 21–36.

[7] Cash, J. R., *Modified extended backward differentiation formulae for the numerical solution of stiff initial value problems in ODEs and DAEs*, J. Comput. Appl. Math. 125(2000), 117–130.

[8] Cash, J. R., Considine, S., *An MEBDF code for stiff initial value problems*, ACM Trans. Math. Software 18(1992), 142–160.

[9] Cash, J. R., *A comparison of some codes for the stiff oscillatory problem*, Comput. Math. Appl. 36 (1998), 51–57.

[10] D'Ambrosio, R., Izzo, G., Jackiewicz, Z. *Perturbed mebdf methods, Comput. Math.*, Appl. 63 (2012), 851–861.

[11] Ebadi, M., Gokhale, M. Y., *Hybrid BDF methods for the numerical solutions of ordinary differential equations*, Numer. Algorithms 55(2010), 1–17 . DOI 10.1007/s11075-009-9354-4

[12] Enright, W. H., Pryce, J. D., *Two Fortran packages for assessing initial value methods*, ACM Trans. Math. Software 13(1987), 1–27.

[13] Galimberti, G., Pereyra, V., *Solving confluent Vandermonde systems of Hermite type*, Numer. Math. 18(1971), 44–60.

[14] Gear, C. W., *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, Englewood Cliffs, NJ, (1971).

[15] Hairer, E., Wanner, G., *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, corr. sec. print., Springer-Verlag, Berlin, (2002).

[16] Hindmarsh, A. C. *Avoiding bdf stability barriers in the mol solution of advection dominated problems*, Appl. Numer. Math. 17 (1995), 311–318.

[17] Hojjati, G., Rahimi, M. Y., Hosseini, S. M., *A-EBDF: an adaptive method for numerical solution of stiff systems of ODEs*, Math. Comput. Simulation 66(2004), 33–41.

[18] Hull, T. E., Enright, W. H., Fellen, B. M., Sedgwick, A. E., *Comparing numerical methods for ordinary differential equations*, SIAM J. Numer. Anal. 9(1972), 603–637.

[19] Krogh, F. T., *Changing stepsize in the integration of differential equations using modified divided differences*, in Proc. Conf. on the Numerical Solution of Ordinary Differential Equations, University of Texas at Austin 1972 (Ed. D.G.

Bettis), Lecture Notes in Mathematics No. 362, Springer-Verlag, Berlin (1974), 22–71.

[20] Lambert, J. D., *Numerical Methods for Ordinary Differential Systems*, Wiley, Chichester, UK, (1991).

[21] Nguyen-Ba, T., Kengne, E., Vaillancourt, R., *One-step 4-stage Hermite–Birkhoff–Taylor ODE solver of order 12*, Can. Appl. Math. Q., 16(1)(2008), 77–94.

[22] Nguyen-Ba, T., Giordano, T., Vaillancourt, R., *Variable-step 4-stage Hermite–Birkhoff solver of order 9 and 10 for stiff ODEs*, Acta Universitatis Apulensis 41 (2015), 177–220. DOI:10.17114/j.aua.2015.41.14

[23] Nordsieck, A., *On numerical integration of ordinary differential equations*, Math. Comp. 16(1962), 22–49.

[24] Petzold, L. R., *A description of DASSL: A differential/algebraic system solver*, In Proceedings of IMACS World Congress, Montréal, Canada, (1982).

[25] Sharp, P. W., *Numerical comparison of explicit Runge–Kutta pairs of orders four through eight*, ACM Trans. Math. Software 17(1991), 387–409.

[26] Warming, R. F., Beam, M., *An extension of a-stability to alternating direction implicit methods*, BIT 19 (1979), 395–417.

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Table 12: Coefficients of the implicit predictors P_i, $i = 2, 3, 4, 5$ and of the integration formulae of HB(p), $p = 6, 7, 8$.

k	4	5	6
coeffs\\p	6	7	8
c_2	1.0	1.0	9.500000000000000e-01
a_{22}	5.9545454545454546e-01	8.4545454545455279e-01	1.0954545454544657e+00
α_{20}	1.4196969696969697e+00	-4.2500000000005045e-01	-3.4345831477265278e+00
α_{21}	-3.4318181818181803e-01	5.0772727272728631e+00	1.6399514578595941e+01
α_{22}	-1.6818181818181829e-01	-6.4863636363637811e+00	-2.5100776079541731e+01
α_{23}	9.1666666666666702e-02	3.5954545454546198e+00	2.0007094971587986e+01
α_{24}		-7.6136363636365156e-01	-8.2824588257563718e+00
α_{25}			1.4112085028407044e+00
c_3	9.509999999999998e-01	1.201000000000000e+00	1.101000000000000e+00
a_{32}	-1.2280128558798009e-01	-4.8312242883334472e-01	-8.7221988964764896e-01
α_{30}	1.8299014074115494e+00	3.0227340367018267e+00	3.4604277345811916e+00
α_{31}	-1.2851128590403549e+00	-3.9693730192643493e+00	-5.5427333975997444e+00
α_{32}	5.5886823597949609e-01	2.8959844491502889e+00	5.3090130975561891e+00
α_{33}	-1.0365678435069055e-01	-1.1361181039360437e+00	-3.0963582633928031e+00
α_{34}		1.8677263734827756e-01	1.0122374958032396e+00
α_{35}			-1.4258666694807259e-01
c_4	6.519999999999997e-01	7.519999999999996e-01	1.652000000000000e+00
a_{43}	-1.4790603895342971e-01	-2.2693831726222627e-01	-1.2834072588317600e+00
α_{40}	1.2912890617869559e+00	1.0510170052111643e+00	8.1365511804473609e+00
α_{41}	-3.9776417220530924e-01	1.2842152511456736e-01	-1.8256332841983692e+01
α_{42}	1.2611265254863535e-01	-3.0465030443372110e-01	1.9978834808154467e+01
α_{43}	-1.9637542130281804e-02	1.5345178448675673e-01	-1.2516339483954063e+01
α_{44}		-2.8240010378767104e-02	4.2787027225199790e+00
α_{45}			-6.2141638518405173e-01
α_{46}			
c_5	8.530000000000003e-01	9.530000000000004e-01	9.530000000000004e-01
a_{54}	3.7073572420945988e-01	2.4762392824339385e-01	8.4229579713816921e-02
a_{53}	-3.5771214821044267e-01	-3.6380529669799960e-01	1.4242935698456041e-01
a_{52}	-1.5095484033513835e-02	-5.1067969144802314e-02	-1.1543003702584997e+00
α_{50}	1.3921662374048833e+00	1.3811212392506116e+00	3.2526385842981971e+00
α_{51}	-5.5801348824042107e-01	-5.0497022581716511e-01	-5.1491327892570098e+00
α_{52}	1.9914562684614415e-01	1.4013626907669907e-01	5.0302335866768546e+00
α_{53}	-3.3298376010606215e-02	-1.5052025559493845e-02	-2.9781891887947745e+00
α_{54}		-1.2352569506518000e-03	9.8420274120169438e-01
α_{55}			-1.3975293412496195e-01
b_5	-1.6347743716641421e+00	-2.0459926629584766e+00	1.3525647203287863e+00
b_4	1.7457839486436524e+00	1.8379417108761216e+00	7.7095324061908319e-02
b_3	2.0095645015192828e-01	2.1626959119817182e-01	-1.7899912350139222e+00
α_0	1.1107586899351263e+00	1.1921233554274981e+00	1.3993496774288885e+00
α_1	-1.3118022630551504e-01	-2.4951856742191617e-01	-5.9010491579581947e-01
α_2	2.2663810219667249e-02	7.0463940441495648e-02	2.6211821640050331e-01
α_3	-2.2422738492785029e-03	-1.4538784897604632e-02	-8.8306874983794470e-02
α_4		1.4700564505271006e-03	1.8807021973675956e-02
α_5			-1.8631250234538996e-03

Table 13: Coefficients of the implicit predictors P_i, $i = 2, 3, 4, 5$ of HB(p), $p = 9, 10$.

k	7	8
coeffs\p	9	10
c_2	8.500000000000000e-01	1.0
a_{22}	1.0454545454544011e+00	4.2360474274791637e-01
α_{20}	-4.1115897708731026e+00	2.1784605353788038e+00
α_{21}	2.1377247829077088e+01	-1.6941454753554235e+00
α_{22}	-3.9551714291565546e+01	-5.6535331493571073e-01
α_{23}	4.1343320126289107e+01	3.1777193096985088e+00
α_{24}	-2.5420692720783872e+01	-3.7282687274525639e+00
α_{25}	8.6061271633613714e+00	2.2594987902908383e+00
α_{26}	-1.2426983355050463e+00	-7.2625770060647066e-01
α_{27}		9.8346582982017650e-02
c_3	1.751000000000000e+00	1.551000000000000e+00
a_{32}	-2.5601120534537443e+00	1.3953221183550846e-01
α_{30}	1.6308184540015283e+01	5.2839728582328771e+00
α_{31}	-4.4941366141892324e+01	-1.3233302882770326e+01
α_{32}	6.0942613459693874e+01	2.0324280451556358e+01
α_{33}	-5.0634597009539995e+01	-2.0551629130148555e+01
α_{34}	2.5878624719491970e+01	1.3787724348060081e+01
α_{35}	-7.5005312717702317e+00	-5.9327224328176404e+00
α_{36}	9.4707170400141971e-01	1.4872564186758865e+00
α_{37}		-1.6557963078868065e-01
c_4	1.502000000000000e+00	1.452000000000000e+00
a_{43}	-3.7499011290603812e-01	2.5639011174276943e-02
α_{40}	3.4732301015197198e+00	5.2214052315693849e+00
α_{41}	-6.0229278965897688e+00	-1.2863630636569201e+01
α_{42}	6.7697677465684514e+00	1.9502342945452011e+01
α_{43}	-5.0267657030055508e+00	-1.9559748890148530e+01
α_{44}	2.3803006541177756e+00	1.3050180129871856e+01
α_{45}	-6.5258074421054590e-01	-5.5932994109592507e+00
α_{46}	7.8975841599918925e-02	1.3980427101442936e+00
α_{47}		-1.5529207936056433e-01
c_5	9.530000000000004e-01	9.530000000000004e-01
a_{54}	-2.6176277404401462e+00	-3.4110394419945989e-01
a_{53}	2.9603441535565462e+00	3.1654376688408081e-01
a_{52}	-6.8434788951141252e+00	-1.4781054885223396e-01
α_{50}	3.2916424214263287e+01	3.5397954956884989e+00
α_{51}	-9.5378956147659579e+01	-7.3362458564569719e+00
α_{52}	1.3127655044159829e+02	1.0670993521404315e+01
α_{53}	-1.0993884327061177e+02	-1.0526992199610547e+01
α_{54}	5.6468976708172875e+01	6.9648294313441426e+00
α_{55}	-1.6423081981642067e+01	-2.9704657072342946e+00
α_{56}	2.0789300358789702e+00	7.4011696419880957e-01
α_{57}		-8.2031649333952530e-02

Table 14: Coefficients of the integration formulae of HB(p), $p = 9, 10$.

k	7	8
coeffs\ p	9	10
b_5	-7.1376451203220892e-02	5.8961559344410308e-01
b_4	-5.2219295224276951e-01	-9.8627913548955615e-01
b_3	1.9079760073720756e-01	6.2459702553550611e-01
α_0	1.6094720086352379e+00	1.6185042823909392e+00
α_1	-1.0101582667633460e+00	-1.0785341697667015e+00
α_2	6.1082553892183045e-01	7.5235609762454214e-01
α_3	-2.8728104287593442e-01	-4.3272551202619663e-01
α_4	9.4451776020869599e-02	1.8706274754564486e-01
α_5	-1.9086039841573393e-02	-5.6153086156063112e-02
α_6	1.7760259029158479e-03	1.0376305282931491e-02
α_7		-8.8666489509660578e-04