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 $\alpha > 75^\circ$. 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.

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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($p$), $p = 4, 5, \ldots, 9$. 

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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

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

(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 $\alpha > 75^\circ$. 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 \(p = 4, 5, \ldots, 10\).

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 \([c_1, c_2, \ldots, c_6]^T\) defines the off-step points \(t_n + c_jh_{n+1}\) with \(c_1 = 0\) and \(c_6 = 1\). Following the approach of Cash [4], \(c_i\) are allowed to be \(0 \leq c_i \leq 2\), \(i = 3, 4, 5\).

Let \(F_1 = f_n\) and \(F_j := f(t_n + c_jh_{n+1}, Y_j), j = 2, 3, 4, 5\), denote the \(j\)th 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 \(p - 3\),

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

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

\[
y_{n+1} = h_{n+1}b_6f(t_n + h_{n+1}, y_{n+1}) + \sum_{j=0}^{p-3} \alpha_{j}y_{n-j} + h_{n+1}\left[\sum_{j=3}^{5} b_jF_j\right]. \tag{3}
\]

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

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

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]:

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

where the Jacobian \( J_{n+1}^0 \) at iteration \( l = 0 \),

\[
J_{n+1}^0 = \left[ I - h a_{22} \frac{\partial f(t_n + c_2 h_{n+1}, Y_2^0)}{\partial y} \right], \quad (6)
\]

computed at \( t_n + c_2 h_{n+1} \), 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

\[
a_{22} = a_{33} = a_{44} = a_{55} = b_6, \quad (7)
\]

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:

\[
B_i(j) = \sum_{\ell=1}^{p-3} \alpha_{i\ell} \frac{\eta_{\ell+1}^j}{j!}, \quad \left\{ \begin{array}{l}
i = 2, 3, 4, 5, \\
j = 1, 2, \ldots, p,
\end{array} \right. \quad (8)
\]

and

\[
\eta_j = -\frac{1}{h_{n+1}} (t_n - t_{n+1-j}) = -\frac{1}{h_{n+1}} \sum_{i=0}^{j-2} h_{n-i}, \quad j = 2, 3, \ldots, p - 2. \quad (9)
\]
In the sequel, \( \eta_j \) 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:

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

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

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

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

\[
\sum_{i=2}^{6} b_i c_i^k + k! B(k + 1) = \frac{1}{k+1}, \quad k = 0, 1, \ldots, p - 1, \tag{12}
\]

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

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

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

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

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

\[
B(j) = \sum_{\ell=1}^{p-3} \alpha_{\ell j} \eta_{\ell+1}^j, \quad j = 1, 2, \ldots, p + 1. \tag{17}
\]

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) $p = 4, 5, \ldots, 9$.

<table>
<thead>
<tr>
<th>$c_i$</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_2$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$c_3$</td>
<td>9.500000000000000e-01</td>
<td>8.500000000000000e-01</td>
<td>9.500000000000000e-01</td>
</tr>
<tr>
<td>$c_4$</td>
<td>7.510000000000000e-01</td>
<td>9.510000000000000e-01</td>
<td>6.519999999999999e-01</td>
</tr>
<tr>
<td>$c_5$</td>
<td>9.530000000000000e-01</td>
<td>9.530000000000000e-01</td>
<td>8.530000000000000e-01</td>
</tr>
<tr>
<td>$a_{22}$</td>
<td>9.545454545454545e-01</td>
<td>9.545454545454545e-01</td>
<td>6.954545454545454e-01</td>
</tr>
</tbody>
</table>

4.2. Integration formula IF

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

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

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

$$M^1 u^1 = r^1,$$  \hspace{1cm} (18)

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.
where

\[
M^1 = \begin{bmatrix}
1 & 1 & 1 & \cdots & 1 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & \cdots & \eta_{p-2} & 1 & 1 & 1 \\
0 & \frac{\eta_2}{2!} & \frac{\eta_3}{3!} & \cdots & \frac{\eta_{p-2}}{(p-2)!} & c_5 & c_4 & c_3 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \vdots \\
0 & \frac{\eta_p}{p!} & \frac{\eta_p}{p!} & \cdots & \frac{\eta_{p-2}}{(p-2)!} & \frac{c_{p-1}}{(p-1)!} & \frac{c_{p-1}}{(p-1)!} & \frac{c_{p-1}}{(p-1)!}
\end{bmatrix},
\]

and \( r^1 = r_1(1 : p + 1) \) has components

\[
r_1(1) = 1, \\
r_1(i) = \frac{1}{(i-1)!} - b_0 \frac{c_{i-2}}{(i-2)!}, \quad i = 2, 3, \ldots, p + 1.
\]

The leading error term of IF is

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

### 4.3. Predictor \( P_2 \)

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

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

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

\[
M^2 u^2 = r^2,
\]

where

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

and \( r^2 = r_2(1 : p - 2) \) has components

\[
r_2(1) = 1, \\
r_2(i) = \frac{c_{i-1}^2}{(i-1)!} - a_{22i} \frac{c_{i-2}^2}{(i-2)!}, \quad i = 2, 3, \ldots, p - 2.
\]
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
\[
S(2, j) = a_{22} \frac{c_2^{j-1}}{(j-1)!} + M^2(j + 1, 1 : p - 2) \mathbf{u}^2 \\
= a_{22} \frac{c_2^{j-1}}{(j-1)!} + r_2(j + 1) = \frac{c_2^j}{j!}, \quad j = 1, 2, \ldots, p - 3.
\]

We define
\[
S(2, j) = a_{22} S(2, j - 1) + \sum_{i=1}^{p-3} \alpha_{2i} \eta_{i+1}^j, \quad j = p - 2, p - 1, \quad (22)
\]
\[
S_{e^{p-2}}(2, p - 1) = a_{22} c_2^{p-2} + \sum_{i=1}^{p-3} \alpha_{2i} \eta_{i+1}^{p-1} \frac{1}{(p-1)!}. \quad (23)
\]

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 \( S_{e^{p-2}}(2, p - 1) \) and \( S_{e^{p-2}}(i, p - 1), i = 3, 4, 5 \), 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
\[
S(2, j) = c_2^j/j!, \quad j = 0, 1, \ldots, p - 3,
\]
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 \( i = 3 \),
\[
\mathbf{u}^3 = [a_{30}, a_{31}, \ldots, a_{3,p-3}, a_{32}]^T,
\]
is the solution of the Vandermonde-type system of order conditions
\[
M^3 \mathbf{u}^3 = \mathbf{r}^3, \quad (24)
\]

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where

\[
M^3 = \begin{bmatrix}
1 & 1 & 1 & \ldots & 1 & 0 \\
0 & \eta_2 & \eta_3 & \ldots & \eta_{p-2} & 1 \\
0 & \frac{\eta_2^2}{2!} & \frac{\eta_3^2}{2!} & \ldots & \frac{\eta_{p-2}^2}{2!} & c_2 \\
0 & \frac{\eta_2^3}{3!} & \frac{\eta_3^3}{3!} & \ldots & \frac{\eta_{p-2}^3}{3!} & c_3^2 \\
\vdots \\
0 & \frac{\eta_{p-2}^2}{(p-2)!} & \frac{\eta_{p-2}^3}{(p-2)!} & \ldots & \frac{\eta_{p-2}^p}{(p-2)!} & c_{p-3}^{p-3} \\
\end{bmatrix}.
\]  

(25)

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

\[
r_3(1) = 1,
\]

\[
r_3(i) = \frac{(i-1)!}{c_3^i} - a_{33} \frac{(i-2)!}{c_3^{i-2}}, \quad i = 2, 3, \ldots, p - 1.
\]

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

\[
\sum_{j=0}^{p+1} S(3, j) h_n^j y_n^{(j)}
\]

with coefficients

\[
S(3, j) = a_{33} \frac{c_3^{j-1}}{(j-1)!} + M^3(j + 1, 1 : p - 1) u^3
\]

\[
= a_{33} \frac{c_3^{j-1}}{(j-1)!} + r_3(j + 1) = \frac{c_3^j}{j!}, \quad j = 1, 2, \ldots, p - 2.
\]

We define

\[
S(3, j) = a_{33} S(3, j - 1) + a_{32} S(2, j - 1) + \sum_{i=1}^{p-3} \alpha_{3i} \frac{\eta_{i+1}^j}{j!}, \quad j = p - 2, p - 1,
\]

\[
S_{c^p-2}(3, p - 1) = a_{33} c_3^{p-2} + a_{32} c_2^{p-2} + \sum_{i=1}^{p-3} \alpha_{3i} \frac{\eta_{i+1}^{p-1}}{(p-1)!},
\]

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

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

\[ u^4 = [α_{40}, α_{41}, \ldots, α_{4,p-3}, a_{43}]^T, \]

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

\[ M^4 u^4 = r^4, \quad (26) \]

where

\[
M^4 = \begin{bmatrix}
1 & 1 & 1 & \cdots & 1 & 0 \\
0 & η_2 & η_3 & \cdots & η_{p-2} & 1 \\
0 & c_2 \frac{η_2}{2} & c_2 \frac{η_3}{3} & \cdots & c_2 \frac{η_{p-2}}{(p-2)!} & c_3 \\
0 & c_3 \frac{η_2}{2} & c_3 \frac{η_3}{3} & \cdots & c_3 \frac{η_{p-2}}{(p-2)!} & c_4 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & c_{p-2} \frac{η_2}{2} & c_{p-2} \frac{η_3}{3} & \cdots & c_{p-2} \frac{η_{p-2}}{(p-2)!} & c_{p-1} \frac{η_{p-1}}{(p-1)!} \\
\end{bmatrix}. \quad (27) \]

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

\[
r_4(1) = 1, \\
r_4(i) = \frac{c_i^{i-1}}{(i-1)!} - a_{44} \frac{c_i^{i-2}}{(i-2)!}, \quad i = 2, 3, \ldots, p-1. \\
\]

We define

\[
S(4,j) = a_{44} \frac{c_4^{j-1}}{(j-1)!} + a_{43} \frac{c_3^{j-1}}{(j-1)!} + a_{42} \frac{c_2^{j-1}}{(j-1)!} + \sum_{i=1}^{p-3} α_{4i} \frac{η_i^{j+1}}{j!} = \frac{c_j}{j!}, \\
\]

\(j = 1, 2, \ldots, p-3,\)

\[
S(4,j) = a_{44}S(4,j-1) + a_{43}S(3,j-1) + a_{42}S(2,j-1) + \sum_{i=1}^{p-3} α_{4i} \frac{η_i^{j+1}}{j!}, \\
\]

\(j = p-2, p-1,\)

\[
S_{p-2}(4,p-1) = a_{44}c_4^{p-2} + a_{43}c_3^{p-2} + a_{42}c_2^{p-2} + \sum_{i=1}^{p-3} α_{4i} \frac{η_i^{p-1}}{(p-1)!}, \\
\]

which will be used in subsequent formulae.

4.6. Predictor P

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

\[ u^5 = [α_{50}, α_{51}, \ldots, α_{5,p-3}, a_{54}, a_{53}, a_{52}]^T, \]
is the solution of the Vandermonde-type system of order conditions

\[ M^5 u^5 = r^5, \]  

(28)

where

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

(29)

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

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

and the \(p\)th and \((p + 1)\)th component are

\[
r_5(p) = S_{c_5^{p-2}}(5, p - 1) - a_{55} \frac{c_5^{p-2}}{(p - 2)!},
\]

(30)

\[
r_5(p + 1) = S(5, p - 1) - a_{55} S(5, p - 2),
\]

(31)

where

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

\[
S_{c_5^{p-2}}(5, p - 1) = \frac{1}{b_5} \left[ \frac{1}{p!} - b_2 S_{c_5^{p-2}}(2, p - 1) - b_3 S_{c_5^{p-2}}(3, p - 1) \\
- b_4 S_{c_5^{p-2}}(4, p - 1) - b_6 \frac{c_5^{p-1}}{(p - 1)!} - B(p) \right].
\]

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),

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

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

\[
M^6 u^6 = r^6,
\]

where

\[
M^6 = \begin{bmatrix}
1 & 1 & 1 & \ldots & 1 & 0 & 0 \\
0 & \eta_2 & \eta_3 & \ldots & \eta_{p-2} & 1 & 1 \\
0 & \eta_2^2 & \eta_3^2 & \ldots & \eta_{p-2}^2 & c_4 & c_3 \\
0 & \eta_2^3 & \eta_3^3 & \ldots & \eta_{p-2}^3 & c_4^2 & c_3^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & \eta_2^{p-1} & \eta_3^{p-1} & \ldots & \eta_{p-2}^{p-1} & c_4^{p-2} & c_3^{p-2}
\end{bmatrix},
\]

and \( r^6 = r_6(1 : p) \) has components

\[
r_6(1) = 1, \\
r_6(i) = \frac{1}{(i-1)!} - \frac{(b_6 + \omega_6)}{(i-2)!} - \frac{(b_5 + \omega_5)}{(i-2)!},
\]

\( i = 2, 3, \ldots, p. \)

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

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

5. Symbolic construction of elementary matrix functions

Consider the matrices

\[
M^\ell \in \mathbb{R}^{m_\ell \times m_\ell}, \quad \ell = 1, 2, \ldots, 6,
\]

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

\[
m_1 = p + 1, \quad m_2 = p - 2, \quad m_3 = p - 1, \\
m_4 = p - 1, \quad m_5 = p + 1, \quad m_6 = p,
\]

\[34\]
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

- $M^{\ell}$ into a diagonal+last-3-column matrix, $W_{3}^{\ell}$, $\ell = 1, 5$, which will be further diagonalized by a Gaussian elimination,
- $M^{2}$ into the identity matrix $I^{2}$,
- $M^{\ell}$ into a diagonal+last-1-column matrix, $W_{1}^{\ell}$, $\ell = 3, 4$, 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 $M^{\ell}u^{\ell} = r^{\ell}$, $\ell = 1, 2, \ldots, 6$ in $O(p^{2})$ operations.

Since the Vandermonde-type matrices $M^{\ell}$ 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 $M^{\ell}$, $\ell = 1, 2, 3, 4, 6$

We first describe the zeroing process of a general vector $x = [x_{1}, x_{2}, \ldots, x_{m}]^{T}$ with no zero elements. The lower bidiagonal matrix

$$L_{k} = \begin{bmatrix}
I_{k-1} & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
0 & -\tau_{k+1} & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & -\tau_{m} & 1
\end{bmatrix}, \quad (36)
$$

defined by the multipliers $\tau_{i} = \frac{x_{i}}{x_{i-1}} = -L_{k}(i, i - 1)$, $i = k + 1, k + 2, \ldots, m$, zeros the last $(m - k)$ components, $x_{k+1}, x_{k+2}, \ldots, x_{m}$, of $x$. This zeroing process will be applied recursively on $M^{\ell}$, $\ell = 1, 2, 3, 4, 6$, as follows. For $k = 2, 3, \ldots$, left multiplying $T_{k}^{\ell} = L_{k-1}^{\ell}L_{k-2}^{\ell} \cdots L_{3}^{\ell}L_{2}^{\ell}M^{\ell}$ by $L_{k}^{\ell}$ zeros the last $(m_{\ell} - k)$ components.
of the $k$th column of $T^\ell_k$. Thus we obtain the upper triangular matrix
\begin{align}
L^1 M^1 &= L^1_{m_1-3} \cdots L^1_3 L^1_2 M^1, \\
L^\ell M^\ell &= L^\ell_{m_\ell-1} \cdots L^\ell_3 L^\ell_2 M^\ell, \quad \ell = 2, 3, 4, \\
L^6 M^6 &= L^6_{m_6-2} \cdots L^6_3 L^6_2 M^6, \quad (37)
\end{align}
in $(m_1 - 4), (m_\ell - 2)$, $\ell = 2, 3, 4$ and $(m_6 - 3)$ steps respectively. We note that $L^\ell$ does not change the first two rows of $M^\ell$.

Process 1. At the $k$th step, starting with $k = 2$,
\begin{itemize}
  \item $M^{\ell(k-1)} = L^\ell_{k-1} L^\ell_{k-2} \cdots L^\ell_2 M^\ell$ is an upper triangular matrix in columns 1 to $k - 1$.
  \item The multipliers in $L^\ell_k$ are obtained from $M^{\ell(k-1)}(k+1 : m_\ell, k)$ since $M^\ell(i, k) \neq 0$ for $i = k + 1, k + 2, \ldots, m_\ell$.
\end{itemize}

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

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, $x = [x_1, x_2, \ldots, x_{m-1}, x_m = x_{m-1}]^T$ 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{equation}
\begin{bmatrix}
0 & \cdots & 0 & -\tau_{m-1} & 1 & 0 \\
0 & \cdots & 0 & -\tau_m & 0 & 1
\end{bmatrix}, \quad (40)
\end{equation}
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, $x_{k+1}, x_{k+2}, \ldots, x_m$, of $x$.

We, thus, obtain the upper triangular matrix
\[ L^5 M^5 = L^5_{m_5-3} \cdots L^5_3 L^5_2 M^5, \quad (41) \]
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 $L_k = L^5_k$, $k = 2, 3, \ldots, m_5 - 3$.  

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

For matrix $L^\ell M^\ell$, $\ell = 1, 2, \ldots, 6$, we construct recursively upper bidiagonal matrices $U_1^\ell, U_2^\ell, \ldots, U_{p-3}^\ell$ such that right multiplying $L^\ell M^\ell$ by the upper triangular matrix $U^\ell = U_1^\ell U_2^\ell U_3^\ell \cdots U_{p-3}^\ell$ transforms $L^\ell M^\ell$ into a matrix $W_{C_\ell}^\ell = L^\ell M^\ell U^\ell$ with nonzero diagonal elements, $W_{C_\ell}^\ell(i, i) \neq 0$, $i = 1, 2, \ldots, m_\ell$, the last $C_\ell$ nonzero columns $W_{C_\ell}^\ell(1 : m_\ell, j) \neq 0$, $j = m_\ell - C_\ell + 1, m_\ell - C_\ell + 2, \ldots, m_\ell$, and zero elsewhere. We call such a matrix a “diagonal+last-$C_\ell$-column matrix”. Here

$$C_\ell = 3, \text{ for } \ell = 1, 5, \quad C_2 = 0, \quad C_\ell = 1, \text{ for } \ell = 3, 4, \quad C_6 = 2. \quad (42)$$

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

$$(L^\ell M^\ell)(k : k + 1, 1 : m_\ell) U_k^\ell U_{k+1}^\ell \cdots U_{p-3}^\ell = \begin{bmatrix} y_{k1} & \cdots & y_{kk-1} & 1 & \cdots & 1 & y_{k,m_\ell-C_\ell+1} & y_{k,m_\ell-C_\ell+2} & \cdots & y_{k,m_\ell} \\ y_{k+1,1} & \cdots & y_{kk-1} & y_{k+1,k} & \cdots & y_{k+1,m_\ell-C_\ell+1} & y_{k+1,m_\ell-C_\ell+2} & \cdots & y_{k+1,m_\ell} \end{bmatrix}. \quad (43)$$

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

$$U_k^\ell = \begin{bmatrix} I_{k-1} & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -\sigma_{k+1} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \sigma_{k+1} & -\sigma_{k+2} & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma_{m_\ell-C_\ell-1} & -\sigma_{m_\ell-C_\ell} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & \sigma_{m_\ell-C_\ell} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}. \quad (44)$$

Right multiplying (43) by $U_k^\ell$ zeros the 1’s in position $k + 1, k + 2, \ldots, m_\ell - C_\ell$ in the first row and puts 1’s in position $k + 1, k + 2, \ldots, m_\ell - C_\ell$ in the second row:

$$(L^\ell M^\ell)(k : k + 1, 1 : m_\ell) U_k^\ell U_2^\ell U_3^\ell \cdots U_{p-3}^\ell U_k^\ell = \begin{bmatrix} y_{k1} & \cdots & y_{kk-1} & 1 & 0 & \cdots & 0 & y_{k,m_\ell-C_\ell+1} & y_{k,m_\ell-C_\ell+2} & \cdots & y_{k,m_\ell} \\ y_{k+1,1} & \cdots & y_{kk-1} & y_{k+1,k} & 1 & \cdots & 1 & y_{k+1,m_\ell-C_\ell+1} & y_{k+1,m_\ell-C_\ell+2} & \cdots & y_{k+1,m_\ell} \end{bmatrix}. \quad (45)$$

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-$C_\ell$-column matrix

$$W_{C_\ell}^\ell = L^\ell M^\ell U_1^\ell U_2^\ell \cdots U_{p-3}^\ell. \quad (46)$$

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in \((p - 3)\) steps.

**Process 2.** At the \(k\)th step, starting with \(k = 1\),

- \(M^{\ell(k)} = L^{\ell}M^{\ell}U^{\ell}_{1}U^{\ell}_{2} \ldots U^{\ell}_{k}\) is a diagonal+last-\(C\ell\)-column matrix in rows 1 to \(k\).
- The divisors in \(U^{\ell}_{k}\) are obtained from \(M^{\ell(k-1)}(k+1, k : m_{\ell} - C\ell)\) since \(M^{\ell(k-1)}(k+1, j) - M^{\ell(k-1)}(k+1, j-1) \neq 0, j = k+1, k+2, \ldots, m_{\ell} - C\ell\).

Algorithm 3 in Appendix A describes this process for \(M^{\ell}, \ell = 1, 2, \ldots, 6\). The input is \(M = M^{\ell}; m = m_{\ell}\). The output is \(U^{k}_{k} = U^{\ell}_{k}, k = 1, 2, \ldots, p - 3\).

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

Symbolic elementary matrix functions \(L^{\ell}_{k}\) and \(U^{\ell}_{k}, \ell = 1, 2, \ldots, 6\), are constructed once as functions of \(\eta_{j}\), for \(j = 2, 3, \ldots, p - 2\), by Algorithms 1 to 3 in Appendix A to factor

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

Here \(C\ell\) is defined in (42).

These elementary matrix functions are used, first, to find the solution \(u^{\ell}, \ell = 1, 2, \ldots, 6\) in elementary matrix functions form and, then, to construct fast Algorithms 4, 5, 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 \(M^{\ell}u^{\ell} = r^{\ell}, \ell = 1, 5\)

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 \(M^{\ell}, \ell = 1, 5\), to construct \(m_{\ell} \times m_{\ell}\) lower tridiagonal matrices \(L^{\ell}_{k}, k = 2, 3, \ldots, m_{\ell} - 3\), with multipliers

- (1.a) for \(\ell = 1\), \(\tau_{i} = \frac{M^{1(2,k)}}{i-1} = -L^{1}_{k}(i, i-1)\), \(i = k+1, k+2, \ldots, m_{1}\),
- (1.b) for \(\ell = 5\), \(\tau_{i} = \frac{M^{5(2,k)}}{m_{5}-2} = -L^{5}_{k}(i, i-2)\), \(i = k+1, k+2, \ldots, m_{5} - 1\), and \(\tau_{m_{5}} = \frac{M^{5(2, m_{5})}}{m_{5}-2} = -L^{5}_{k}(m_{5}, m_{5} - 2)\).

Left multiplying the coefficient matrix \(M^{\ell}\) by the lower triangular matrix \(L^{\ell} = L^{\ell}_{m_{\ell} - 3} \ldots L^{\ell}_{2}\) transforms \(M^{\ell}\) 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 $U_k^\ell$, $k = 1, 2, \ldots, p - 3$, with multipliers

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

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

(3) A factored Gaussian elimination, $L_{m_\ell-1}^\ell L_{m_\ell-2}^\ell$, will transform $W_3^\ell$ 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,

$$L_{m_\ell-2}(i, i) = 1, \quad i = 1, 2, \ldots, m_\ell - 3,$$

$$L_{m_\ell-2}(m_\ell - 2, m_\ell - 2) = 1/W_3^\ell(m_\ell - 2, m_\ell - 2),$$

$$L_{m_\ell-2}(i, i) = 1, \quad i = m_\ell - 1, m_\ell.$$

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,

$$L_{m_\ell-1}(i, m_\ell - 2) = -W_3^\ell(i, m_\ell - 2), \quad i = 1, 2, \ldots, m_\ell - 3,$$

$$L_{m_\ell-1}(i, i) = 1, \quad i = 1, 2, \ldots, m_\ell,$$

$$L_{m_\ell-1}(i, m_\ell - 2) = -W_3^\ell(i, m_\ell - 2), \quad i = m_\ell - 1, m_\ell.$$

(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 $W_2^\ell$ 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 $L_k^\ell$, $k = m_\ell, m_\ell + 1, m_\ell + 2, m_\ell + 3$ 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 $M^\ell$ into the identity matrix

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

Thus we have the following factorization of $M^\ell$ into the product of elementary matrices:

$$M^\ell = \left( L_{m_\ell+3}^\ell L_{m_\ell+2}^\ell \cdots L_2^\ell \right)^{-1} \left( U_2^\ell U_2^\ell \cdots U_{p-3}^\ell \right)^{-1}.$$
Table 2: The nonzero entries of Gaussian elimination matrices $L^\ell_k$, $k = m_\ell - 2, m_\ell - 1, \ldots, m_\ell + 3$ for $\ell = 1, 5$.

<table>
<thead>
<tr>
<th>Gaussian elimination matrices</th>
<th>$L^\ell_{m_\ell-2}$</th>
<th>$L^\ell_{m_\ell-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^\ell_{m_\ell-2}(i, i) = 1$, $i = 1, 2, \ldots, m_\ell - 3$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L^\ell_{m_\ell-2}(m_\ell - 2, m_\ell - 2) = 1/W^\ell_2(m_\ell - 2, m_\ell - 2)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L^\ell_{m_\ell-2}(i, i) = 1$, $i = m_\ell - 1, m_\ell$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Gaussian elimination matrices</th>
<th>$L^\ell_{m_\ell}$</th>
<th>$L^\ell_{m_\ell+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^\ell_{m_\ell}(i, i) = 1$, $i = 1, 2, \ldots, m_\ell - 2$</td>
<td>$L^\ell_{m_\ell+1}(1 : m_\ell - 2, m_\ell - 1) = -W^\ell_2(1 : m_\ell - 2, m_\ell - 1)$</td>
<td></td>
</tr>
<tr>
<td>$L^\ell_{m_\ell}(m_\ell - 1, m_\ell - 1) = 1/W^\ell_2(m_\ell - 1, m_\ell - 1)$</td>
<td>$L^\ell_{m_\ell+1}(i, i) = 1$, $i = 1, 2, \ldots, m_\ell$</td>
<td>$L^\ell_{m_\ell+1}(m_\ell, m_\ell - 1) = -W^\ell_3(m_\ell, m_\ell - 1)$</td>
</tr>
<tr>
<td>$L^\ell_{m_\ell}(m_\ell, m_\ell) = 1.$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gaussian elimination matrices</th>
<th>$L^\ell_{m_\ell+2}$</th>
<th>$L^\ell_{m_\ell+3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^\ell_{m_\ell+2}(i, i) = 1$, $i = 1, 2, \ldots, m_\ell - 1$</td>
<td>$L^\ell_{m_\ell+3}(i, i) = 1$, $i = 1, 2, \ldots, m_\ell$</td>
<td>$L^\ell_{m_\ell+3}(1 : m_\ell - 1, m_\ell) = -W^\ell_2(1 : m_\ell - 1, m_\ell)$</td>
</tr>
<tr>
<td>$L^\ell_{m_\ell+2}(m_\ell, m_\ell) = 1/W^\ell_2(m_\ell, m_\ell)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

and the solution is

$$u^\ell = U^\ell_1 U^\ell_2 \cdots U^\ell_{p-3} L^\ell_{m_\ell+3} L^\ell_{m_\ell+2} \cdots L^\ell_2 r^\ell,$$

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 $M = M^\ell$; $m = m_\ell$; $r = r^\ell$; $L_k = L^\ell_k$, $k = 2, 3, \ldots, m_\ell + 3$; $U_k = U^\ell_k$, $k = 1, 2, \ldots, p - 3$. The output is $u = u^\ell$, $\ell = 1, 5$.

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 $P_6$. 

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6.2. Solution of $M^2u^2 = r^2$

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 $L^2 M^2$ in column 1 to $m_2 - 1$ of the form (38). Next, the right-product of the $U^2_k$, $k = 1, 2, \ldots, p - 3$, will transform $L^2 M^2$ 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:

$$M^2 = (L^2_{m_2-1} \cdots L^2_2)^{-1} (U^2_1 U^2_2 \cdots U^2_{p-3})^{-1},$$

and the solution is

$$u^2 = U^2_1 U^2_2 \cdots U^2_{p-3} L^2_{m_2-1} \cdots L^2_2 r^2, \quad (49)$$

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 $M = M^2$; $m = m_2$; $r = r^2$; $L_k = L^2_k$, $k = 2, 3, \ldots, m_2 - 1$; $U_k = U^2_k$, $k = 1, 2, \ldots, p - 3$. The output is $u = u^2$.

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

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 $L^\ell = L^\ell_{m_\ell-1} \cdots L^\ell_3 L^\ell_2$ transforms the coefficient matrix $M^\ell$ 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 $U^\ell_k$, $k = 1, 2, \ldots, p - 3$, will transform $L^\ell M^\ell$ into a diagonal+last-1-column matrix $W^\ell_1$ 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 $m_\ell$ of $W^\ell_1$ and transform $W^\ell_1$ into the identity matrix $I^\ell = L^\ell_{m_\ell+1} L^\ell_{m_\ell} W^\ell_1$ where $L^\ell_k$, $k = m_\ell, m_\ell + 1$ have nonzero entries listed in Table 3 and zeros elsewhere.

This procedure transforms $M^\ell$ into the identity matrix

$$I^\ell = L^\ell_{m_\ell+1} L^\ell_{m_\ell} \cdots L^\ell_2 M^\ell U^\ell_1 U^\ell_2 \cdots U^\ell_{p-3}.$$

Thus we have the following factorization of $M^\ell$ into the product of elementary matrices:

$$M^\ell = \left( L^\ell_{m_\ell+1} L^\ell_{m_\ell} \cdots L^\ell_2 \right)^{-1} \left( U^\ell_1 U^\ell_2 \cdots U^\ell_{p-3} \right)^{-1},$$
Table 3: The nonzero entries of Gaussian elimination matrices \( L^\ell_k, k = m_\ell, m_\ell + 1, \ell = 3, 4 \).

<table>
<thead>
<tr>
<th>Gaussian elimination matrices</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L^\ell_m )</td>
</tr>
<tr>
<td>( L^\ell_m(i, i) = 1, \ i = 1, 2, \ldots, m_\ell - 1 )</td>
</tr>
<tr>
<td>( L^\ell_m(m_\ell, m_\ell) = 1/W^\ell(m_\ell, m_\ell) )</td>
</tr>
<tr>
<td>( L^\ell_{m+1} )</td>
</tr>
<tr>
<td>( L^\ell_{m+1}(i, i) = 1, \ i = 1, 2, \ldots, m_\ell )</td>
</tr>
<tr>
<td>( L^\ell_{m+1}(1 : m_\ell - 1, m_\ell) = -W^\ell(1 : m_\ell - 1, m_\ell) )</td>
</tr>
</tbody>
</table>

and the solution is

\[
\mathbf{u}^\ell = U^\ell_1 U^\ell_2 \cdots U^\ell_{p-3} L^\ell_{m+1} L^\ell_{m_\ell} \cdots L^\ell_2 \mathbf{r}^\ell,
\]

(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 \( M = M^\ell; m = m_\ell; \mathbf{r} = \mathbf{r}^\ell; L_k = L^\ell_k, k = 2, 3, \ldots, m_\ell + 1; U_k = U^\ell_k, k = 1, 2, \ldots, p - 3 \). The output is \( \mathbf{u} = \mathbf{u}^\ell, \ell = 3, 4 \).

6.4. Solution of \( M^6 \mathbf{u}^6 = \mathbf{r}^6 \)

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

(1) Similar to steps (1) and (2) of Subsection 6.1, the matrix \( L^6 = L^6_{m_6-2} \cdots L^6_2 L^6_2 \) 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 \( U^6_1 U^6_2 \cdots U^6_{p-3} \), will transform \( L^6 M^6 \) into a diagonal+last-2-column matrix \( W^6_2 \) of the form (46).

(3) Similar to steps (3) and (4) of Subsection 6.1, factored Gaussian eliminations, \( L^6_{m_6-1} \cdots L^6_{m_6+1} \) will eliminate columns \((m_6-1)\) and \((m_6)\) respectively of \( W^6_2 \) and transform \( W^6_2 \) into the identity matrix

\[
I^6 = L^6_{m_6+2} L^6_{m_6+1} L^6_{m_6} L^6_{m_6-1} W^6_2,
\]

where \( L^6_k, k = m_6 - 1, m_6, m_6 + 1, m_6 + 2 \) have nonzero entries listed in Table 4 and zeros elsewhere. In Table 4, \( W^6_1 = L^6_{m_6-1} W^6_2 \).

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

\[
I^6 = L^6_{m_6+2} L^6_{m_6+1} \cdots L^6_2 M^6 = U^6_1 U^6_2 \cdots U^6_{p-3}.
\]
Table 4: The nonzero entries of Gaussian elimination matrices $L^6_k$, $k = m_6 - 1, m_6, m_6 + 1, m_6 + 2$. 

<table>
<thead>
<tr>
<th>Gaussian elimination matrices $L^6_{m_6-1}$</th>
<th>$L^6_{m_6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I^6_{m_6-1}(i, i) = 1$, $i = 1, 2, \ldots, m_6 - 2$,</td>
<td>$L^6_{m_6}(1 : m_6 - 2, m_6 - 1) = -W^6_2(1 : m_6 - 2, m_6 - 1)$,</td>
</tr>
<tr>
<td>$F^6_{m_6-1}(m_6 - 1, m_6 - 1) = 1/W^6_2(m_6 - 1, m_6 - 1)$,</td>
<td>$L^6_{m_6}(i, i) = 1$, $i = 1, 2, \ldots, m_6$,</td>
</tr>
<tr>
<td>$L^6_{m_6-1}(m_6, m_6) = 1$.</td>
<td>$L^6_{m_6}(m_6, m_6 - 1) = -W^6_2(m_6, m_6 - 1)$.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gaussian elimination matrices $L^6_{m_6+1}$</th>
<th>$L^6_{m_6+2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I^6_{m_6+1}(i, i) = 1$, $i = 1, 2, \ldots, m_6 - 1$,</td>
<td>$L^6_{m_6+2}(i, i) = 1$, $i = 1, 2, \ldots, m_6$,</td>
</tr>
<tr>
<td>$F^6_{m_6+1}(m_6, m_6) = 1/W^6_1(m_6, m_6)$.</td>
<td>$L^6_{m_6+2}(1 : m_6 - 1, m_6) = -W^6_1(1 : m_6 - 1, m_6)$.</td>
</tr>
</tbody>
</table>

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

$$M^6 = (L^6_{m_6+2} \cdots L^6_2)^{-1} (U^6_1 U^6_2 \cdots U^6_{p-3})^{-1},$$

and the solution is

$$u^6 = U^6_1 U^6_2 \cdots U^6_{p-3} T^6_{m_6+2} \cdots T^6_2 r^6,$$

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 $M = M^6$; $m = m_6$; $r = r^6$; $L_k = L^6_k$, $k = 2, 3, \ldots, m_6 + 2$; $U_k = U^6_k$, $k = 1, 2, \ldots, p - 3$. The output is $u = u^6$.

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

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

where

$$F^1 = \begin{bmatrix} y_n, y_{n-1}, \ldots, y_{n-(p-3)}, h_{n+1} F_5, h_{n+1} F_4, h_{n+1} F_3 \end{bmatrix},$$

$$G^1 = \begin{bmatrix} h_{n+1} f(t_n + h, y_{n+1}) \end{bmatrix}.$$
\( \mathbf{u}^1 = [\alpha_0, \alpha_1, \ldots, \alpha_{p-3}, b_5, b_4, b_3]^T, \)
\( \mathbf{v}^1 = [b_6]. \)

It is interesting to note the three decomposition forms of the system \( F \mathbf{u} \):

\[
\begin{align*}
F(ULr) & \quad \text{(generalized Lagrange interpolation)}, \\
(FU)Lr & \quad \text{(generalized divided differences)}, \\
(FUL)r & \quad \text{(Nordsieck’s formulation)}. \\
\end{align*}
\]

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 \( \text{HB}(p), p = 4, 5, \ldots, 10 \), 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

\[
y' = \lambda y, \quad y_0 = 1.
\]

This gives the following difference equation and corresponding characteristic equation

\[
\sum_{j=0}^{k} \eta_j(z) y_{n+j} = 0, \quad \sum_{j=0}^{k} \eta_j(z) r^j = 0,
\]
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 \( \eta_j(z), j = 0, 1, \ldots, k \) in (52) are rational functions of the form

\[
\eta_k(z) = 1, \quad \eta_j(z) = \frac{\sum_{\ell=0}^{j-1} n_{j\ell} z^\ell}{\sum_{\ell=0}^{5} d_{j\ell} z^\ell}, \quad j = 0, 1, \ldots, k - 1.
\]

Hence, in the difference equation of (52), \( y_{n+k} \to 0 \) as \( z \to \infty \). This implies that \( \text{HB}(p), p = 4, 5, \ldots, 10 \) 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 \( \alpha \) angles of \( A(\alpha) \)-stability for HB(\( p \)), FPMEBDF(\( p \)), PMEBDF(\( p \)), HBDF(\( p \)) and MEBDF(\( p \)), respectively.

<table>
<thead>
<tr>
<th>( k )</th>
<th>( p )</th>
<th>( \alpha )</th>
<th>( k )</th>
<th>( p )</th>
<th>( \alpha )</th>
<th>( k )</th>
<th>( p )</th>
<th>( \alpha )</th>
<th>( k )</th>
<th>( p )</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>90.00°</td>
<td>1</td>
<td>2</td>
<td>90.00°</td>
<td>2</td>
<td>2</td>
<td>90.00°</td>
<td>1</td>
<td>2</td>
<td>90.00°</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>90.00°</td>
<td>2</td>
<td>3</td>
<td>90.00°</td>
<td>3</td>
<td>3</td>
<td>90.00°</td>
<td>3</td>
<td>4</td>
<td>90.00°</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>90.00°</td>
<td>4</td>
<td>5</td>
<td>89.71°</td>
<td>4</td>
<td>5</td>
<td>89.32°</td>
<td>5</td>
<td>5</td>
<td>89.77°</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>90.00°</td>
<td>5</td>
<td>6</td>
<td>88.01°</td>
<td>5</td>
<td>6</td>
<td>86.19°</td>
<td>6</td>
<td>6</td>
<td>88.36°</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
<td>90.00°</td>
<td>6</td>
<td>7</td>
<td>84.67°</td>
<td>6</td>
<td>7</td>
<td>80.60°</td>
<td>7</td>
<td>7</td>
<td>85.97°</td>
</tr>
<tr>
<td>6</td>
<td>8</td>
<td>90.00°</td>
<td>7</td>
<td>8</td>
<td>78.70°</td>
<td>7</td>
<td>8</td>
<td>72.63°</td>
<td>8</td>
<td>8</td>
<td>82.42°</td>
</tr>
<tr>
<td>7</td>
<td>9</td>
<td>90.00°</td>
<td>8</td>
<td>9</td>
<td>65.01°</td>
<td>8</td>
<td>9</td>
<td>60.60°</td>
<td>9</td>
<td>9</td>
<td>77.75°</td>
</tr>
<tr>
<td>8</td>
<td>10</td>
<td>75.38°</td>
<td></td>
<td>9</td>
<td>9</td>
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<td>10</td>
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<td>70.18°</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>11</td>
<td>58.96°</td>
<td></td>
<td>12</td>
<td>12</td>
<td>46.12°</td>
<td></td>
<td>12</td>
<td>12</td>
<td>46.12°</td>
<td></td>
</tr>
</tbody>
</table>

Table 5 lists the \( \alpha \) 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, \( \alpha \) of HB methods compare favorably with \( \alpha \) of the considered methods of the same order.

8. Controlling step size

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

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

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 \( \eta_2, \eta_3, \ldots, \eta_{p-2} \), 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 \(\tilde{y}_{n+1}\) are obtained by formulae (2)–(4).

(e) The step is accepted if \(\|y_{n+1} - \tilde{y}_{n+1}\|_\infty\) 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,

\[
EPE = \{\|y_{\text{end}} - z_{\text{end}}\|_\infty\},
\]

where \(y_{\text{end}}\) is the numerical value obtained by the numerical method at the endpoint \(t_{\text{end}}\) of the integration interval and \(z_{\text{end}}\) is the “exact solution” obtained by MATLAB’s `ode15s` with stringent tolerance \(5 \times 10^{-14}\).

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

Computations were performed on a PC with the following characteristics: Memory: 5.8 GB, Processor 0,1,\ldots,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\((p)\), \(p = 4,5,\ldots,9\) are suitable for such problems.

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

Problem 1.

\[
\begin{align*}
y_1' &= -10y_1 + \alpha y_2, & y_1(0) &= 1, \\
y_2' &= -\alpha y_1 - 10y_2 & y_2(0) &= 1, \\
y_3' &= -4y_3 & y_3(0) &= 1, \\
y_4' &= -y_4 & y_4(0) &= 1, \\
y_5' &= -0.5y_5 & y_5(0) &= 1, \\
y_6' &= -0.1y_6 & y_6(0) &= 1, \\
\end{align*}
\]

with \(\alpha = 500\) and \(t_{\text{end}} = 20\).
(2) As above with $\alpha = 1000$.

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

Problem 2.

\[
\begin{align*}
y_1' &= -\alpha y_1 - \beta y_2 + (\alpha + \beta - 1)e^{-t} \quad y_1(0) = 1, \\
y_2' &= \beta y_1 - \alpha y_2 + (\alpha - \beta - 1)e^{-t} \quad y_2(0) = 1, \\
y_3' &= 1 \\
y_3(0) &= 0,
\end{align*}
\]

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]),

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

where $NFE_{1,ij}$ and $NFE_{2,ij}$ are the estimates of NFE of methods 1 and 2, respectively, associated with problem $i$, and estimate of EPE = $10^{-j}$. To compute $NFE_{2,j}$ and $NFE_{1,j}$ 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 α = 500.

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

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 α = 1000.

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

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

<table>
<thead>
<tr>
<th>Problem</th>
<th>NFE PEG of HB(8) over: MEBDF(4)</th>
<th>NFE PEG of HB(9) over: MEBDF(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prob. B5 with α = 500</td>
<td>176%</td>
<td>213%</td>
</tr>
<tr>
<td>Prob. B5 with α = 1000</td>
<td>181%</td>
<td>180%</td>
</tr>
</tbody>
</table>
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, $\alpha$ 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, $\alpha$ angles of $L(\alpha)$-stability of HB($p$), $p = 4, 5, \ldots, 10$ compare favorably with $\alpha$ 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.

Acknowledgment

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.
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 $t$.

<table>
<thead>
<tr>
<th></th>
<th>HB methods</th>
<th>MEBDF methods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$</td>
<td>\text{Error in } y_1</td>
</tr>
<tr>
<td>$p = 4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.791 \times 10^{-7}$</td>
<td>$0.477 \times 10^{-7}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.533 \times 10^{-9}$</td>
<td>$0.321 \times 10^{-9}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.359 \times 10^{-11}$</td>
<td>$0.216 \times 10^{-11}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.242 \times 10^{-13}$</td>
<td>$0.145 \times 10^{-13}$</td>
</tr>
<tr>
<td>$p = 5$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.161 \times 10^{-8}$</td>
<td>$0.227 \times 10^{-9}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.108 \times 10^{-10}$</td>
<td>$0.153 \times 10^{-11}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.731 \times 10^{-13}$</td>
<td>$0.103 \times 10^{-13}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.492 \times 10^{-15}$</td>
<td>$0.697 \times 10^{-16}$</td>
</tr>
<tr>
<td>$p = 6$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.255 \times 10^{-10}$</td>
<td>$0.652 \times 10^{-12}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.171 \times 10^{-12}$</td>
<td>$0.443 \times 10^{-14}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.115 \times 10^{-14}$</td>
<td>$0.298 \times 10^{-16}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.779 \times 10^{-17}$</td>
<td>$0.201 \times 10^{-18}$</td>
</tr>
<tr>
<td>$p = 7$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.484 \times 10^{-11}$</td>
<td>$0.335 \times 10^{-11}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.326 \times 10^{-13}$</td>
<td>$0.226 \times 10^{-13}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.220 \times 10^{-15}$</td>
<td>$0.152 \times 10^{-15}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.148 \times 10^{-17}$</td>
<td>$0.102 \times 10^{-17}$</td>
</tr>
<tr>
<td>$p = 8$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.194 \times 10^{-12}$</td>
<td>$0.138 \times 10^{-12}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.129 \times 10^{-14}$</td>
<td>$0.929 \times 10^{-15}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.872 \times 10^{-17}$</td>
<td>$0.626 \times 10^{-17}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.587 \times 10^{-19}$</td>
<td>$0.422 \times 10^{-19}$</td>
</tr>
<tr>
<td>$p = 9$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t = 5.0$</td>
<td>$0.351 \times 10^{-14}$</td>
<td>$0.476 \times 10^{-15}$</td>
</tr>
<tr>
<td>$t = 10.0$</td>
<td>$0.242 \times 10^{-16}$</td>
<td>$0.271 \times 10^{-17}$</td>
</tr>
<tr>
<td>$t = 15.0$</td>
<td>$0.166 \times 10^{-18}$</td>
<td>$0.201 \times 10^{-19}$</td>
</tr>
<tr>
<td>$t = 20.0$</td>
<td>$0.109 \times 10^{-20}$</td>
<td>$0.130 \times 10^{-21}$</td>
</tr>
</tbody>
</table>
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 $t$.

<table>
<thead>
<tr>
<th>$p$</th>
<th>HB methods</th>
<th>MEBDF methods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$</td>
<td>\text{Error in } y_1</td>
</tr>
<tr>
<td>4</td>
<td>$t = 5.0$</td>
<td>$0.852 \times 10^{-7}$, $0.109 \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.590 \times 10^{-9}$, $0.106 \times 10^{-9}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.316 \times 10^{-11}$, $0.333 \times 10^{-11}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.278 \times 10^{-13}$, $0.125 \times 10^{-13}$</td>
</tr>
<tr>
<td>5</td>
<td>$t = 5.0$</td>
<td>$0.166 \times 10^{-8}$, $0.274 \times 10^{-9}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.112 \times 10^{-10}$, $0.184 \times 10^{-11}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.757 \times 10^{-13}$, $0.124 \times 10^{-13}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.510 \times 10^{-15}$, $0.839 \times 10^{-16}$</td>
</tr>
<tr>
<td>6</td>
<td>$t = 5.0$</td>
<td>$0.570 \times 10^{-10}$, $0.138 \times 10^{-11}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.782 \times 10^{-13}$, $0.140 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.281 \times 10^{-14}$, $0.237 \times 10^{-14}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.464 \times 10^{-17}$, $0.273 \times 10^{-16}$</td>
</tr>
<tr>
<td>7</td>
<td>$t = 5.0$</td>
<td>$0.516 \times 10^{-11}$, $0.357 \times 10^{-11}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.341 \times 10^{-13}$, $0.237 \times 10^{-13}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.230 \times 10^{-15}$, $0.159 \times 10^{-15}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.155 \times 10^{-17}$, $0.107 \times 10^{-17}$</td>
</tr>
<tr>
<td>8</td>
<td>$t = 5.0$</td>
<td>$0.538 \times 10^{-12}$, $0.310 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.380 \times 10^{-14}$, $0.652 \times 10^{-15}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.770 \times 10^{-16}$, $0.161 \times 10^{-16}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.688 \times 10^{-18}$, $0.693 \times 10^{-18}$</td>
</tr>
<tr>
<td>9</td>
<td>$t = 5.0$</td>
<td>$0.230 \times 10^{-13}$, $0.122 \times 10^{-13}$</td>
</tr>
<tr>
<td></td>
<td>$t = 10.0$</td>
<td>$0.144 \times 10^{-14}$, $0.134 \times 10^{-14}$</td>
</tr>
<tr>
<td></td>
<td>$t = 15.0$</td>
<td>$0.651 \times 10^{-16}$, $0.118 \times 10^{-15}$</td>
</tr>
<tr>
<td></td>
<td>$t = 20.0$</td>
<td>$0.162 \times 10^{-17}$, $0.905 \times 10^{-17}$</td>
</tr>
</tbody>
</table>
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 \( \eta_j \), \( j = 2, 3, \ldots, p - 2 \).

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 \( \eta_j \), \( j = 2, 3, \ldots, p - 2 \).

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 \( IF, P_i, i = 2, 3, \ldots, 6 \)) as functions of \( \eta_j \), \( j = 2, 3, \ldots, p - 2 \).

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

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

for \( k = 2, 3, \ldots, m - 3 \), compute

\[
r(i) = r(i) + r(i - 1)L_k(i, i - 1), \quad i = m, m - 1, \ldots, k + 1.
\]
Step (2) This step forms the two matrices $L_{m-2}$ and $L_{m-1}$ which transform $W_{2}^{3}$ into a diagonal+last-2-column matrix $W_{2}^{4} = L_{m-1}L_{m-2}W_{2}^{3}$ (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 $L_{m-3}L_{m-4} \cdots L_{2}G_{m-2}(1 : m)$: for $k = 3, 4, \ldots, m − 3$, 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 $r$ with $L_{m-1}L_{m-2}r$:

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

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 $W_{2}^{3}$ into a diagonal+last-1-column matrix $W_{2}^{4} = L_{m+1}L_{m}W_{2}^{3}$ (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 $r$ with $L_{m+1}L_{m}r$:

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

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 $W_{2}^{3}$ into the identity matrix $I^{3} = L_{m+3}L_{m+2}W_{2}^{3}$ (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 $r$ with $L_{m+3}L_{m+2}r$:

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

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 $r = r(1 : m)$ with $U_{1}U_{2} \cdots U_{p-3}r$:

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

$$r(i) = r(i)U_{k}(i, i), \quad i = k + 1, k + 2, \ldots, p - 2,$$

$$r(i) = r(i) - r(i + 1), \quad i = k, k + 1, \ldots, p - 3.$$
**Definition 5.** This algorithm solves the systems for $P_2$ in $O(m^2)$ operations.

Given $[n_2, n_3, \ldots, n_p - 2]$ and $r = r(1 : m)$, the following algorithm overwrites $r$ with the solution $u = u(1 : m)$ of the system $Mu = r$.

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

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

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

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

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

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

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

Given $[n_2, n_3, \ldots, n_p - 2]$ and $r = r(1 : m)$, the following algorithm overwrites $r$ with the solution $u = u(1 : m)$ of the system $Mu = r$.

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

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

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

Step (2) Similar to Step (2) of Algorithm 4, this step forms the two matrices $L_m$ and $L_{m+1}$ which transform $W_1^\ell$ into the identity matrix $I^\ell = L_{m+1}L_m W_1^\ell$ (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 $r$ with $L_{m+1}L_m r$:

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

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 $r = r(1 : m)$ with $U_1U_2\cdots U_{p-2}r$:

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

$$r(i) = r(i)U_k(i, i), \quad i = k, k + 1, \ldots, p - 2,$$

$$r(i) = r(i) - r(i + 1), \quad i = k, k + 1, \ldots, p - 3.$$ 

**Definition 7.** This algorithm solves the systems for $P_6$ in $O(m^2)$ operations.

Given $[n_2, n_3, \ldots, n_p - 2]$ and $r = r(1 : m)$, the following algorithm overwrites $r$ with the solution $u = u(1 : m)$ of the system $Mu = r$. 

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Step (1) The following iteration overwrites $\mathbf{r} = r(1 : m)$ with $L_{m-2}L_{m-3} \cdots L_3 L_2 \mathbf{r}$:

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

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

Step (2) Similar to Step (2) of Algorithm 4, this step forms the two matrices $L_{m-1}$ and $L_m$ which transform $W_2^1$ into a diagonal+last-1-column matrix $W_2^1 = L_m L_{m-1} W_2^1$ (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 $L_{m-1}$ and $L_m$ by means of the formulae in Table 4.

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

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

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 (4) Similar to Step (2) of Algorithm 4, this step forms the two matrices $L_{m+1}$ and $L_{m+2}$ which transform $W_2^1$ into the identity matrix $I^4 = L_{m+2} L_{m+1} W_2^1$ (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 $L_{m+1}$ and $L_{m+2}$ by means of the formulae in Table 4.

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

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

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

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

Step (6) The following iteration overwrites $\mathbf{r} = r(1 : m)$ with $U_1 U_2 U_3 \cdots U_{p-3} \mathbf{r}$:

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

$$r(i) = r(i)U_k(i, i), \quad i = k + 1, k + 2, \ldots, p - 2,$$

$$r(i) = r(i) - r(i + 1), \quad i = k, k + 1, \ldots, p - 3.$$ 

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

The appendix lists the coefficients of HB($p$), of order $p = 4, 5, \ldots, 10$, 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$(p)$, $p = 4, 5$.

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References


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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($p$), $p = 6, 7, 8.$

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

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| $\alpha_{31}$ | -3.491366118922240e+00 | -3.233430888270326e+00 |
| $\alpha_{32}$ | 6.9922614796593874e+00 | 2.023248951556358e+00 |
| $\alpha_{33}$ | -5.8651497908953995e+00 | -2.365162910148855e+00 |
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| $c_4$ | 1.052000000000000e+00 | 1.452000000000000e+00 |
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| $\alpha_{43}$ | -5.2627657036055580e+00 | -1.95594890148530e+00 |
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| $\alpha_{56}$ | 2.078030358789702e+00 | 7.401169641988057e+01 |
| $\alpha_{57}$ | -8.203164933952530e-02 | 1.3980427101442936e+00 |
Table 14: Coefficients of the integration formulae of HB($p$), $p = 9, 10$.

<table>
<thead>
<tr>
<th>coeffs$p$</th>
<th>$\gamma$</th>
<th>9</th>
<th>10</th>
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<tr>
<td>$b_3$</td>
<td>-7.1376451203220892e-02</td>
<td>5.8961559344410308e-01</td>
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<td>$b_4$</td>
<td>-5.2219295224276951e-01</td>
<td>-9.862791354955615e-01</td>
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<td>$b_5$</td>
<td>1.9079760073720756e-01</td>
<td>6.2459702553550611e-01</td>
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<td>$\alpha_0$</td>
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<td>1.6185042823909392e+00</td>
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<td>-1.0101582667631400e+00</td>
<td>-1.0785341697667015e+00</td>
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<td>$\alpha_2$</td>
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<td>7.5235609762454214e-01</td>
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<td>-4.3472594292619663e-01</td>
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<td>1.8706274745664486e-01</td>
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<tr>
<td>$\alpha_5$</td>
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<td>-5.6153086156631126e-02</td>
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<tr>
<td>$\alpha_6$</td>
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<td>1.0376365282931491e-02</td>
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<tr>
<td>$\alpha_7$</td>
<td>-8.8666489590660578e-04</td>
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