Interpolating Runge-Kutta methods for vanishing delay differential equations

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Abstract. In the numerical solution of delay differential equations by a continuous explicit Runge-Kutta method a difficulty arises when the delay vanishes or becomes smaller than the stepsize the method would like to use. In this situation the standard explicit sequential process of computing the Runge-Kutta stages become an implicit process and an iteration scheme must be adopted. We will consider several alternative iteration schemes and investigate their order.

Key Words: Runge-Kutta methods, interpolations, iterations, delay differential equations

AMS Subject Classifications: 65L05, 65L06

1. Introduction

Consider the following delay differential equations (DDEs):

$$\begin{aligned} y'(x) &= f(x, y(x), y(x - \sigma(x, y(x)))), \quad x \geq x_0, \\ y(x) &= \phi(x), \qquad\qquad\qquad\qquad\quad x \leq x_0, \end{aligned} \tag{1.1}$$

where y, f, ϕ are n-vector functions. DDEs emerge from mathematical models for various real life problems ranging from population dynamics to two-body problem of electrodynamics. There are two main challenges to integrate the system (1.1) numerically: vanishing delays and derivative discontinuities. In this paper, we will focus on dealing with the former problem with Runge-Kutta methods. A vanishing delay occurs when $\sigma(x, y) \to 0$. In such cases, a delay may fall in the current step where there is no available approximant for computing the delayed argument, $(x - \sigma(x, y(x)))$, or the solution value at the delayed argument (required for the associated derivative evaluation). This situation can also arise particularly at relaxed tolerance when the delay does not vanish but the actual optimal stepsize is larger than the size of the delay. Several authors have investigated numerical methods for vanishing delay problems, for example, Tavernini [14], Paul [12], Hayashi & Enright [5], Karoui & Vaillancourt [8]. We shall propose a new approach which combines an iteration method and an interpolation technique based on two timesteps for Runge-Kutta methods. Our numerical tests show favorable aspects compared with the existing approaches.

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An s-stage explicit Runge-Kutta formula, when applied to standard initial value problems, has the form for $n \geq 0$

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i f(x_n + c_i h_n, Y_i) \tag{1.2}$$

where

$$Y_i = y_n + h_n \sum_{j=1}^{i-1} a_{i,j} f(x_n + c_j h_n, Y_j). \tag{1.3}$$

The formula can be represented by the tableau

$$\begin{array}{c|ccccc} 0 & 0 & & & & \\ c_2 & a_{2,1} & 0 & & & \\ c_3 & a_{3,1} & a_{3,2} & 0 & & \\ \vdots & & & & & \\ c_s & a_{s,1} & a_{s,2} & \ldots & a_{s,s-1} & 0 \\ \hline & b_1 & b_2 & \ldots & b_{s-1} & b_s \end{array}$$

Continuous Runge-Kutta methods, i.e, Runge-Kutta methods with interpolants, have been investigated extensively (See for example, [6], [4], [11], [15]). By appending an additional $\bar{s} - s$ stages to the discrete RK formula, the general form of a continuous Runge-Kutta formula is

$$u(x_n + \tau h_n) = y_n + h_n \sum_{i=1}^{\bar{s}} \bar{b}_i(\tau) f(x_n + c_i h_n, Y_i) \tag{1.4}$$

where $\tau = (x - x_n)/h_n$ and $0 \leq \tau \leq 1$. The corresponding continuous tableau is

$$\begin{array}{c|cccccc} 0 & 0 & & & & & \\ c_2 & a_{2,1} & 0 & & & & \\ c_3 & a_{3,1} & a_{3,2} & 0 & & & \\ \vdots & & & & & & \\ c_s & a_{s,1} & a_{s,2} & \ldots & a_{s,s-1} & 0 & \\ 1 & b_1 & b_2 & \ldots & b_{s-1} & b_s & 0 \\ \vdots & & & & & & \\ c_{\bar{s}+1} & a_{\bar{s}+1,1} & a_{\bar{s}+1,2} & \ldots & & a_{\bar{s}+1,\bar{s}} & 0 \\ \hline & \bar{b}_1(\tau) & \bar{b}_2(\tau) & \ldots & & \bar{b}_{\bar{s}}(\tau) & \bar{b}_{\bar{s}+1}(\tau) \end{array}$$

Note that with $c_{s+1} = 1$ and the weights $a_{s+1,j} = b_j = \bar{b}_j(1)$, we have $Y_{s+1} = y_{n+1}$ and the corresponding derivative value will be re-used as the first stage of the next step. With this form of the continuous tableau it is also easy to define the $\bar{b}_i(\tau)$ so that $u(t)$ will interpolate the solution and derivative at x_n and x_{n+1}.

2. Interpolations based on two timestep intervals

The above standard continuous Runge-Kutta method can be used effectively in solving non-vanishing delay problems, but are not directly suitable for vanishing delay problems, since the interpolant can only be constructed after all the stage values on the current step are available. For the vanishing delay problem, the delay may fall in the current step, and the associated delayed solution values required in the evaluation of the current stage values are not available. We may consider extending the interpolant from the last step to the current step, but it is not always suitable due to the large local truncation error on the interval $[x_{n-1}, x_{n-1} + 2h_{n-1}]$, compared to that on the interval $[x_{n-1}, x_{n-1} + h_{n-1}]$. We can illustrate this by considering the interpolant for a sixth order Runge-Kutta formula in [4], the local error on $[x_{n-1}, x_{n-1} + 2h_{n-1}]$ can be 90 times larger than that on $[x_{n-1}, x_{n-1} + h_{n-1}]$.

Although it may not be appropriate to extend an interpolant over the next complete step, it may be appropriate to extend the interpolant to one stage. Our main idea is to provide special interpolants based on all the available information from the last step and the early stages of the current step. When computing the stage value $f(x_n + c_{i+1}h_n, Y_i, y(\cdot))$ in which the delay falls in the current step, we construct an interpolant on $[x_{n-1}, x_n + c_ih_n]$ based on the last step and the i stages of the current step. This interpolant is then extended to the interval $[x_{n-1}, x_n + c_{i+1}h_n]$ in order to determine any delay values associated with this stage value. That is, we provide an interpolant for each stage in the current step when necessary. Note that we are assuming here that at least for the first few stages (small m) $c_2 < c_3 < \cdots < c_m < 1$ and c_2 satisfies $c_2h_n < h_{n-1}$. This condition is satisfied for most commonly used RK formulas and for most stepsize control strategies.

If the delay falls in the interval $[x_n, x_n + c_2h_n]$ no new information is available and therefore when computing the second stage, we just extend the interpolant from the last step. In that case, we make use of the standard continuous Runge-Kutta formula, for example, those discussed in Enright et al [4].

After the second stage, when the delay falls on the interval $[x_n + c_2h_n, x_n + h_n]$ in the computation of the $(i+2)$-th stage, we construct an interpolant of the form

$$u_i(x_{n-1} + \tau h_{n-1}) = y_{n-1} + h_{n-1}\sum_{j=1}^{s} b_{i,j}(\tau)\tilde{Y}_j + h_{n-1}\sum_{j=1}^{i+1} b_{i,s+j}(\tau)Y_j, \quad 0 \le \tau \le 1 + rc_{i+1}, \quad (2.1)$$

where $\tilde{Y}_j, Y_j$ are the stages associated with the last and current step respectively; and $r = h_n/h_{n-1}$. For simplicity, we do not make use of the $\bar{s} - s$ appended stages in constructing the special interpolants (the order cannot be increased through the use of the appended stages). We denote u_1 as the interpolant on the interval $[x_{n-1}, x_n + c_2h_n]$, u_i as the interpolant on the interval $[x_{n-1}, x_n + c_{i+1}h_n]$, for $i = 1, 2, \ldots, s_1$ where s_1 is the maximum number of interpolants necessary. Since (1.2) and (1.3) hold for all $n \ge 0$, we have

$$
\begin{aligned}
Y_i &= y_n + h_n \sum_{j=1}^{i-1} a_{i,j} f(x_n + h_n c_i, Y_j) \\
&= y_{n-1} + h_{n-1} \sum_{j=1}^{s} b_i f(x_{n-1} + c_j h_{n-1}, \tilde{Y}_j) \\
&\quad + h_{n-1} \sum_{j=1}^{i-1} a_{i,j} \frac{h_n}{h_{n-1}} f(x_{n-1} + h_{n-1}(1 + \frac{h_n}{h_{n-1}} c_i), Y_j).
\end{aligned}
$$

Such an interpolation scheme can then be represented by the tableau

0	0									
c_2	$a_{2,1}$	0								
c_3	$a_{3,1}$	$a_{3,2}$	0							
$\vdots$										
c_s	$a_{s,1}$	$a_{s,2}$	$\ldots$	$a_{s-1,s}$	0					
1	b_1	b_2	$\ldots$	b_{s-1}	b_s	0				
$1 + rc_2$	b_1	b_2	$\ldots$	b_{s-1}	b_s	$ra_{2,1}$	0			
$1 + rc_3$	b_1	b_2	$\ldots$	b_{s-1}	b_s	$ra_{3,1}$	$ra_{3,2}$	0		
$\vdots$										
$1 + rc_{i+1}$	b_1	b_2	$\ldots$	b_{s-1}	b_s	$ra_{i+1,1}$	$ra_{i+1,2}$	$\ldots$	$ra_{i+1,i}$	0
	$b_{i,1}(\tau)$	$b_{i,2}(\tau)$	$\ldots$	$b_{i,s-1}(\tau)$	$b_{i,s}(\tau)$	$b_{i,s+1}(\tau)$	$b_{i,s+2}(\tau)$	$\ldots$	$b_{i,s+i}(\tau)$	$b_{i,s+i+1}(\tau)$

where the coefficients

$$
b_{i,j}(\tau) = \sum_{\ell=1}^{p} b_{i,j,\ell} \tau^{\ell}. \tag{2.2}
$$

The above tableau has the same form as the standard continuous Runge-Kutta so that the approach ([11], [15]) for analyzing the order and local error can be adopted here. The order condition for the interpolants is

$$
\sum_{j=1}^{s+i+1} b_{i,j}(\tau) \phi_j(\tau) = \frac{\tau^{r(t)}}{\gamma(t)}
$$

for all real $\tau \in \mathbb{R}$, and each tree $t \in T$ such that $1 \leq r(t) \leq p$ where $\phi_j(t)$ is the elementary weight for stage j. That is, the coefficients $b_{i,j,\ell}$ satisfy

$$
\sum_{j=1}^{s+i+1} b_{i,j,\ell} \phi_j(\tau) = \frac{\delta_{j,\ell}}{\gamma(t)} \tag{2.3}
$$

where $\delta_{j,\ell}$ is Kronecker delta. Solving the order equation (2.3), we get the coefficients $b_{i,j,\ell}$ as rational functions of r. There are some free parameters $b_{i,j,\ell}$ to be determined for minimizing the local truncation error.

Define the local solution $y_{n-1}(x)$ to the initial value problem $y' = f(x, y(x))$, $y(x_{n-1}) = y_{n-1}$, then the local truncation error for an interpolant of order p can be written as

$$\begin{aligned} &|y_{n-1}(x_{n-1} + \tau h_{n-1}) - u(x_{n-1} + \tau h_{n-1})| \\ &\quad = \frac{h_{n-1}^{p+1}}{(p+1)!} \left| \sum_{i=1}^{N_{p+1}} e_i(\tau) \alpha_i F_i(x_{n-1}, y_{n-1}) \right| + \mathcal{O}(h_{n-1}^{p+2}), \end{aligned} \tag{2.4}$$

where $F_i := F(t_i)$ is the elementary differential corresponding to the tree t_i, $\alpha_i := \alpha(t_i)$ is a positive integer weight corresponding to the tree t_i and $e_i(\tau)$, $i = 1, \ldots, N_{p+1}$ are the error polynomials given by

$$e_i(\tau) = \tau^{\rho(t_i)} - \gamma(t_i) \sum_{j=1}^{s} \phi_{i,j} b_{i,j}(\tau), \quad i = 1, \ldots, N_{p+1}. \tag{2.5}$$

In the literature, the way to minimize the 'size' of the coefficient of h_{n-1}^{p+1} in (2.4) is not consistent. For example, Enright et al [4] consider minimizing

$$\max_{i \le N_{p+1}} \{ \max_{\tau \in [0,1]} |e_i(\tau)| \} \text{ and } \max_{i \le N_{p+1}} \{ \max_{\tau \in [0,2]} |e_i(\tau)| \}$$

while Calvo et al [1] minimize the quantity

$$g^* = \int_0^1 g(\tau) d\tau$$

over the free parameters, where

$$g(\tau) = \sqrt{\frac{\sum_{i=1}^{N_{p+1}} [e_i(\tau)\alpha(t_i)]^2}{\sum_{i=1}^{N_{p+1}} [e_i(1)\alpha(t_i)]^2}}.$$

Since our coefficients $b_{i,j}(\tau)$ are functions of the variable τ and r, it is more complicated than the interpolation for one timestep. For convenience we choose to minimize the quantity

$$\int_0^{1+rc_{i+2}} \sum_{i=1}^{N_{p+1}} [e_i(\tau)\alpha(t_i)]^2 d\tau, \tag{2.6}$$

in which the variable τ is eliminated by integration. Since the coefficients are continuous functions of r and the stepsize does not change dramatically in practice, we can consider minimizing (2.6) at fixed $r = 1$. Then (2.6) is reduced to a quadratic form of the free parameters $b_{i,j,\ell}$ and optimal values can be determined numerically.

In deriving suitable u_i for low values of i ($i = 1$ or $i = 2$) a special difficulty arises because of the low order of accuracy associated with the corresponding Y_i. As the 'suitability' of u_1 and u_2 require that we use information associated with the 'extended' interval, $[x_{n-1} + h_{n-1}, x_{n-1} + (1 + r)c_i h_{n-1}]$ for $i = 1$ and $i = 2$ respectively, we are forced to either use Y_1 and Y_2 directly or use them indirectly (by introducing extra intermediate stages) in defining their interpolants. In either case u_1 and u_2 will be of lower order than desired and an overall iteration will be required to ensure that the full order of the continuous formula is realized.

3. An example of the special interpolants for a RK formula

According to the procedure described in section 2, we constructed interpolants for the seven-stage RK formula of order six developed by Verner and used in the subroutine DVERK [7]. Its coefficient tableau is the following

0	0						
$\frac{1}{6}$	$\frac{1}{6}$	0					
$\frac{4}{15}$	$\frac{4}{75}$	$\frac{16}{75}$	0				
$\frac{2}{3}$	$\frac{5}{6}$	$\frac{-8}{3}$	$\frac{5}{2}$	0			
$\frac{5}{6}$	$\frac{-165}{64}$	$\frac{55}{6}$	$\frac{-425}{64}$	$\frac{85}{96}$	0		
$\frac{1}{15}$	$\frac{-8263}{15000}$	$\frac{124}{75}$	$\frac{-643}{680}$	$\frac{-81}{250}$	$\frac{2484}{10625}$	0	
1	$\frac{3501}{1720}$	$\frac{-300}{43}$	$\frac{297275}{52632}$	$\frac{-319}{2322}$	$\frac{24068}{84065}$	$\frac{3850}{26703}$	0
	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$

The original DVERK is an eight-stage RK formula-pair with order five and six. We only make use of the sixth order formula since we adopt defect error control (see [2]). The sixth stage is then not used for the sixth order formula. The standard interpolant u based on one step has been developed for DVERK in [4]. We use the modification of u proposed in [3]), where the corresponding code is called CRK6N, since the latter interpolant does not use the sixth stage. The interpolant u is used on the interval $[x_{n-1}, x_n + h_n/6]$ and its coefficients can be found in [3].

Now we construct the interpolants u_1, u_2, u_3, u_4 (here $s_1 = 4$) based on the intervals $[x_{n-1}, x_n + h_n/6]$, $[x_{n-1}, x_n + 4h_n/15]$, $[x_{n-1}, x_n + 2h_n/3]$, $[x_{n-1}, x_n + 5h_n/6]$ and use them on the intervals $[x_{n-1}, x_n + 4h_n/15]$, $[x_{n-1}, x_n + 2h_n/3]$, $[x_{n-1}, x_n + 5h_n/6]$ and $[x_{n-1}, x_n + h_n]$ respectively. The resulting code for delay differential equations with vanishing delay will be called DDRK6N. Once u_4 is constructed, we shall use it for the calculation of all subsequent stages, $Y_6, Y_7, \ldots, Y_{11}$ required before the initial approximation to the standard interpolant can be derived. If we do not introduce intermediate stages, the interpolants u_3, u_4 are of order 5, while u_1, u_2 are only of order 3 and 4 respectively. We have found it effective to introduce one intermediate stage to construct each of u_1, u_2 such that they are of order 4 and 5 respectively. To solve the order equation (2.3) for the corresponding interpolants, we modified a MAPLE program (developed by J. Butcher and J. Verner with modifications by P. Sharp). There were some free parameters $b_{i,j,\ell}$, which were determined by minimizing the quantity (2.6) for $r = 1$. The subroutine 'DUMINF' in the IMSL library was then called to numerically solve the optimization problem, which is a quadratic form with respect to the free parameters $b_{i,j,\ell}$.

The resulting numerical method need only construct $u_i, i = 1, \ldots, 4$ when necessary, i.e., the delay in the corresponding stage falls beyond x_n. The 'extra' intermediate stages at $1 + r/6$ and $1 + 4r/15$ only contribute to u_1 and u_2 respectively. That is, the extra stage at $1 + r/6$ is not computed unless u_1 is required, neither is the extra stage at $1 + 4r/15$ unless u_2 is required.

Table 1: Tableau for DDRK6N

0	0										
$\frac{1}{6}$	$\frac{1}{6}$	0									
$\frac{4}{15}$	$\frac{4}{75}$	$\frac{16}{75}$	0								
$\frac{2}{3}$	$\frac{5}{6}$	$\frac{-8}{3}$	$\frac{5}{2}$	0							
$\frac{5}{6}$	$\frac{-165}{64}$	$\frac{55}{6}$	$\frac{-425}{64}$	$\frac{85}{96}$	0						
$\frac{1}{15}$	$\frac{-8263}{15000}$	$\frac{124}{75}$	$\frac{-643}{680}$	$\frac{-81}{250}$	$\frac{2484}{10625}$	0					
1	$\frac{3501}{1720}$	$\frac{-300}{43}$	$\frac{297275}{52632}$	$\frac{-319}{2322}$	$\frac{24068}{84065}$	$\frac{3850}{26703}$	0				
1	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	0			
$1+\frac{r}{6}$	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	$\frac{r}{6}$	0		
$1+\frac{r}{6}$	$\bar{b}_{1,1}$	$\bar{b}_{1,2}$	$\bar{b}_{1,3}$	$\bar{b}_{1,4}$	$\bar{b}_{1,5}$	$\bar{b}_{1,6}$	$\bar{b}_{1,7}$	$\bar{b}_{1,8}$	$\bar{b}_{1,9}$	0	
u_1	$b_{1,1}(\tau)$	$b_{1,2}(\tau)$	$b_{1,3}(\tau)$	$b_{1,4}(\tau)$	$b_{1,5}(\tau)$	$b_{1,6}(\tau)$	$b_{1,7}(\tau)$	$b_{1,8}(\tau)$	$b_{1,9}(\tau)$	$b_{1,10}(\tau)$	
$1+\frac{4r}{15}$	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	$\frac{4r}{75}$	$\frac{16r}{75}$	0	
$1+\frac{4r}{15}$	$\bar{b}_{2,1}$	$\bar{b}_{2,2}$	$\bar{b}_{2,3}$	$\bar{b}_{2,4}$	$\bar{b}_{2,5}$	$\bar{b}_{2,6}$	$\bar{b}_{2,7}$	$\bar{b}_{2,8}$	$\bar{b}_{2,9}$	$\bar{b}_{2,10}$	0
u_2	$b_{2,1}(\tau)$	$b_{2,2}(\tau)$	$b_{2,3}(\tau)$	$b_{2,4}(\tau)$	$b_{2,5}(\tau)$	$b_{2,6}(\tau)$	$b_{2,7}(\tau)$	$b_{2,8}(\tau)$	$b_{2,9}(\tau)$	$b_{2,10}(\tau)$	$b_{2,11}(\tau)$
$1+\frac{2r}{3}$	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	$\frac{5r}{6}$	$-\frac{8r}{3}$	$\frac{5r}{2}$	0
u_3	$b_{3,1}(\tau)$	$b_{3,2}(\tau)$	$b_{3,3}(\tau)$	$b_{3,4}(\tau)$	$b_{3,5}(\tau)$	$b_{3,6}(\tau)$	$b_{3,7}(\tau)$	$b_{3,8}(\tau)$	$b_{3,9}(\tau)$	$b_{3,10}(\tau)$	$b_{3,11}(\tau)$
$1+\frac{5r}{6}$	$\frac{3}{40}$	0	$\frac{875}{2244}$	$\frac{23}{72}$	$\frac{264}{1955}$	$\frac{125}{11592}$	$\frac{43}{616}$	$-\frac{165r}{64}$	$\frac{55r}{6}$	$-\frac{425r}{64}$	$\frac{85r}{96}$
u_4	$b_{4,1}(\tau)$	$b_{4,2}(\tau)$	$b_{4,3}(\tau)$	$b_{4,4}(\tau)$	$b_{4,5}(\tau)$	$b_{4,6}(\tau)$	$b_{4,7}(\tau)$	$b_{4,8}(\tau)$	$b_{4,9}(\tau)$	$b_{4,10}(\tau)$	$b_{4,11}(\tau)$

The tableau for the corresponding interpolants u_1, u_2, u_3, u_4 is listed in table 1, while the coefficients $\bar{b}_{i,j}$ and $b_{i,j}(\tau)$ are listed in the appendix A.

4. Numerical results

Denote the stage values

$$k_i = f(x_n + c_i h_n, Y_i, u(x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i))),$$

where u is an interpolant (or other kind of approximation) for the delay values. The Runge-Kutta formula (1.2)–(1.3) for solving delay differential equations (1.1) can be written as

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i k_i,$$

and

$$Y_i = y_n + h_n \sum_{j=1}^{i-1} a_{i,j} k_j.$$

We list an outline of the algorithm in the following, which is based on the continuous Runge-Kutta methods described in section 1. In the outline, u_0 is the standard interpolant constructed on each step and available as a piecewise polynomial on $[x_0, x_n]$ while s_1 is the maximum number of the special interpolants described in section 2 for each step. Recall that when the delay falls in the interval $[x_n, x_n + c_2 h_n]$, we make use of u_0 (from step $n-1$) rather than construct a new interpolant.

Outline of the algorithm: one step from x_n to $x_{n+1} = x_n + h_n$

Part 1. Compute stage values

$k_1^{(0)} = f(x_n, y_n, u_0(x_n - \sigma(x_n, y_n)))$
do $i = 2, \bar{s}$
  $Y_i^{(0)} = y_n + h_n \sum_{j=1}^{i-1} a_{i,j} k_j^{(0)}$
  if $x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(0)}) \le x_n + c_2 h_n$
    $k_i^{(0)} = f(x_n + c_i h_n, Y_i^{(0)}, u_0(x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(0)})))$
  else
    if $i \le s_1 + 1$
      $k_i^{(0)} = f(x_n + c_i h_n, Y_i^{(0)}, u_{i-2}(x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(0)})))$
    else
      $k_i^{(0)} = f(x_n + c_i h_n, Y_i^{(0)}, u_{s_1}(x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(0)})))$
    end if
  end if
end do

Part 2. Iterate (only if a delay in current step is detected and
  at least one of the special interpolants was constructed in part 1)

do while (errest $\geq$ tol) or ($\ell \leq$ maximum iteration number)
  do $i = imin, \bar{s}$ (update stage values)
    $k_i^{(\ell)} = f(x_n + c_i h_n, Y_i^{(\ell)}, \tilde{u}_i^{(\ell)}(x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(\ell)})))$
  end do
end do

where $imin$ is the minimum i for which $x_n + c_i h_n - \sigma(x_n + c_i h_n, Y_i^{(0)}) \geq x_n$; $\tilde{u}_i^{(\ell)}$ is the standard interpolant on $[x_n, x_{n+1}]$ using $k_1^{(0)}, \ldots, k_{imin-1}^{(0)}, k_{imin}^{(\ell)}, \ldots, k_{i-1}^{(\ell)}, k_i^{(\ell-1)}, \ldots, k_{\bar{s}}^{(\ell-1)}$; and errest is the estimated of the magnitude of the defect used in the stepsize control strategy. We tested several alternative stopping criteria for the iteration scheme and found that it is effective to set the maximum number of iterations as 2 or 3 dependent on whether the value of $imin$ is greater than 4 or not.

For the original DVERK and CRK6N, the stepsize h_n is determined from the estimated error and the desired tolerance. When dealing with vanishing delay problems, an iteration scheme must be adopted. There is a trade off between the stepsize and the number of iterations required for convergence, the larger the stepsize, the more iterations are likely to be required. We found that it is better to consider this potential extra work when considering increasing h_n. We do not increase the stepsize in any of the following situations: 1. more than two iterations are used in the current step; 2. one iteration is used and the estimated error is between the allowed tolerance and a factor (0.1–0.5) of the tolerance in the current step.

We tested the program on several examples and report the results below. For comparison we also report the corresponding results for other related methods that are available.

DDRK6N — the six order Runge-Kutta code described in section 3.

DDVSS6 — a six order Runge-Kutta code from the Verner class. The discrete coefficients was chosen by Sharp and Smart [13] as being near-optimal (as a discrete formula pair) from Verner class. The continuous extensions was developed in [3]. The option for handling vanishing delay is the same as that for DDRK6N and the specific coefficients are given in the appendix B.

DDVERK — a code described in [5] with the same discrete and continuous coefficients as DDVSS6. The vanishing delay is dealt with by using lower order interpolation based on the information on one step only.

DRKLAG — a code developed by K.W. Neves and S. Thompson [10]. This is a fourth order Runge-Kutta code and uses extrapolation to deal with the vanishing delay.

SYSDEL — a code developed by Karoui and Vaillancourt [8], which deals with the vanishing delay by using an extrapolation polynomial.

The reported statistics in tables 2–4 are:

Tol: requested error tolerance;
NS: total number of steps;
NF: total number of function evaluations;
ERR: maximum relative error over mesh points.
(For SYSDEL, the error reported is that associated with the end points)

The results of SYSDEL is from [8], where example 2 is not considered, so the corresponding

Table 2: Numerical results for example 1

Tol		DDVSS6	DDRK6N	DDVERK	DRKLAG	SYSDEL
	NS	13	14	12	34	
10^{-4}	NF	214	315	302	242	498
	ERR	2.56E-4	1.37E-4	2.96E-4	4.82E-7	4.05E-3
	NS	19	20	20	80	
10^{-6}	NF	299	350	446	527	568
	ERR	2.11E-6	7.31E-7	2.40E-4	7.56E-9	6.69E-5
	NS	32	38	37	194	
10^{-8}	NF	465	742	657	1222	631
	ERR	4.64E-7	2.00E-8	3.02E-6	3.69E-11	1.07E-7
	NS	64	73	74	479	
10^{-10}	NF	835	1163	1219	2949	1030
	ERR	2.71E-8	5.69E-9	2.06E-9	1.03E-13	1.83E-9
	NS	137	145	144	1195	
10^{-12}	NF	1724	2050	2369	7271	1947
	ERR	7.49E-11	2.25E-11	9.43E-10	2.65E-14	5.81E-12

entries are left as blank. The other blank entries in the tables correspond to the failure of the methods on problems with certain tolerance. Examples 2 with tolerance $tol = 10^{-12}$ can not be solved by DDVERK due to the stepsize being smaller than the minimum stepsize allowed in the code. The blank entries corresponding for DRKLAG on example 2 are caused by the effect of round error on the delay argument, the code returns an error message when $\sigma(x, y) < 0$ is detected.

Example 1. (Vanishing delay at $x = 1$) [9]

$$\begin{aligned} y'(x) &= 1 - y(\exp(1 - \frac{1}{x})), \quad x \in [0.1, 10] \\ y(x) &= \ln(x), \qquad\qquad\qquad\quad x \in [0, 0.1] \end{aligned}$$

The exact solution is $y(x) = \ln(x)$.

Example 2. (Vanishing delay at $x = 1$) [10]

$$\begin{aligned} y_1'(x) &= y_2(x), & x \in [0.1, 5] \\ y_2'(x) &= -y_2(\exp(1 - y_2(x)))y_2^2(x)\exp(1 - y_2(x)), & x \in [0.1, 5] \\ y_1(x) &= \ln(x), & x \in [0, 0.1] \\ y_2(x) &= \frac{1}{x}, & x \in [0, 0.1] \end{aligned}$$

The exact solution is $y_1(x) = \ln(x), y_2(x) = \frac{1}{x}$.

Table 3: Numerical results for example 2

Tol		DDVSS6	DDRK6N	DDVERK	DRKLAG	SYSDEL
	NS	19	28	17	46	
10^{-4}	NF	264	511	286	313	
	ERR	7.80E-5	6.44E-5	2.32E-5	5.88E-6	
	NS	26	46	30		
10^{-6}	NF	358	656	499		
	ERR	1.90E-6	7.11E-7	1.82E-6		
	NS	42	86	59		
10^{-8}	NF	561	1144	974		
	ERR	1.92E-8	1.08E-7	6.85E-8		
	NS	79	170	119	491	
10^{-10}	NF	966	2147	1750	3010	
	ERR	7.85E-10	5.97E-10	4.89E-9	9.21E-12	
	NS	175	355			
10^{-12}	NF	2160	4312			
	ERR	3.59E-11	9.58E-12			

Table 4: Numerical results for example 3

Tol		DDVSS6	DDRK6N	DDVERK	DRKLAG	SYSDEL
	NS	32	40	52	323	
10^{-4}	NF	831	1135	1283	2013	10585
	ERR	2.70E-4	2.55E-4	1.71E-5	4.54E-4	4.00E-5
	NS	38	59	56	343	
10^{-6}	NF	1281	2605	1445	2160	13945
	ERR	8.19E-5	3.64E-6	2.28E-6	6.47E-6	6.80E-7
	NS	72	150	95	725	
10^{-8}	NF	1997	5086	2271	4464	18950
	ERR	1.72E-6	4.30E-8	4.75E-8	8.59E-10	1.96E-8
	NS	144	207	172	1820	
10^{-10}	NF	4947	9044	3928	11189	22051
	ERR	2.61E-9	6.49E-10	9.71E-11	1.83E-12	1.94E-10
	NS	328	421	298	4567	
10^{-12}	NF	9127	17686	7408	28062	23402
	ERR	5.07E-11	8.58E-12	1.01E-11	6.78E-14	1.09E-12

Example 3. (Asymptotically vanishing delay) [8]

$$\begin{aligned} y'(x) &= (1+e^{-x})y(x-e^{-x})\exp\left(e^{-x+e^{-x}}\right), \quad x \in [1,30], \\ y(x) &= e^{x-e^{-x}}, \qquad\qquad\qquad\qquad\qquad\qquad\quad x \in [0,1] \end{aligned}$$

The exact solution is $y(x) = e^{x-e^{-x}}$.

Conclusions: For the first two test problems, which have smooth solutions, DDVSS6 is the best for almost all tolerance because of the high order of both the original method and the interpolants. Since the coefficients are near-optimal, DDVSS6 is also better than DDRK6N for all problems, which is in accordance with the comparison in [3]. For the last test problem, where $h > \sigma$ on almost every step and the solutions increase significantly, DDVSS6 and DDVERK are comparable and they are better than the other codes. The numerical results confirm our analysis and show the codes developed in this paper are at least comparable with the widely used codes.

The vanishing delay can be handled automatically by the codes so that users do not need to know where the delay vanishes. However, the codes developed in this paper are not helpful for vanishing delay that arise on the first step or after a discontinuity since the interpolants are based on two timesteps. In many cases the derivative discontinuities will be smoothed before a vanishing point as discussed in Neves and Thompson [10, p.13]. For the vanishing delay close to discontinuous points or on the first step, we would recommend adopting a technique using one-step information, such as those in [14], [12], [5].

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Appendix

The fortran format of the following coefficients can be obtained through an anonymous ftp: ftp.cs.utoronto.ca in the directory: /cs/ftp/pub/reports.

A. Coefficients of interpolants for DDRK6N

A.1. Interpolant u_1

(1) Coefficients of intermediate stage at $1 + \frac{r}{6}$

```
bbar(1,1) = 0.6416251416924154D1*r-0.7537408691442648D1+0.1302026859368352D1*r**2
     +25.D0/288.D0*r**3
bbar(1,2) = -0.265759835208D-4*r**2
bbar(1,3) = -0.278478852760468D1+0.2916506103432895D1*r+0.503466685558988*r**2
     +25/864*r**3
bbar(1,4) = 0.802651649208283D-1
bbar(1,5) = 0.181737691056607D0
bbar(1,6) = -0.180546696894382D1*r**2+0.1073843815164611D2-0.9166090853690383D1*r
     -25/216*r**3
bbar(1,7) = 0.1447676295599D0
bbar(1,8) = 0.176962005880341D0
bbar(1,9) = 0.265759835208D-4
```

(2) Coefficients of interpolant u_1

```
b(1,1,1) = 0.5224608628061679D1-0.3073538089540367D1*r-0.124737747140437D1*r**2
     -0.12473774714043*r**3
```

$b_{1,1,2}$ = −0.2279134082777135D2+0.580054455139579*r**3+0.580054455139579D1*r**2
+0.1429254177463924D2*r
$b_{1,1,3}$ = 0.3138273055235956D2−0.2021305827433477D2*r−0.820335157237612D1*r**2
−0.820335157237612*r**3
$b_{1,1,4}$ = 0.3664562413806474D1*r**2+0.9029481787619152D1*r−0.1379209968842256D2
+0.366456241380647*r**3
$b_{1,2,1}$ = 0.D0
$b_{1,2,2}$ = 0.D0
$b_{1,2,3}$ = 0.D0
$b_{1,2,4}$ = 0.D0
$b_{1,3,1}$ = 0.3027155443000343D1−0.657708121285940*r**2−0.190508559269031D1*r
−0.566989759729259D−1*r**3
$b_{1,3,2}$ = −0.1017201966691113D2+0.3058468945281419D1*r**2+0.263661115972536*r**3
+0.8859013496677214D1*r
$b_{1,3,3}$ = 0.1366857333688706D2−0.4325403556343774D1*r**2−0.125287551287199D2*r
−0.37287961692618 7*r**3
$b_{1,3,4}$ = −0.617206263271556D1+0.1932223818188868D1*r**2+0.166571018809385*r**3
+0.5596786231995342D1*r
$b_{1,4,1}$ = −0.506693191111390D0
$b_{1,4,2}$ = 0.1710000989879487D1
$b_{1,4,3}$ = −0.775758599372477D0
$b_{1,4,4}$ = −0.978233164667996D−1
$b_{1,5,1}$ = −0.477419359932993D0
$b_{1,5,2}$ = 0.1281964940762434D1
$b_{1,5,3}$ = −0.710011299482372D0
$b_{1,5,4}$ = 0.416911580619513D−1
$b_{1,6,1}$ = −0.6638630352752823D1+0.1853246528943635D1*r**2+0.4704395035010766D1*r
+0.178196781629195*r**3
$b_{1,6,2}$ = −0.2187633945097843D2*r+0.3103624367509208D2−0.828649221627970*r**3
−0.8617951904930895D1*r**2
$b_{1,6,3}$ = 0.3093835450153281D2*r−0.4396010312468449D2+0.1218783662181595D2*r**2
+0.1171907367482303D1*r**3
$b_{1,6,4}$ = −0.5444492729083904D1*r**2−0.1382063538921299D2*r+0.1965421949809919D2
−0.523508916258067*r**3
$b_{1,7,1}$ = −0.1914250776913554D1+0.419066991328121*r**2+0.1056583797284732D1*r
+0.4049494863011104D−1*r**3
$b_{1,7,2}$ = 0.8074621413025866D1−0.1948741907677241D1*r**2−0.188309280085832*r**3
−0.4913317362973469D1*r
$b_{1,7,3}$ = −0.1063597673295039D2+0.2755985209811473D1*r**2+0.6948601007716162D1*r
+0.2663141736431*r**3
$b_{1,7,4}$ = 0.456105309575011D1−0.1231140677536064D1*r**2−0.1189666080243 18*r**3
−0.3104046176340927D1*r
$b_{1,8,1}$ = 0.2764222558668017D1−0.367227927581446*r**2−0.782355150064820*r
−0.3725500714594384D−1*r**3
$b_{1,8,2}$ = −0.1136687963181338D2+0.1707680315930922D1*r**2+0.173242930601687*r**3
+0.3638101542635442D1*r
$b_{1,8,3}$ = 0.1418063287103553D2−0.2415066702907531D1*r**2−0.5145142106194304D1*r
−0.245006766961633*r**3
$b_{1,8,4}$ = −0.5602170081208019D1+0.1078847174624626D1*r**2+0.109448264092353*r**3
+0.229841354593942D1*r

$b_{1,9,1}$ = 0.D0
$b_{1,9,2}$ = 0.D0
$b_{1,9,3}$ = 0.D0
$b_{1,9,4}$ = 0.D0
$b_{1,10,1}$ = −0.47899294901927
$b_{1,10,2}$ = 0.2227409107735985D1
$b_{1,10,3}$ = −0.3150087003792431D1
$b_{1,10,4}$ = 0.1407191966901686D1

A.2. Interpolant u_2

(1) Coefficients of intermediate stage at $1 + \frac{4r}{15}$

$\bar{b}_{2,1}$ = 0.306159149077685−0.703437066309108*r**2+0.1024795806772862D1*r
−0.486120300979827*r**3−16/225*r**4
$\bar{b}_{2,2}$ = 0.D0
$\bar{b}_{2,3}$ = 0.552875697485929−0.497610251124600*r**2+0.635204012462517*r
−0.26406141627029*r**3−16/495*r**4
$\bar{b}_{2,4}$ = 0.2984285093978D0
$\bar{b}_{2,5}$ = 0.101502827694766D0
$\bar{b}_{2,6}$ = −0.35142282319549+0.1106566815976707D1*r**2−0.1568565010366626D1*r
+0.728320006690759*r**3+32.D0/315.D0*r**4
$\bar{b}_{2,7}$ = −0.4707626002237131D−1−0.352291923320028*r+0.247015929333958*r**2
+0.167573451083173*r**3+149984.D0/6496875.D0*r**4
$\bar{b}_{2,8}$ = 0.3971512617462346D−1+0.527523781117940*r−0.15253542787695*r**2
−0.145711740523812*r**3−1792.D0/84375.D0*r**4
$\bar{b}_{2,9}$ = 0.D0
$\bar{b}_{2,10}$ = 0.998177733869671D−1

(2) Coefficients of interpolant u_2

$b_{2,1,1}$ = 1
$b_{2,1,2}$ =(−24192*r**3−197280*r**2−469800*r−303750)/(675+1080*r+480*r**2+64*r**3)/120.D0
$b_{2,1,3}$ =(27648*r**3+270720*r**2+712800*r+486000)/(675+1080*r+480*r**2+64*r**3)/120.D0
$b_{2,1,4}$ =(−10560*r**3−158400*r**2−486000*r−354375)/(675+1080*r+480*r**2+64*r**3)/120.D0
$b_{2,1,5}$ =(31680*r**2+123120*r+97200)/(675+1080*r+480*r**2+64*r**3)/120.D0
$b_{2,2,1}$ = 0.D0
$b_{2,2,2}$ = 0.D0
$b_{2,2,3}$ = 0.D0
$b_{2,2,4}$ = 0.D0
$b_{2,2,5}$ = 0.D0
$b_{2,3,1}$ = 0.D0
$b_{2,3,2}$ = 125.D0/13464.D0*(6720*r**2+32256*r+26460)/(16*r**2+60*r+45)
$b_{2,3,3}$ = 125.D0/13464.D0*(−10752*r**2−68544*r−60480)/(16*r**2+60*r+45)
$b_{2,3,4}$ = 125.D0/13464.D0*(4704*r**2+52920*r+51030)/(16*r**2+60*r+45)
$b_{2,3,5}$ = 125.D0/13464.D0*(−14112*r−15120)/(16*r**2+60*r+45)
$b_{2,4,1}$ = 0.D0
$b_{2,4,2}$ = −(1104*r**2+8280*r+15525)/(16*r**2+60*r+45)/108.D0
$b_{2,4,3}$ = −(−4416*r**2−33120*r−62100)/(16*r**2+60*r+45)/108.D0
$b_{2,4,4}$ = −(5520*r**2+62100*r+139725)/(16*r**2+60*r+45)/216.D0
$b_{2,4,5}$ = −(−8280*r−24840)/(16*r**2+60*r+45)/108.D0
$b_{2,5,1}$ = 0.D0

$b_{2,5,2}$ = 176.D0/1955.D0*(−168*r**2−990*r−1350)/(16*r**2+60*r+45)
$b_{2,5,3}$ = 176.D0/1955.D0*(432*r**2+3060*r+4725)/(16*r**2+60*r+45)
$b_{2,5,4}$ = 88.D0/1955.D0*(−480*r**2−5400*r−10125)/(16*r**2+60*r+45)
$b_{2,5,5}$ = 176.D0/1955.D0*(720*r+1755)/(16*r**2+60*r+45)
$b_{2,6,1}$ = 0.D0
$b_{2,6,2}$ = −125.D0/17388.D0*(−384*r**2−1908*r−1755)/(16*r**2+60*r+45)
$b_{2,6,3}$ = −125.D0/8694.D0*(336*r**2+2196*r+2295)/(16*r**2+60*r+45)
$b_{2,6,4}$ = −125.D0/34776.D0*(−624*r**2−7020*r−8505)/(16*r**2+60*r+45)
$b_{2,6,5}$ = −125.D0/8694.D0*(468*r+675)/(16*r**2+60*r+45)
$b_{2,7,1}$ = 0.D0
$b_{2,7,2}$ = −43.D0/924.D0*(288*r**2+1620*r+2025)/(16*r**2+60*r+45)
$b_{2,7,3}$ = −43.D0/462.D0*(−336*r**2−2340*r−3375)/(16*r**2+60*r+45)
$b_{2,7,4}$ = −43.D0/1848.D0*(720*r**2+8100*r+14175)/(16*r**2+60*r+45)
$b_{2,7,5}$ = −43.D0/462.D0*(−540*r−1215)/(16*r**2+60*r+45)
$b_{2,8,1}$ = 0.D0
$b_{2,8,2}$ = 3.D0/8.D0*(64*r**3+400*r**2+660*r+225)/r/(16*r**2+60*r+45)
$b_{2,8,3}$ = −(128*r**3+960*r**2+1800*r+675)/r/(16*r**2+60*r+45)/2.D0
$b_{2,8,4}$ = 5.D0/8.D0*(64*r**3+720*r**2+1620*r+675)/r/(16*r**2+60*r+45)
$b_{2,8,5}$ = −15.D0/4.D0/r*(32*r**2+96*r+45)/(16*r**2+60*r+45)
$b_{2,9,1}$ = 0.D0
$b_{2,9,2}$ = 0.D0
$b_{2,9,3}$ = 0.D0
$b_{2,9,4}$ = 0.D0
$b_{2,9,5}$ = 0.D0
$b_{2,10,1}$ = 0.D0
$b_{2,10,2}$ = 0.D0
$b_{2,10,3}$ = 0.D0
$b_{2,10,4}$ = 0.D0
$b_{2,10,5}$ = 0.D0
$b_{2,11,1}$ = 0.D0
$b_{2,11,2}$ = −10125.D0/8.D0/r/(675+1080*r+480*r**2+64*r**3)
$b_{2,11,3}$ = 10125.D0/2.D0/r/(675+1080*r+480*r**2+64*r**3)
$b_{2,11,4}$ = −50625.D0/8.D0/r/(675+1080*r+480*r**2+64*r**3)
$b_{2,11,5}$ = 10125.D0/4.D0/r/(675+1080*r+480*r**2+64*r**3)

A.3. Interpolant u_3

$b_{3,1,1}$ = 1.D0
$b_{3,1,2}$ = −(245*r**3+1096*r**2+1740*r+900)/(r**3+4*r**2+6*r+3)/80.D0
$b_{3,1,3}$ =(65*r**3+376*r**2+660*r+360)/(r**3+4*r**2+6*r+3)/20.D0
$b_{3,1,4}$ = −(15*r**3+176*r**2+360*r+210)/(r**3+4*r**2+6*r+3)/16.D0
$b_{3,1,5}$ = −(7*r**3−88*r**2−228*r−144)/(r**3+4*r**2+6*r+3)/40.D0
$b_{3,2,1}$ = 0.D0
$b_{3,2,2}$ = 0.D0
$b_{3,2,3}$ = 0.D0
$b_{3,2,4}$ = 0.D0
$b_{3,2,5}$ = 0.D0
$b_{3,3,1}$ = 0.D0
$b_{3,3,2}$ = 25.D0/8976.D0*(1459*r**3+6384*r**2+10920*r+5880)/(r**3+4*r**2+6*r+3)
$b_{3,3,3}$ = −25.D0/2244.D0*(619*r**3+3024*r**2+5880*r+3360)/(r**3+4*r**2+6*r+3)
$b_{3,3,4}$ = 125.D0/8976.D0*(255*r**3+1568*r**2+3696*r+2268)/(r**3+4*r**2+6*r+3)
$b_{3,3,5}$ = −25.D0/4488.D0*(59*r**3+784*r**2+2520*r+1680)/(r**3+4*r**2+6*r+3)

```
b3,4,1 = 0.D0
b3,4,2 = -(65*r**3+276*r**2+690*r+690)/(r**3+4*r**2+6*r+3)/72.D0
b3,4,3 =(65*r**3+276*r**2+690*r+690)/(r**3+4*r**2+6*r+3)/18.D0
b3,4,4 = -5.D0/72.D0*(42*r**3+184*r**2+552*r+621)/(r**3+4*r**2+6*r+3)
b3,4,5 =(19*r**3+92*r**2+414*r+552)/(r**3+4*r**2+6*r+3)/36.D0
b3,5,1 = 0.D0
b3,5,2 = -264.D0/1955.D0*(5*r**3+36*r**2+75*r+60)/(r**3+4*r**2+6*r+3)
b3,5,3 = 528.D0/1955.D0*(5*r**3+52*r**2+120*r+105)/(r**3+4*r**2+6*r+3)
b3,5,4 = -264.D0/391.D0*(16*r**2+45*r+45)/(r**3+4*r**2+6*r+3)
b3,5,5 = -528.D0/1955.D0*(2*r**3-8*r**2-33*r-39)/(r**3+4*r**2+6*r+3)
b3,6,1 = 0.D0
b3,6,2 = -25.D0/5796.D0*(r**3-186*r**2-330*r-195)/(r**3+4*r**2+6*r+3)
b3,6,3 = 25.D0/2898.D0*(47*r**3-192*r**2-390*r-255)/(r**3+4*r**2+6*r+3)
b3,6,4 = -125.D0/11592.D0*(69*r**3-104*r**2-258*r-189)/(r**3+4*r**2+6*r+3)
b3,6,5 = 25.D0/2898.D0*(41*r**3-26*r**2-90*r-75)/(r**3+4*r**2+6*r+3)
b3,7,1 = 0.D0
b3,7,2 = -129.D0/308.D0*(r**3+10*r**2+20*r+15)/(r**3+4*r**2+6*r+3)
b3,7,3 = 43.D0/154.D0*(r**3+40*r**2+90*r+75)/(r**3+4*r**2+6*r+3)
b3,7,4 = 645.D0/616.D0*(r**3-8*r**2-22*r-21)/(r**3+4*r**2+6*r+3)
b3,7,5 = -129.D0/154.D0*(r**3-2*r**2-8*r-9)/(r**3+4*r**2+6*r+3)
b3,8,1 = 0.D0
b3,8,2 =(16*r**4+128*r**3+288*r**2+288*r+81)/(r**3+4*r**2+6*r+3)/r/16.D0
b3,8,3 = -(8*r**4+96*r**3+240*r**2+264*r+81)/(r**3+4*r**2+6*r+3)/r/4.D0
b3,8,4 = 5.D0/16.D0*(64*r**3+192*r**2+240*r+81)/(r**3+4*r**2+6*r+3)/r
b3,8,5 =(8*r**4-32*r**3-144*r**2-216*r-81)/(r**3+4*r**2+6*r+3)/r/8.D0
b3,9,1 = 0.D0
b3,9,2 = 0.D0
b3,9,3 = 0.D0
b3,9,4 = 0.D0
b3,9,5 = 0.D0
b3,10,1 = 0.D0
b3,10,2 = -75.D0/16.D0/(r**3+4*r**2+6*r+3)/r
b3,10,3 = 75.D0/4.D0/(r**3+4*r**2+6*r+3)/r
b3,10,4 = -375.D0/16.D0/(r**3+4*r**2+6*r+3)/r
b3,10,5 = 75.D0/8.D0/(r**3+4*r**2+6*r+3)/r
b3,11,1 = 0.D0
b3,11,2 = -3.D0/8.D0/(r**3+4*r**2+6*r+3)/r
b3,11,3 = 3.D0/2.D0/(r**3+4*r**2+6*r+3)/r
b3,11,4 = -15.D0/8.D0/(r**3+4*r**2+6*r+3)/r
b3,11,5 = 3.D0/4.D0/(r**3+4*r**2+6*r+3)/r
```

A.4. Interpolant u_4

```
b4,1,1 =(139881465216+139881465216*r-8590337269*r**4-9598142200*r**3
      +43747712412*r**2-1199767775*r**5+527897821*r**6)/(r**2+3*r+3)/46627155072.D0
b4,1,2 =(-368193101940*r-86456233090*r**4-111153626195*r**3
      -245606335776*r**2-190444707900-46535808840*r**5-3193633940*r**6
      +2509283810*r**7)/(r**3+4*r**2+6*r+3)/16928418480.D0
b4,1,3 = -(-1493510106240-2738101861440*r-1011221601625*r**4
      -963375574460*r**3-1719976185684*r**2-544298698500*r**5
      -37353832250*r**6+29349439625*r**7)/(r**3+4*r**2+6*r+3)/82972783680.D0
```

$b_{4,1,4}$ =(−240753540960*r−100168077501*r**4−78748284480*r**3
−133559474276*r**2−140439565560−53916326676*r**5−3700140066*r**6
+2907252909*r**7)/(r**3+4*r**2+6*r+3)/10700157376.D0
$b_{4,1,5}$ = −(−101437942368*r−40918133527*r**4−24956164588*r**3
−45629291308*r**2−64066068864−22024536252*r**5−1511487782*r**6
+1187597543*r**7)/(r**3+4*r**2+6*r+3)/17796130240.D0
$b_{4,2,1}$ = 0.D0
$b_{4,2,2}$ = 0.D0
$b_{4,2,3}$ = 0.D0
$b_{4,2,4}$ = 0.D0
$b_{4,2,5}$ = 0.D0
$b_{4,3,1}$ = 352872875.D0/1538696117376.D0*r**2*(2213*r**2+2800*r+840+595*r**3+107*r**4)/
(r**2+3*r+3)
$b_{4,3,2}$ = 25.D0/1899368553456.D0*(1244238758280+24408487970*r**7
+1139076856429*r**3+1542505831104*r**2+2310729122520*r+1143549067230*r**4
+640551721680*r**5+160137930420*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,3,3}$ = −25.D0/9309546328896.D0*(13939427658240+285490003625*r**7+12280004039896*r**3
+14786714827416*r**2+24393998401920*r+13375340076375*r**4+7492111497000*r**5
+1873027874250*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,3,4}$ = 125.D0/6002788287936.D0*(1516747308048+28279641933*r**7+1132570175340*r**3
+1270623826808*r**2+2471736353856*r+1324914439347*r**4+742142378952*r**5
+185535594738*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,3,5}$ = −25.D0/1996725812928.D0*(747437470080+11552085191*r**7+419236115424*r**3
+439493419624*r**2+1121156205120*r+541220589369*r**4+303161263704*r**5
+75790315926*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,4,1}$ = −239953555.D0/209822197824.D0*(37*r**4+119*r**3+403*r**2+920*r+690)*r**2/
(r**2+3*r+3)
$b_{4,4,2}$ = −(8440318270*r**7+35586206760*r**6+119076922620*r**5
+301798407330*r**4+381022243115*r**3+215803573656*r**2+146007609390*r
+146007609390)/(r**3+4*r**2+6*r+3)/15235576632.D0
$b_{4,4,3}$ =(98720842375*r**7+416228416500*r**6+1392764316750*r**5
+3529937147625*r**4+4565352255710*r**3+2986034718534*r**2+2862561036960*r
+2862561036960)/(r**3+4*r**2+6*r+3)/74675505312.D0
$b_{4,4,4}$ = −5.D0/48150708192.D0*(9778941603*r**7+41230132164*r**6
+137962365318*r**5+349663236237*r**4+453604020702*r**3+305415855934*r**2
+369155429472*r+415299858156)/(r**3+4*r**2+6*r+3)
$b_{4,4,5}$ =(3994646281*r**7+16842292428*r**6+56356901586*r**5
+142835595399*r**4+182274256794*r**3+115425854522*r**2+184189947984*r
+245586597312)/(r**3+4*r**2+6*r+3)/16016517216.D0
$b_{4,5,1}$ = 2822983.D0/5585544618.D0*(87*r**4+85*r**3−553*r**2−1430*r−990)*r**2/
(r**2+3*r+3)
$b_{4,5,2}$ = 8.D0/137896075535.D0*(9923076885*r**7+19618037060*r**6
−53379310140*r**5−226177717965*r**4−287659506805*r**3−196713442926*r**2
−174574315575*r−139659452460)/(r**3+4*r**2+6*r+3)
$b_{4,5,3}$ = −(232127386125*r**7+458918510500*r**6−1248685249500*r**5
−5290903525125*r**4−6685051872620*r**3−5014471179498*r**2−5476203722880*r
−4791678257520)/(r**3+4*r**2+6*r+3)/168970616765.D0
$b_{4,5,4}$ = 3.D0/65371273969.D0*(22993727553*r**7+45458863668*r**6
−123690396492*r**5−524098410777*r**4−639595639980*r**3−497056224082*r**2
−662072237640*r−662072237640)/(r**3+4*r**2+6*r+3)

$b_{4,5,5}$ = −3.D0/108723233185.D0*(9392816931*r**7+18569707036*r**6
−50526877284*r**5−214091447979*r**4−241695716196*r**3−185186751926*r**2
−322999763856*r−381726993648)/(r**3+4*r**2+6*r+3)
$b_{4,6,1}$ = −5998838875.D0/16890686924832.D0*r**2*(−37*r**2−125*r−60+109*r**3+68*r**4)/
(r**2+3*r+3)
$b_{4,6,2}$ = −25.D0/1226463918876.D0*(−41263020045+15511936280*r**7−41989986119*r**3
−53045575566*r**2−69829726230*r−36954907020*r**4+16424403120*r**5
+40376657670*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,6,3}$ = 25.D0/6011378177616.D0*(−528951495960+181432899500*r**7−396111191051*r**3
−558357214164*r**2−808984640880*r−432237201750*r**4+192105423000*r**5
+472259164875*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,6,4}$ = −125.D0/3876132009456.D0*(−63197804502+17972108892*r**7−25822493673*r**3
−50633254612*r**2−86270018844*r−42815906478*r**4+19029291768*r**5
+46780342263*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,6,5}$ = 25.D0/1289329635888.D0*(−33367744200+7341512084*r**7−1732197909*r**3
−18045289436*r**2−40041293040*r−17490072906*r**4+7773365736*r**5
+19109524101*r**6)/(r**3+4*r**2+6*r+3)
$b_{4,7,1}$ = 10318002865.D0/299190911712.D0*r**2*(−10+3*r**3−5*r**2−15*r+2*r**4)/(r**2+3*r+3)
$b_{4,7,2}$ = 43.D0/21724803716.D0*(−4232104620*r−4562334200*r**4−5914522981*r**3
−4397219410*r**2−456233420*r**5+1140583550*r**6+456233420*r**7−3174078465)/
(r**3+4*r**2+6*r+3)
$b_{4,7,3}$ = −43.D0/106481739056.D0*(−62229587760*r−53362617500*r**4−67394711739*r**3
−54338903310*r**2−51857989800−5336261750*r**5+13340654375*r**6
+5336261750*r**7)/(r**3+4*r**2+6*r+3)
$b_{4,7,4}$ = 645.D0/205978029488.D0*(−7356358196*r−7021978278−5285914380*r**4
−6273013057*r**3−5317996534*r**2−528591438*r**5+1321478595*r**6
+528591438*r**7)/(r**3+4*r**2+6*r+3)
$b_{4,7,5}$ = −129.D0/68515101424.D0*(−3559226048*r−2159268260*r**4−2254182069*r**3
−1969440642*r**2−215926826*r**5+539817065*r**6+215926826*r**7−4004129304)/
(r**3+4*r**2+6*r+3)
$b_{4,8,1}$ = −47990711.D0/46627155072.D0*(−1017*r−560*r**4−1760*r**3−2049*r**2
−207+80*r**5+80*r**6)/(r**2+3*r+3)
$b_{4,8,2}$ = −(−70386338322*r−17140023711+3649867360*r**8−177164993374*r**4
−166966636140*r**3−116785277136*r**2−105846153440*r**5−21899204160*r**6
+7299734720*r**7)/(r**3+4*r**2+6*r+3)/r/3385683696.D0
$b_{4,8,3}$ = (−1205701362801*r+42690094000*r**8−2065771214047*r**4−2034367214214*r**3
−1648831842360*r**2−336039773904−1238012726000*r**5−256140564000*r**6
+85380188000*r**7)/(r**3+4*r**2+6*r+3)/r/16594556736.D0
$b_{4,8,4}$ = −(−857221017033*r+21143657520*r**8−1006702393671*r**4−1024333821974*r**3
−965507402616*r**2−270847733580−613166068080*r**5−126861945120*r**6
+42287315040*r**7)/(r**3+4*r**2+6*r+3)/r/10700157376.D0
$b_{4,8,5}$ = (−502843942971*r+8637073040*r**8−393436509877*r**4−402200345218*r**3
−452477561832*r**2−250475118160*r**5−51822438240*r**6+17274146080*r**7
−180185818680)/(r**3+4*r**2+6*r+3)/r/17796130240.D0
$b_{4,9,1}$ = 0.D0
$b_{4,9,2}$ = 0.D0
$b_{4,9,3}$ = 0.D0
$b_{4,9,4}$ = 0.D0
$b_{4,9,5}$ = 0.D0

$b_{4,10,1}$ = −352872875.D0/46627155072.D0*(83*r**2+147*r+45)/(r**2+3*r+3)
$b_{4,10,2}$ = −25.D0/3385683696.D0*(1113746290*r**4+3086284900*r**3+2576376960*r**2
+603838350*r+634815693)/r/(r**3+4*r**2+6*r+3)
$b_{4,10,3}$ = 25.D0/16594556736.D0*(13026756625*r**4+36098241250*r**3+30134184000*r**2
+7062699375*r+12445917552)/r/(r**3+4*r**2+6*r+3)
$b_{4,10,4}$ = −375.D0/10700157376.D0*(430128327*r**4+1191921870*r**3+994995648*r**2
+233202105*r+668759836)/r/(r**3+4*r**2+6*r+3)
$b_{4,10,5}$ = 25.D0/3559226048.D0*(527115487*r**4+1460681470*r**3+1219351488*r**2+285785505*r
+1334709768)/r/(r**3+4*r**2+6*r+3)
$b_{4,11,1}$ = −239953555.D0/23313577536.D0*(r**2−3*r−9)/(r**2+3*r+3)
$b_{4,11,2}$ = −(228116710.D0*r**4−456233420*r**3−2737400520*r**2−2053050390*r+634815693)/
(r**3+4*r**2+6*r+3)/r/1692841848.D0
$b_{4,11,3}$ = (2668130875*r**4−5336261750*r**3−32017570500*r**2−24013177875*r
+12445917552)/(r**3+4*r**2+6*r+3)/r/8297278368.D0
$b_{4,11,4}$ = −15.D0/5350078688.D0*(88098573*r**4−176197146*r**3−1057182876*r**2−792887157*r
+668759836)/(r**3+4*r**2+6*r+3)/r
$b_{4,11,5}$ = (107963413*r**4−215926826*r**3−1295560956*r**2−971670717*r+1334709768)/
(r**3+4*r**2+6*r+3)/r/1779613024.D0
$b_{4,12,1}$ = 2822983.D0/242849766.D0
$b_{4,12,2}$ = 10734904.D0/70535077.D0
$b_{4,12,3}$ = −31389775.D0/86429983.D0
$b_{4,12,4}$ = 46640421.D0/167189959.D0
$b_{4,12,5}$ = −19052367.D0/278064535.D0

B. Coefficients of interpolants for DDVSS6

B.1. Tableau for DDVSS6

Table 5: Tableau for DDVSS6

0	0											
c_2	$a_{2,1}$	0										
c_3	$a_{3,1}$	$a_{3,2}$	0									
c_4	$a_{4,1}$	$a_{4,2}$	$a_{4,3}$	0								
c_5	$a_{5,1}$	$a_{5,2}$	$a_{5,3}$	$a_{5,4}$	0							
c_6	$a_{6,1}$	$a_{6,2}$	$a_{6,3}$	$a_{6,4}$	$a_{6,5}$	0						
c_7	$a_{7,1}$	$a_{7,2}$	$a_{7,3}$	$a_{7,4}$	$a_{7,5}$	$a_{7,6}$	0					
1	b_1	b_2	b_3	b_4	b_5	b_6	b_7	0				
$1+rc_2$	b_1	b_2	b_3	b_4	b_5	b_6	b_7	$ra_{2,1}$	0			
$1+rc_2$	$\bar{b}_{1,1}$	$\bar{b}_{1,2}$	$\bar{b}_{1,3}$	$\bar{b}_{1,4}$	$\bar{b}_{1,5}$	$\bar{b}_{1,6}$	$\bar{b}_{1,7}$	$\bar{b}_{1,8}$	$\bar{b}_{1,9}$	0		
u_1	$b_{1,1}(\tau)$	$b_{1,2}(\tau)$	$b_{1,3}(\tau)$	$b_{1,4}(\tau)$	$b_{1,5}(\tau)$	$b_{1,6}(\tau)$	$b_{1,7}(\tau)$	$b_{1,8}(\tau)$	$b_{1,9}(\tau)$	$b_{1,10}(\tau)$		
$1+rc_3$	b_1	b_2	b_3	b_4	b_5	b_6	b_7	$ra_{3,1}$	$ra_{3,2}$	0		
$1+rc_3$	$\bar{b}_{2,1}$	$\bar{b}_{2,2}$	$\bar{b}_{2,3}$	$\bar{b}_{2,4}$	$\bar{b}_{2,5}$	$\bar{b}_{2,6}$	$\bar{b}_{2,7}$	$\bar{b}_{2,8}$	$\bar{b}_{2,9}$	$\bar{b}_{2,10}$	0	
u_2	$b_{2,1}(\tau)$	$b_{2,2}(\tau)$	$b_{2,3}(\tau)$	$b_{2,4}(\tau)$	$b_{2,5}(\tau)$	$b_{2,6}(\tau)$	$b_{2,7}(\tau)$	$b_{2,8}(\tau)$	$b_{2,9}(\tau)$	$b_{2,10}(\tau)$	$b_{2,11}(\tau)$	
$1+rc_4$	b_1	b_2	b_3	b_4	b_5	b_6	b_7	$ra_{4,1}$	$ra_{4,2}$	$ra_{4,3}$	0	
u_3	$b_{3,1}(\tau)$	$b_{3,2}(\tau)$	$b_{3,3}(\tau)$	$b_{3,4}(\tau)$	$b_{3,5}(\tau)$	$b_{3,6}(\tau)$	$b_{3,7}(\tau)$	$b_{3,8}(\tau)$	$b_{3,9}(\tau)$	$b_{3,10}(\tau)$	$b_{3,11}(\tau)$	
$1+rc_5$	b_1	b_2	b_3	b_4	b_5	b_6	b_7	$ra_{5,1}$	$ra_{5,2}$	$ra_{5,3}$	$ra_{5,4}$	0
u_4	$b_{4,1}(\tau)$	$b_{4,2}(\tau)$	$b_{4,3}(\tau)$	$b_{4,4}(\tau)$	$b_{4,5}(\tau)$	$b_{4,6}(\tau)$	$b_{4,7}(\tau)$	$b_{4,8}(\tau)$	$b_{4,9}(\tau)$	$b_{4,10}(\tau)$	$b_{4,11}(\tau)$	$b_{4,12}(\tau)$
$1+rc_6$	b_1	b_2	b_3	b_4	b_6	b_6	b_7	$ra_{6,1}$	$ra_{6,2}$	$ra_{6,3}$	$ra_{6,4}$	$ra_{6,5}$
u_5	$b_{5,1}(\tau)$	$b_{5,2}(\tau)$	$b_{5,3}(\tau)$	$b_{5,4}(\tau)$	$b_{5,5}(\tau)$	$b_{5,6}(\tau)$	$b_{5,7}(\tau)$	$b_{5,8}(\tau)$	$b_{5,9}(\tau)$	$b_{5,10}(\tau)$	$b_{5,11}(\tau)$	$b_{5,12}(\tau)$

0	
0	0
0	0
0	0

B.2. Interpolant u_1

(1) Coefficients of intermediate stage at $1 + rc_2$

$\bar{b}_{1,1}$ = 0.848563888816329*r−0.108945715262257 6D1+0.234167218704346*r**2
+0.2103681442524418D−1*r**3
$\bar{b}_{1,2}$ = −0.1185351484863983D−14*r−0.1035631880326596D−14+0.3068624633921216D−4*r**2
−0.9708461538461548D−17*r**3
$\bar{b}_{1,3}$ = 0.3333955668376459D1−0.566485711593429*r**2−0.2265925464653765D1*r
−0.436918453447379D−1*r**3
$\bar{b}_{1,4}$ = −0.18707376692863D1+0.332287806642743*r**2+0.1599179757655619D1*r
+0.2265503091949373D−1*r**3
$\bar{b}_{1,5}$ = 0.976621634274615D−1
$\bar{b}_{1,6}$ = 0.162336719307402
$\bar{b}_{1,7}$ = 0.166827907930443
$\bar{b}_{1,8}$ = 0.199443049113449
$\bar{b}_{1,9}$ = −0.306862463394D−4

(2) Coefficients of interpolant u_1

$b_{1,1,1}$ = 0.1009831612996394D1−0.7076714743197776D−2*r−0.2131153802031142D−1*r**2
−0.4833088738352169D−2*r**3−0.2081405741466123D−7*r**4
$b_{1,1,2}$ = 0.1559692808471255D−6*r**4−0.2863702495497748D1+0.362165511401035D−1*r**3
+0.5302907007834695D−1*r+0.159697131249036*r**2
$b_{1,1,3}$ = −0.871819937107136D−1*r−0.2564199757187689D−6*r**4+0.2950780096996873D1
−0.262548716611523*r**2−0.5954151428745298D−1*r**3
$b_{1,1,4}$ = 0.4126704035063487D−1*r+0.124421209984893*r**2+0.2821960510611802D−1*r**3
+0.121551586213357D−6*r**4−0.1022734829963082D1
$b_{1,3,1}$ = 0.1910469212557484D−2*r**3−0.6429776229724033D−1*r+0.1309759041516834D−3*r**2
−0.3963058476658892D−1+0.9601541115193398D−7*r**4
$b_{1,3,2}$ = −0.7194875237088394D−6*r**4+0.1717935327918952D1−0.143160222549052D−1*r**3
+0.481812630079324*r−0.9814625362016468D−3*r**2
$b_{1,3,3}$ = −0.79211997538817*r+0.1182867372070581D−5*r**4−0.2007412963843347D1
+0.1613565173441945D−2*r**2+0.2353613518671168D−1*r**3
$b_{1,3,4}$ = 0.375724284155254*r+0.612278500749974−0.6454446676555764D−3*r**2
−0.1114291312426212D−1*r**3−0.5607184266833242D−6*r**4
$b_{1,4,1}$ = 0.1819489835414961D−1*r**3+0.269617780202832*r+0.147360952386272*r**2
+0.5222893278709695D−1−0.156750432448538 5D−6*r**4
$b_{1,4,2}$ = 0.1174602901030404D−5*r**4+0.3569858599788832D1−0.2020369716680659D1*r
−0.1104243219414049D1*r**2−0.136342720443555*r**3
$b_{1,4,3}$ = 0.3321571727973626D1*r−0.1931095955085073D−5*r**4−0.6760846514693342D1
+0.18154217161987D1*r**2+0.224153095248509*r**3
$b_{1,4,4}(4,4)$ = −0.1574840761461756D1*r−0.860697851695618*r**2−0.106269138278591*r**3
+0.9154036295839457D−6*r**4+0.333106356693915D1
$b_{1,5,1}$ = −0.2987873081448477D−1*r**3−0.518641429424248*r−0.257285012965914*r**2
−0.4048214245276534D−1+0.2562672239794297D−6*r**4
$b_{1,5,2}$ = 0.388641816217176D1*r−0.498150842038882D1+0.1927954634004752D1*r**2
+0.223895037133 77*r**3−0.192032787420902D−5*r**4
$b_{1,5,3}(5,3)$ = −0.6389432876553726D1*r+0.1091939869559572D2−0.3169637493699437D1*r**2
−0.368092740272789*r**3+0.3157098783826488D−5*r**4

$b_{1,5,4}$ = 0.174509583869641*r**3+0.3029267239118462D1*r−0.5734559482841803D1
+0.1502714689756679D1*r**2−0.149656969559674D−5*r**4
$b_{1,6,1}$ = 0.861166219608901D−2*r**3+0.9339627527138385D−1*r+0.6385010965186993D−1*r**2
+0.1481271048655561D−1−0.1852788924560673D−6*r**4
$b_{1,6,2}$ = −0.699861137003354*r+0.2169287550091448D1−0.478458163442821*r**2
−0.6453113551403363D−1*r**3+0.1388379739558582D−5*r**4
$b_{1,6,3}$ = 0.1150600777167189D1*r−0.3608719407162703D1+0.786605092913821*r**2
+0.106091867012144*r**3−0.2282553956602431D−5*r**4
$b_{1,6,4}$ = −0.5031246683596637D−1*r**3−0.545886801221966*r+0.1635395254773291D1
−0.373078172549436*r**2+0.1082006396985598D−5*r**4
$b_{1,7,1}$ = 0.2243012611435583D−2*r**3+0.1171151292684852D−2*r+0.1346299479602771D−1*r**2
−0.2768275174862666D−1−0.9024638506025246D−7*r**4
$b_{1,7,2}$ = −0.8775973912446844D−2*r+0.95598480179897−0.100884396278543*r**2
−0.1680792250002232D−1*r**3+0.6762575646104242D−6*r**4
$b_{1,7,3}$ = 0.144280656121243D−1*r−0.1482352310791144D1+0.165858137600199*r**2
+0.2763292268791725D−1*r**3−0.1111795523805767D−5*r**4
$b_{1,7,4}$ = −0.1311023623926729D−1*r**3−0.7085520955180939D−2*r+0.610512991618768
−0.7872832991219188D−1*r**2+0.5270280097511508D−6*r**4
$b_{1,8,1}$ = 0.375177717860525 4D−2*r**3+0.225830699697785*r+0.5379151824790475D−1*r**2
+0.239132881590276+0.1008071322481559D−6*r**4
$b_{1,8,2}$ = −0.1692253034732972D1*r−0.2128073349334664D1−0.403084523582173*r**2
−0.281137875613592D−1*r**3−0.7553940881286766D−6*r**4
$b_{1,8,3}$ = 0.2782134274899676D1*r+0.2554215574135783D1+0.662687698424797*r**2
+0.4622023442495863D−1*r**3+0.1241899255314971D−5*r**4
$b_{1,8,4}$ = −0.218944344976724D−1*r**3−0.1318445479985448D1*r−0.647786145787110
−0.313986100916669*r**2−0.5887015002539538D−6*r**4
$b_{1,10,1}$ = −0.208210658892342
$b_{1,10,2}$ = 0.156021798562303D1
$b_{1,10,3}$ = −0.2565063170237841D1
$b_{1,10,4}$ = 0.1215830144510811D1

B.3. Interpolant u_2

(1) Coefficients of intermediate stage at $1 + rc_3$

$\bar{b}_{2,1}$ = 0.2115656017407523D−1*r−0.8081458474192313D−2*r**2−0.1199437026528283D−1*r**3
−0.4491900159420196D−2*r**4+0.5203924849357778D−1
$\bar{b}_{2,2}$ = −0.2203491823505498D−16*r−0.2491520233564422D−15*r**2−0.2298818999416907D−15*r**3
−0.2214912303264025D−16*r**4−0.229043251865977D−15
$\bar{b}_{2,3}$ = 0.2705002965329429D−1*r+0.110031587589639*r**2+0.4420922034526149D−1*r**3
+0.1050541976249062D−1*r**4+0.382403409995255
$\bar{b}_{2,4}$ = −0.262319439063368*r−0.275509885192244*r**2−0.4361652128991576D−1*r**3
+0.3656896527661707D−1−0.6146073769929776D−2*r**4
$\bar{b}_{2,5}$ = 0.623627686821084*r+0.40949317454614 0*r**2+0.110901754637046*r**3
+0.7746369995067088D−2*r**4+0.3948857710763621
$\bar{b}_{2,6}$ = −0.161824293427029*r−0.304216899683929*r**2−0.138318204743442*r**3
+0.5028117370254531D−1−0.1120882825056163D−1*r**4
$\bar{b}_{2,7}$ = −0.109941258146079*r−0.142175505815687*r**2−0.6036033071799415D−1*r**3
−0.4671771089329218D−2*r**4−0.4171020317912413D−2

$\bar{b}_{2,8}$ = 0.8447293621024614D−1*r−0.107424556129085+0.210458987030274*r**2
+0.9917845203432746D−1*r**3+0.826678351168313 7D−2*r**4
$\bar{b}_{2,9}$ = 0
$\bar{b}_{2,10}$ = 0.195417007902640

(2) Coefficients of interpolant u_2

temp(1) = 0
temp(2) = 0.8022639275488D−1*r**3+0.2358267754770+0.11501991792814D−1*r**4
+0.4192476008481*r+0.2678526338751*r**2+0.63899954404509D−3*r**5
temp(3) = temp(2)
temp(4) = 0.69011950756882D−1*r**4+0.14149606528624D1+0.25154856050887D1*r
+0.4813583565292*r**3+0.1607115803251D1*r**2+0.38339972642706D−2*r**5
temp(5) = 0.8384952016962*r+0.4716535509541+0.23003983585627D−1*r**4
+0.12779990880902D−2*r**5+0.1604527855097*r**3+0.5357052677503*r**2
$b_{2,1,1}$ = 0.1D1
$b_{2,1,2}$ = (−0.9633901077311*r**2−0.9003930458265−0.15578292549371D1*r−0.2781956239439*r**3
−0.38321389492707D−1*r**4−0.20389301777847D−2*r**5)/temp(2)
$b_{2,1,3}$ = (0.14185917025673D1*r**2+0.14577410202959D1+0.24200616188412D1*r
+0.3834681906640*r**3+0.48724367273797D−1*r**4+0.23467656724158D−2*r**5)/temp(3)
$b_{2,1,4}$ = (−0.55260945460427D1*r**2−0.64310924230863D1−0.10146968400629D2*r
−0.13444786771339D1*r**3−0.1458581663318*r**4−0.54021543085845D−2*r**5)/temp(4)
$b_{2,1,5}$ = (0.4348862018321*r**2+0.5916524816050+0.8803486611686*r+0.88831760492114D−1*r**3
+0.64825851703028D−2*r**4)/temp(5)
$b_{2,3,2}$ = (0.20845118808666D−2*r**5+0.18604038627342D1*r+0.11313266732844D1
+0.10950124837715D1*r**2+0.3029286236283*r**3+0.40280126639107D−1*r**4)/temp(2)
$b_{2,3,3}$ = (−0.34333136861332D−2*r**5−0.42236195802615D1*r−0.27151840158825D1
−0.23241081288211D1*r**2−0.5959251612361*r**3−0.72835297484412D−1*r**4)/temp(3)
$b_{2,3,4}$ = (0.91963759449988D−2*r**5+0.20816410788432D2*r+0.14254716083383D2
+0.10492007370014D2*r**2+0.239114970946D1*r**3+0.2483021505150*r**4)/temp(4)
$b_{2,3,5}$ = (−0.19710224707887D1*r−0.1448098141804D1−0.8849488644357*r**2
−0.16487262794*r**3−0.11035651134001D−1*r**4)/temp(5)
$b_{2,4,2}$ = (0.62114894949483D−3*r**5+0.4245164851704*r+0.1910324183266+0.2830109901136*r**2
+0.83855108181819D−1*r**3+0.1164654280303D−1*r**4)/temp(2)
$b_{2,4,3}$ = (−0.75918204938254D−3*r**5−0.566021980227*r−0.1273549455510−0.4087936523863*r**2
−0.118794736590*r**3−0.15528723737373D−1*r**4)/temp(3)
$b_{2,4,4}$ = (0.15528723737368D−2*r**5+0.1528259346613D1*r−0.5730972549810
+0.13301516535339D1*r**2+0.3710588537045*r**3+0.41927554090903D−1*r**4)/temp(4)
$b_{2,4,5}$ = (−0.67922637627197D−1*r+0.1528259346614−0.90563516836344D−1*r**2
−0.23479430290906D−1*r**3−0.18634468484845D−2*r**4)/temp(5)
$b_{2,5,2}$ = (−0.29263336849147D−3*r**5−0.5039914768018*r−0.4319926944016−0.2346626981934*r**2
−0.54517596549987D−1*r**3−0.63208807594179D−2*r**4)/temp(2)
$b_{2,5,3}$ = (0.97544456163846D−3*r**5+0.18879680718294D1*r+0.16559719952064D1
+0.8568743979488*r**2+0.1935769732572*r**3+0.21771922615776D−1*r**4)/temp(3)
$b_{2,5,4}$ = (−0.35116004218984D−2*r**5−0.11663802748844D2*r−0.11015813707243D2
−0.48319182855293D1*r**2−0.9742057470455*r**3−0.94813211391285D−1*r**4)/temp(4)
$b_{2,5,5}$ = (0.12479788949381D1*r+0.1295978083205D1+0.4479924238239*r**2
+0.71109908543471D−1*r**3+0.42139205062789D−2*r**4)/temp(5)
$b_{2,6,2}$ = (−0.76053986548402D−3*r**5−0.10915410750654D1*r−0.8771312210346
−0.537107513127*r**2−0.1309079243464*r**3−0.15828735950388D−1*r**4)/temp(2)

$b_{2,6,3}$ = (0.20914846300809D−2*r**5+0.37424265430812D1*r+0.31576723957248D1
+0.17499309298666D1*r**2+0.4042744722464*r**3+0.46202796828158D−1*r**4)/temp(3)
$b_{2,6,4}$ = (−0.71300612389114D−2*r**5−0.22454559258487D2*r−0.20524870572211D2
−0.95379898702136D1*r**2−0.19578435155933D1*r**3−0.1925116534506*r**4)/temp(4)
$b_{2,6,5}$ = (0.23702034772847D1*r+0.23857969212143D1+0.8732328600522*r**2
+0.1416885769396*r**3+0.85560734866949D−2*r**4)/temp(5)
$b_{2,7,2}$ = (−0.5720567346691D−3*r**5−0.7037370442808*r−0.5278027832106−0.3649006896270*r**2
−0.92673191016404D−1*r**3−0.1158414887705D−1*r**4)/temp(2)
$b_{2,7,3}$ = (0.13347990475611D−2*r**5+0.21894041377625D1*r+0.1759342610702D1
+0.10599496222501D1*r**2+0.2509898923360*r**3+0.29174893468125D−1*r**4)/temp(3)
$b_{2,7,4}$ = (−0.42904255100174D−2*r**5−0.12667266797054D2*r−0.11083858447423D2
−0.55517033493263D1*r**2−0.11642069621435D1*r**3−0.1158414887704*r**4)/temp(4)
$b_{2,7,5}$ = (0.13136424826575D1*r+0.12667266797054D1+0.5004352314885*r**2
+0.83405871914757D−1*r**3+0.51485106120215D−2*r**4)/temp(5)
$b_{2,8,2}$ = (0.9584993160678D−3*r**5+0.15983814782335D1*r+0.5306102448233/r
+0.16507874283395D1+0.72203753479*r**2+0.1695106040466*r**3
+0.20128485637426D−1*r**4)/temp(2)
$b_{2,8,3}$ = (−0.25559981761806D−2*r**5−0.55550307112376D1*r−0.21224409792935D1/r
−0.61314961624038D1−0.23524448714255D1*r**2−0.5175896306766*r**3
−0.57509958964072D−1*r**4)/temp(3)
$b_{2,8,4}$ = (0.95849931606762D−2*r**5+0.3537401632156D2*r+0.15918307344702D2/r
+0.42448819585872D2+0.13625547027564D2*r**2+0.26785263387517D1*r**3
+0.2587948153383*r**4)/temp(4)
$b_{2,8,5}$ = (−0.3878040307845D1*r−0.21224409792935D1/r−0.51881890604954D1
−0.12810343359248D1*r**2−0.1966840596571*r**3−0.11501991792813D−1*r**4)/temp(5)
$b_{2,11,2}$ = (−0.5306102448233/r−0.26202975053003D−1*r−0.2358267754770)/temp(2)
$b_{2,11,3}$ = (0.1048119002120*r+0.943307101908+0.21224409792936D1/r)/temp(3)
$b_{2,11,4}$ = (−0.7860892515900*r−0.15918307344702D2/r−0.70748032643115D1)/temp(4)
$b_{2,11,5}$ = (0.1048119002120*r+0.943307101908+0.21224409792936D1/r)/temp(5)

B.4. Interpolant u_3

temp(1) = 0
temp(2) = −0.5578827290622*r**2−0.4171085824764D−1*r**4−0.3016588855409−0.6770566097697*r
−0.2212165160633*r**3−0.29793470176882D−2*r**5
temp(3) = temp(2)
temp(4) = −0.13272990963803D1*r**3−0.40623396586187D1*r−0.18099533132459D1
−0.2502651494858*r**4−0.33472963743733D1*r**2−0.17876082106129D−1*r**5
temp(5) = −0.83421716495279D−1*r**4−0.13541132195396D1*r−0.6033177710819
−0.59586940353764D−2*r**5−0.4424330321267*r**3−0.11157654581244D1*r**2
$b_{3,1,1}$ = 0.1D1
$b_{3,1,2}$ = (0.11517418334006D1+0.7633512680320*r**3+0.25109910063769D1*r
+0.98298183916924D−2*r**5+0.19929139748843D1*r**2+0.140199051540*r**4)/temp(2)
$b_{3,1,3}$ = (−0.18646760135709D1−0.10423914374388D1*r**3−0.38890435072148D1*r
−0.12234914850416D−1*r**5−0.29001097298989D1*r**2−0.1816151841338*r**4)/temp(3)
$b_{3,1,4}$ = (0.82263609347787D1+0.35948823916556D1*r**3+0.1624272350706D2*r
+0.34885721457115D−1*r**5+0.11100765774032D2*r**2+0.5658479221094*r**4)/temp(4)
$b_{3,1,5}$ = (−0.7568149454933−0.2299599875152*r**3−0.14025108877519D1*r
−0.12930771410103D−2*r**5−0.851250618812*r**2−0.2842945620212D−1*r**4)/temp(5)

$b_{3,3,2}$ = (−0.22421762238379D1*r**2−0.10879146927559D−1*r**5−0.14471416265408D1
−0.1536540738888*r**4−0.29875434912365D1*r−0.837749819273*r**3)/temp(2)
$b_{3,3,3}$ = (0.46865949564713D1*r**2+0.20648176821693D−1*r**5+0.3473139903698D1
+0.2944585431158*r**4+0.67533275905238D1*r+0.16530197686207D1*r**3)/temp(3)
$b_{3,3,4}$ = (−0.20697341129814D2*r**2−0.77680439413871D−1*r**5−0.18233984494415D2
−0.11279066588851D1*r**4−0.33110600415254D2*r−0.66669674235543D1*r**3)/temp(4)
$b_{3,3,5}$ = (0.16891179992552D1*r**2+0.46402891997142D−2*r**5+0.18523412819723D1
+0.70348116408106D−1*r**4+0.31155351284283D1*r+0.4644341126886*r**3)/temp(5)
$b_{3,4,2}$ = (−0.5903857816629*r**2−0.17238799376974D−2*r**5−0.244359981168
−0.31202226872327D−1*r**4−0.6950683908796*r−0.2050555185891*r**3)/temp(2)
$b_{3,4,3}$ = (0.8551593744271*r**2−0.11492532917986D−2*r**5+0.1629066541122
+0.12182084893064D−1*r**4+0.9520988895902*r+0.222897675944*r**3)/temp(3)
$b_{3,4,4}$ = (−0.27983743028642D1*r**2+0.27926854990701D−1*r**5+0.7330799435072
+0.17893873753*r**4−0.2753122454499D1*r−0.2381540133929*r**3)/temp(4)
$b_{3,4,5}$ = (0.1923505234482*r**2−0.46889534305372D−2*r**5−0.1954879849350
−0.37373717049281D−1*r**4+0.1477020330618*r−0.39925059357067D−1*r**3)/temp(5)
$b_{3,5,2}$ = (0.4601467372279*r**2+0.20466126192501D−2*r**5+0.5525854071974
+0.27970372463082D−1*r**4+0.784364286327*r+0.1540075995985*r**3)/temp(2)
$b_{3,5,3}$ = (−0.16702632987098D1*r**2−0.72768448684465D−2*r**5−0.21182440609236D1
−0.99147011332567D−1*r**4−0.29307492707656D1*r−0.5484921819589*r**3)/temp(3)
$b_{3,5,4}$ = (0.92056635613849D1*r**2+0.36839027146524D−1*r**5+0.14090927883535D2
+0.4952802538586*r**4+0.1794981597713D2*r+0.27966961442051D1*r**3)/temp(4)
$b_{3,5,5}$ = (−0.8186450476998*r**2−0.27288168256708D−2*r**5−0.16577562215924D1
−0.35474618733697D−1*r**4−0.18972098980445D1*r−0.2108010997827*r**3)/temp(5)
$b_{3,6,2}$ = (0.10651944626681D1*r**2+0.22162693631573D−2*r**5+0.1121986365099D1
+0.43217252581584D−1*r**4+0.17104058810176D1*r+0.3141561822277*r**3)/temp(2)
$b_{3,6,3}$ = (−0.34307849741693D1*r**2−0.44325387263121D−2*r**5−0.40391509143564D1
−0.1108134681578*r**4−0.58343290985148D1*r−0.9275087284817*r**3)/temp(3)
$b_{3,6,4}$ = (0.18260951417744D2*r**2−0.66488080895076D−2*r**5+0.26254480943317D2
+0.2726011316682*r**4+0.34691818408861D2*r+0.39942714597518D1*r**3)/temp(4)
$b_{3,6,5}$ = (−0.1604800645863D1*r**2+0.5319046471584D−2*r**5−0.30518029130693D1
+0.25708724612668D−1*r**4−0.36182813622925D1*r−0.2034535275378*r**3)/temp(5)
$b_{3,7,2}$ = (0.7309863376317*r**2+0.6751413152584+0.16670155932303D−1*r**4
+0.11102323850917D1*r+0.1900397776283*r**3)/temp(2)
$b_{3,7,3}$ = (−0.20915488976402D1*r**2+0.44453749152851D−2*r**5−0.22504710508616D1
−0.44453749152588D−2*r**4−0.3430718090869D1*r−0.4300900230534*r**3)/temp(3)
$b_{3,7,4}$ = (0.10692238014982D2*r**2−0.60012561356329D−1*r**5+0.14177967620428D2
−0.3400711810192*r**4+0.1966911698453D2*r+0.1245260648143D1*r**3)/temp(4)
$b_{3,7,5}$ = (−0.9261938635990*r**2+0.1066889979668D−1*r**5−0.16203391566204D1
+0.82683973424268D−1*r**4−0.2016422061572D1*r+0.3200669939008D−1*r**3)/temp(5)
$b_{3,8,2}$ = (−0.5555551142046/r−0.14166795069111D1*r**2−0.14896735088433D−2*r**5
−0.2056866697337D1−0.43200531756482D−1*r**4−0.2460816497152D1*r
−0.3787494896236*r**3)/temp(2)
$b_{3,8,3}$ = (0.22222204568187D1/r+0.45509525695198D1*r**2+0.7624149018266D1
+0.8938041053063D−1*r**4+0.84891527690683D1*r+0.10725649263679D1*r**3)/temp(3)
$b_{3,8,4}$ = (−0.1666665342614D2/r−0.25763903335464D2*r**2+0.44690205265368D−1*r**5
−0.5265623435388D2−0.44690205265054D−1*r**4−0.53512796621465D2*r
−0.47259892068083D1*r**3)/temp(4)

$b_{3,8,5}$ = (0.22222204568187D1/r+0.23194216532708D1*r**2−0.11917388070759D−1*r**5
+0.64175134761019D1−0.77463022459944D−1*r**4+0.5780926329989D1*r
+0.1876988621143*r**3)/temp(5)
$b_{3,10,2}$ = (0.20884076691296D−1*r**2+0.1879566902216*r+0.4229025529988)/(r*temp(2))
$b_{3,10,3}$ = (−0.83536306765184D−1*r**2−0.7518267608867*r−0.16916102119954D1)/(r*temp(3))
$b_{3,10,4}$ = (0.6265223007388*r**2+0.56387007066505D1*r+0.12687076589965D2)/(r*temp(4))
$b_{3,10,5}$ = (−0.83536306765182D−1*r**2−0.7518267608867*r−0.16916102119953D1)/(r*temp(5))
$b_{3,11,2}$ = (0.1326525612058+0.65507437632508D−2*r**2+0.58956693869263D−1*r)/(r*temp(2))
$b_{3,11,3}$ = (−0.2358267754770*r−0.26202975053003D−1*r**2−0.5306102448233)/(r*temp(3))
$b_{3,11,4}$ = (0.1965223128975*r**2+0.17687008160779D1*r+0.39795768361754D1)/(r*temp(4))
$b_{3,11,5}$ = (−0.2358267754770*r−0.26202975053003D−1*r**2−0.530610244823)/(r*temp(5))

B.5. Interpolant u_4

temp(1) = −0.2212165160633*r**3−0.6770566097697*r−0.29793470176882D−2*r**5
−0.5578827290622*r**2−0.3016588855409−0.4171085824764D−1*r**4
temp(2) = temp(1)
temp(3) = temp(1)
temp(4) = −0.40623396586187D1*r−0.17876082106129D−1*r**5−0.18099533132459D1
−0.13272990963803D1*r**3−0.33472963743733D1*r**2−0.2502651494858*r**4
temp(5) = −0.83421716495279D−1*r**4−0.59586940353764D−2*r**5−0.4424330321267*r**3
−0.13541132195396D1*r−0.6033177710819−0.11157654581244D1*r**2
$b_{4,1,1}$ = (0.1066863854582*r**5+0.11121397263477D−1*r**7+0.46901788560155D−1*r**6
+0.92419034319773D−1*r**4+0.75864543671986D−4*r**9+0.14134943841429D−2*r**8
−0.5410886467553*r**2−0.6770566097697*r−0.3016588855409−0.1428402525278*r**3)/temp(1)
$b_{4,1,2}$ = (−0.6462224323213*r**5−0.66531427284094D−1*r**7−0.2805801160733*r**6
−0.6622049074724*r**4−0.45384372585352D−3*r**9−0.84559337830611D−2*r**8
+0.1892446898731D1*r**2+0.25109910063769D1*r+0.11517418334006D1
+0.2944817047322*r**3)/temp(2)
$b_{4,1,3}$ = (0.12848842126093D1*r**5+0.1315431611027*r**7+0.5547512945013*r**6
+0.14048644324732D1*r**4+0.89732087199209D−3*r**9+0.16718719337706D−1*r**8
−0.27014704202757D1*r**2−0.38890435072148D1*r−0.18646760135709D1
−0.1153621068040*r**3)/temp(3)
$b_{4,1,4}$ = (−0.61990947354945D1*r**5−0.6321990619060*r**7−0.26661458112661D1*r**6
−0.70588048302161D1*r**4−0.43125420489084D−2*r**9−0.80350499356702D−1*r**8
+0.10146101281034D2*r**2+0.1624272350706D2*r+0.82263609347787D1−0.8604391033835*r**3)/
temp(4)
$b_{4,1,5}$ = (0.5786454361602*r**5+0.58812597601809D−1*r**7+0.2480278288819*r**6
+0.6808813624885*r**4+0.40118977620536D−3*r**9+0.74748949666621D−2*r**8
−0.7624395115922*r**2−0.14025108877519D1*r−0.7568149454933+0.184512361564*r**3)/temp(5)
$b_{4,3,1}$ = (−0.9850785996178D−1*r**6−0.36736754459256D−2*r**8−0.24212259918415D−1*r**7
−0.2542490335192*r**5−0.24931884774407D−3*r**9−0.2429371351924*r**3
−0.59092816668433D−1*r**2−0.3603733954 017*r**4)/temp(1)
$b_{4,3,2}$ = (0.15101123872196D1*r**5+0.1448447683310*r**7+0.5893026178897*r**6
+0.2002204203922D1*r**4+0.14914977314687D−2*r**9+0.21976993088685D−1*r**8
−0.1888665838223D1*r**2−0.29875434912365D1*r−0.14471416265408D1+0.6155706549207*r**3)/
temp(2)
$b_{4,3,3}$ = (−0.29865928005583D1*r**5−0.2863810303378*r**7−0.11651445394724D1*r**6
−0.39680144614377D1*r**4−0.29489270617518D−2*r**9−0.43451993447778D−1*r**8

+0.39876489770339D1*r**2+0.67533275905238D1*r+0.347139903698D1
−0.12204248135107D1*r**3)/temp(3)

$b_{4,3,4}$ = (0.14375179814868D2*r**5+0.13763529567742D1*r**7+0.55997079488139D1*r**6
+0.19357623811018D2*r**4+0.14172602410034D−1*r**9+0.2088311491478*r**8
−0.17338192780186D2*r**2−0.33110600415254D2*r−0.18233984494415D2
+0.7142864680473D1*r**3)/temp(4)

$b_{4,3,5}$ = (−0.13398891565851D1*r**5−0.1280401972770*r**7−0.5209330258863*r**6
−0.18353922315031D1*r**4−0.13184574491438D−2*r**9−0.19427270746851D−1*r**8
+0.13766211101016D1*r**2+0.31155351284283D1*r+0.18523412819723D1−0.820275320498*r**3)/
temp(5)

$b_{4,4,1}$ = (−0.13052071368823D−1*r**6+0.1665972255615D−2*r**8+0.22291178068067D−2*r**7
−0.28051687768846D−1*r**5+0.1877151837313D−3*r**9+0.64673746894956D−1*r**3
+0.33260784117403D−1*r**2+0.17164207112453D−1*r**4)/temp(1)

$b_{4,4,2}$ = (0.1660894604883*r**5−0.13335229895822D−1*r**7+0.78081280311186D−1*r**6
−0.1338834970704*r**4−0.11229667280705D−2*r**9−0.99663297116239D−2*r**8
−0.7893614487930*r**2−0.6950683908796*r−0.244359981168−0.5919526491198*r**3)/temp(2)

$b_{4,4,3}$ = (−0.3329427857016*r**5+0.26365859957258D−1*r**7−0.1543790484341*r**6
+0.2151992065644*r**4+0.22202829437716D−2*r**9+0.19705011125969D−1*r**8
+0.12485657585268D1*r**2+0.9520988895902*r+0.1629066541122+0.9878545339159*r**3)/temp(3)

$b_{4,4,4}$ = (0.1622533204553D1*r**5−0.1267148500278*r**7+0.7419487929271*r**6
−0.7967656076835*r**4−0.10670724212881D−1*r**9−0.94702677389298D−1*r**8
−0.46890932493347D1*r**2−0.27531224544989D1*r+0.7330799435072−0.39145519648638D1*r**3)/
temp(4)

$b_{4,4,5}$ = (−0.1530329596480*r**5+0.11788105889292D−1*r**7−0.69022462115039D−1*r**6
+0.53394698298484D−1*r**4+0.99268260120461D−3*r**9+0.88100580856894D−2*r**8
+0.3682414718492*r**2+0.1477020330618*r−0.1954879849350+0.3020851180893*r**3)/temp(5)

$b_{4,5,1}$ = (0.1141636024694*r**6+0.66671655271127D−2*r**8+0.36873696808022D−1*r**7
+0.2396372433956*r**5+0.48285878469345D−3*r**9+0.2904117017553*r**3+0.1034199945099*r**2
+0.3431547382371*r**4)/temp(1)

$b_{4,5,2}$ = (−0.14315329507958D1*r**5−0.2205891597753*r**7−0.6829598148722*r**6
−0.20248808991298D1*r**4−0.28886014375026D−2*r**9−0.3988491984859D−1*r**8
−0.1585416956598*r**2+0.7843642863274*r+0.5525854071974−0.15833195149751D1*r**3)/temp(2)

$b_{4,5,3}$ = (0.28271368324262D1*r**5+0.4361396796427*r**7+0.13503196402335D1*r**6
+0.39596648398868D1*r**4+0.57112221962809D−2*r**9+0.788587987871D−1*r**8
−0.4470183523437*r**2−0.29307492707656D1*r−0.21182440609236D1+0.28864784755132D1*r**3)/
temp(3)

$b_{4,5,4}$ = (−0.13585409767978D2*r**5−0.20960960191212D1*r**7−0.64896631848603D1*r**6
−0.19011450641782D2*r**4−0.27448248046923D−1*r**9−0.3789969634170*r**8
+0.33267238955696D1*r**2+0.1794981597713D2*r+0.14090927883535D2
−0.13711841503235D2*r**3)/temp(4)

$b_{4,5,5}$ = (0.12645300025783D1*r**5+0.1949968912254*r**7+0.6037243211208*r**6
+0.17792093689856D1*r**4+0.25534722598153D−2*r**9+0.35257559279753D−1*r**8
−0.2717354843*r**2−0.18972098980445D1*r−0.16577562215924D1+0.13249651487877D1*r**3)/
temp(5)

$b_{4,6,1}$ = (0.22285502816639D−1*r**6−0.67874627868019D−2*r**8−0.20814885879528D−1*r**7
+0.2499294630605*r**5−0.6033300254935D−3*r**9+0.5243315002802*r**3+0.1832614952435*r**2
+0.5540832121623*r**4)/temp(1)

$b_{4,6,2}$ = (−0.14929343402076D1*r**5+0.124520690477*r**7−0.1333183479564*r**6
−0.32714693884918D1*r**4+0.36092953761532D−2*r**9+0.40604572981723D−1*r**8

$$
\begin{aligned}
&-0.31129007838021D-1*r**2+0.17104058810176D1*r+0.1121986365099D1\\
&-0.28225470806092D1*r**3)/temp(2)\\
b_{4,6,3} &= (0.29517168411432D1*r**5-0.2461971119023*r**7+0.2635914730690*r**6\\
&+0.64428466084571D1*r**4-0.71361481710822D-2*r**9-0.80281666924675D-1*r**8\\
&-0.12631799672039D1*r**2-0.58343290985148D1*r-0.40391509143564D1\\
&+0.5274250041447D1*r**3)/temp(3)\\
b_{4,6,4} &= (-0.14213961823376D2*r**5+0.11832282414669D1*r**7-0.12668258889602D1*r**6\\
&-0.31224420209104D2*r**4+0.34296470767153D-1*r**9+0.3858352961304*r**8\\
&+0.78433984222253D1*r**2+0.34691818408861D2*r+0.26254480943317D2\\
&-0.25811505166316D2*r**3)/temp(4)\\
b_{4,6,5} &= (0.13270055748441D1*r**5-0.1100740741795*r**7+0.1178510468116*r**6\\
&+0.29558327209777D1*r**4-0.31905528747692D-2*r**9-0.35893719841154D-1*r**8\\
&-0.6356702101522*r**2-0.36182813622926D1*r-0.30518029130693D1+0.25693363301902D1*r**3)/\\
&temp(5)\\
b_{4,7,1} &= (-0.28703350098312D-1*r**6-0.10437581853929D-1*r**8-0.37892960208829D-1*r**7\\
&+0.1114098410929*r**5-0.9076158133851D-3*r**9+0.2705829643653*r**3\\
&+0.91896101105224D-1*r**2+0.2904370602831*r**4)/temp(1)\\
b_{4,7,2} &= (-0.6664860148241*r**5+0.2266866893597*r**7+0.1717117736767*r**6\\
&-0.17208086607173D1*r**4+0.54296213020309D-2*r**9+0.62440644973355D-1*r**8\\
&+0.181237180801*r**2+0.11102323850918D1*r+0.6751413152584-0.14286660730394D1*r**3)/\\
&temp(2)\\
b_{4,7,3} &= (0.13221937052856D1*r**5-0.4481954606352*r**7-0.3395013519183*r**6\\
&+0.34308252215697D1*r**4-0.10735220614017D-1*r**9-0.123455037061*r**8\\
&-0.10046078104712D1*r**2-0.3430718090869D1*r-0.22504710508616D1\\
&+0.27703476224999D1*r**3)/temp(3)\\
b_{4,7,4} &= (-0.63931373798893D1*r**5+0.2154036343575D1*r**7+0.16316502842054D1*r**6\\
&-0.16850050341351D2*r**4+0.51593684876046D-1*r**9+0.5933273760745*r**8\\
&+0.54683774212836D1*r**2+0.1966911698453D2*r+0.14177967620428D2\\
&-0.14136106655526D2*r**3)/temp(4)\\
b_{4,7,5} &= (0.599830674873*r**5-0.2003869988550*r**7-0.1517901518273*r**6\\
&+0.16185843239299D1*r**4-0.47996885953309D-2*r**9-0.55196418846306D-1*r**8\\
&-0.4402253933218*r**2-0.2016422061572D1*r-0.16203391566204D1+0.14629138618729D1*r**3)/\\
&temp(5)\\
b_{4,8,1} &= (-0.43087612417316D-1*r**6+0.11152087919785D-1*r**8-0.54013399851737D-1\\
&+0.32695894128466D-1*r**7-0.4363435439002*r**5+0.10138261745259D-2*r**9\\
&-0.13555308554379D1*r**3-0.9483499007542D0*r**2-0.3480863546000*r\\
&-0.10719522085318D1*r**4)/temp(1)\\
b_{4,8,2} &= (0.26088440888883D1*r**5-0.1955963312128*r**7-0.5555551142046/r+0.2577626070243*r**6\\
&+0.63695287975128D1*r**4-0.60650025182261D-2*r**9-0.66715027700488D-1*r**8\\
&+0.42566249320113D1*r**2-0.3784628646895*r-0.1733742857817D1+0.77304296362834D1*r**3)/\\
&temp(2)\\
b_{4,8,3} &= (-0.51610429635432D1*r**5+0.3867249021725*r**7+0.22222204568187D1/r\\
&-0.5096374679788*r**6-0.12589600361468D2*r**4+0.11991469834807D-1*r**9\\
&+0.13190611681828*r**8-0.6666068171786D1*r**2+0.43720100813225D1*r+0.69852820494779D1\\
&-0.14960565576239D2*r**3)/temp(3)\\
b_{4,8,4} &= (0.24848765861158D2*r**5-0.1858607610761D1*r**7-0.1666665342614D2/r\\
&+0.24493278591401D1*r**6+0.60890744847257D2*r**4-0.5763124374452D-1*r**9\\
&-0.6339436811897*r**8+0.28145322583874D2*r**2-0.33725726559401D2*r-0.49585826930456D2\\
&+0.72329556502976D2*r**3)/temp(4)
\end{aligned}
$$

$b_{4,8,5}$ = (−0.23194059756631D1*r**5+0.1729036755951*r**7+0.22222204568187D1/r
−0.227857556985*r**6−0.57462016166461D1*r**4+0.53613542820187D−2*r**9
+0.58974897102206D−1*r**8−0.26956784980328D1*r**2+0.394016278034D1*r+0.61318777528805D1
−0.6980671159116D1*r**3)/temp(5)
$b_{4,10,1}$ = (0.62801906723396D−2*r**5+0.73709606312205D−1*r**4+0.2957474002145*r**3
+0.4759723456932*r**2+0.3078946111203*r+0.60240250001803D−1)/temp(1)
$b_{4,10,2}$ = (−0.37569923917668D−1*r**6−0.4409522649284*r**5−0.176924681186D1*r**4
−0.28474047600766D1*r**3−0.18210308774833D1*r**2−0.1724179747255*r+0.4229025529988)/
(r*temp(2))
$b_{4,10,3}$ = (0.74281685456987D−1*r**6+0.8718324135215*r**5+0.34980809506659D1*r**4
+0.56297698451624D1*r**3+0.35582210618244D1*r**2−0.39309014858308D−1*r
−0.16916102119953D1)/(r*temp(3))
$b_{4,10,4}$ = (−0.3569992652526*r**6−0.41900440079659D1*r**5−0.16811846978151D2*r**4
−0.27056786419155D2*r**3−0.16875836414152D2*r**2+0.22143261754759D1*r
+0.12687076589965D2)/(r*temp(4))
$b_{4,10,5}$ = (0.33211144078802D−1*r**6+0.389793954188*r**5+0.15639826928692D1*r**4
+0.25170551301835D1*r**3+0.15446837305723D1*r**2−0.4332619709728*r−0.16916102119953D1)/
(r*temp(5))
$b_{4,11,1}$ = (0.21117958169771D−2*r**5+0.25106905824064D−1*r**4+0.1758656627582*r**2
+0.1288195448356*r+0.1033020120471*r**3+0.33260784117391D−1)/temp(1)
$b_{4,11,2}$ = (−0.1501967998794*r**5−0.6179826275413*r**4−0.12633375690793D−1*r**6
−0.10520794533612D1*r**3−0.1400189732607*r−0.7640851733752*r**2+0.1326525612058)/
(r*temp(2))
$b_{4,11,3}$ = (−0.5306102448234+0.14974661951105D1*r**2+0.12218494574945D1*r**4
+0.2969628437294*r**5+0.1575796086224*r+0.2497818311743D−1*r**6
+0.20801275829463D1*r**3)/(r*temp(3))
$b_{4,11,4}$ = (0.39795768361756D1−0.99971347469442D1*r**3−0.71262621781929D1*r**2
−0.58722329184017D1*r**4−0.1220181303919*r−0.14272093634729D1*r**5−0.120045647394*r**6)/
(r*temp(4))
$b_{4,11,5}$ = (−0.5306102448234+0.1327712979111*r**5−0.599358270761D−1*r+0.6550254600237*r**2
+0.11167679263552D−1*r**6+0.9300195120037*r**3+0.546285643975*r**4)/(r*temp(5))
$b_{4,12,1}$ = 0.130901611588997
$b_{4,12,2}$ = −0.783091444939628
$b_{4,12,3}$ = 0.1548295719856576D1
$b_{4,12,4}$ = −0.1240190030203101D1
$b_{4,12,5}$ = 0.346119449985589

B.6. Interpolant u_5

temp(1) = −0.2212165160633*r**3−0.4171085824764D−1*r**4−0.6770566097697*r−0.3016588855409
−0.5578827290622*r**2−0.29793470176882D−2*r**5
temp(2) = temp(1)
temp(3) = temp(1)
temp(4) = −0.33472963743733D1*r**2−0.17876082106129D−1*r**5−0.2502651494858*r**4
−0.13272990963803D1*r**3−0.18099533132459D1−0.40623396586187D1*r
temp(5) = −0.11157654581244D1*r**2−0.6033177710819−0.13541132195396D1*r
−0.83421716495279D−1*r**4−0.4424330321267*r**3−0.59586940353764D−2*r**5
$b_{5,1,1}$ = (0.90760940680027D−1*r**6+0.1933197725522*r**5+0.19950440695987D−3*r**9
+0.33670002207937D−2*r**8−0.5304523821431*r**2−0.6770566097697*r

+0.23777682626708D−1*r**7+0.18502178257505*r**4−0.93201894024397D−1*r**3
−0.3016588855409)/temp(1)

$b_{5,1,2}$ = (−0.5265706244817*r**6−0.11365359227855D1*r**5−0.11326722852018D−2*r**9
−0.19237154452492D−1*r**8+0.18313853365487D1*r**2+0.25109910063769D1*r
−0.1368899073509*r**7−0.11906904773881D1*r**4+0.95136426468954D−2*r**3
+0.11517418334006D1)/temp(2)

$b_{5,1,3}$ = (0.9931468476278*r**6+0.21624946736596D1*r**5+0.20945543689093D−2*r**9
+0.35782175841073D−1*r**8−0.25914415574197D1*r**2−0.38890435072148D1*r
+0.256396155501*r**7+0.23545306922873D1*r**4+0.3981313365499*r**3−0.18646760135709D1)/
temp(3)

$b_{5,1,4}$ = (−0.45283245383429D1*r**6−0.99241907860321D1*r**5−0.94071236953015D−2*r**9
−0.161435409596*r**8+0.9679603181779D1*r**2+0.1624272350706D2*r−0.11629274612268D1*r**7
−0.11087061016175D2*r**4−0.30375379944098D1*r**3+0.82263609347787D1)/temp(4)

$b_{5,1,5}$ = (0.3999443046809*r**6+0.8808613678554*r**5+0.82235820009454D−3*r**9
+0.14156361804493D−1*r**8−0.7249166607768*r**2−0.14025108877519D1*r
+0.1023471531798*r**7+0.1006047529659D1*r**4+0.3596276664904*r**3
−0.7568149454933)/temp(5)

$b_{5,3,1}$ = (−0.63457522249197D−1*r**7−0.2211965777479*r**6−0.72925212217764D−3*r**9
−0.3967975014120*r**3−0.96518311154289D−1*r**2−0.10508775423283D−1*r**8
−0.488455189756*r**5−0.6212158012140*r**4)/temp(1)

$b_{5,3,2}$ = (0.12689365551389D1*r**6+0.28246769833106D1*r**5+0.41147883212819D−2*r**9
+0.59369199866066D−1*r**8−0.16738104127465D1*r**2−0.29875434912365D1*r
+0.3603499302261*r**7+0.34863102099535D1*r**4+0.14988651818793D1*r**3
−0.14471416265408D1)/temp(2)

$b_{5,3,3}$ = (−0.2369082932119D1*r**6−0.53302084469747D1*r**5−0.75652855090859D−2*r**9
−0.109281348898*r**8+0.36004938290365D1*r**2+0.67533275905238D1*r−0.66649221860000*r**7
−0.66310725891244D1*r**4−0.28120626441664D1*r**3+0.3473139903698D1)/temp(3)

$b_{5,3,4}$ = (0.10718959083115D2*r**6+0.24329576417788D2*r**5+0.33824078488447D−1*r**9
+0.4890409790542*r**8−0.15696740383336D2*r**2−0.33110600415254D2*r
+0.29938162864467D1*r**7+0.30656415045682D2*r**4+0.13891057867522D2*r**3
−0.18233984494415D2)/temp(4)

$b_{5,3,5}$ = (−0.9417826334070*r**6−0.21515945184195D1*r**5−0.29476281058337D−2*r**9
−0.42645007743202D−1*r**8+0.12445906184321D1*r**2+0.3115535128428 3D1*r
−0.2617423213045*r**7−0.2749123073143D1*r**4−0.13630673418062D1*r**3
+0.18523412819723D1)/temp(5)

$b_{5,4,1}$ = (0.38360466177299D−1*r**7+0.66240393272557D−1*r**6+0.77420527098602D−3*r**9
+0.105633834673*r**3+0.54325972117595D−1*r**2+0.92675405614798D−2*r**8
+0.60445155255737D−1*r**5+0.75379755425497D−1*r**4)/temp(1)

$b_{5,4,2}$ = (−0.3412507790599*r**6−0.2984199347407*r**5−0.42983399963244D−2*r**9
−0.5092367546743D−1*r**8−0.9102942512235*r**2−0.6950683908796*r−0.2065349360423*r**7
−0.4486928799939*r**4−0.8270997649569*r**3−0.244359981168)/temp(2)

$b_{5,4,3}$ = (0.5711478712625*r**6+0.467564728712*r**5+0.77814450169355D−2*r**9
+0.91258333664381D−1*r**8+0.14664786034964D1*r**2+0.9520988895902*r
+0.3625706732443*r**7+0.7661990299081*r**4+0.14115739546902D1*r**3+0.1629066541122)/
temp(3)

$b_{5,4,4}$ = (−0.23556416698142D1*r**6−0.17975547323483D1*r**5
−0.34363731711938D−1*r**9−0.3996816801004*r**8−0.56129956267924D1*r**2
−0.2753122454499D1*r−0.15606809486488D1*r**7−0.31445176528512D1*r**4
−0.57110288099203D1*r**3+0.7330799435072)/temp(4)

$b_{5,4,5}$ = (0.1933199225036*r**6+0.1380665851641*r**5+0.29688591091086D−2*r**9
+0.34327052099625D−1*r**8+0.4425557104981*r**2+0.1477020330618*r+0.1323585025459*r**7
+0.249367107477*r**4+0.4465850265733*r**3−0.1954879849350)/temp(5)

$b_{5,5,1}$ = (0.19007539248946D−1*r**7+0.82516375684416D−1*r**6+0.23352457216912D−3*r**9
+0.4743393287569*r**3+0.1689194012479*r**2+0.3117676758964 3D−2*r**8+0.2652509437354*r**5
+0.5042778826221*r**4)/temp(1)

$b_{5,5,2}$ = (−0.5438701431002*r**6−0.16302703451623D1*r**5−0.16846706564262D−2*r**9
−0.22692268710247D−1*r**8−0.5345661970452*r**2+0.7843642863274*r−0.1349111215162*r**7
−0.29729013316897D1*r**4−0.26392267006837D1*r**3+0.5525854071974)/temp(2)

$b_{5,5,3}$ = (0.1135402457937D1*r**6+0.32285904667242D1*r**5+0.37325435465493D−2*r**9
+0.50548928600457D−1*r**8+0.2305527220737*r**2−0.29307492707656D1*r
+0.2959148498943*r**7+0.56872452740348D1*r**4+0.47891528056959D1*r**3
−0.21182440609235D1)/temp(3)

$b_{5,5,4}$ = (−0.55529171833771D1*r**6−0.15256483234311D2*r**5−0.18922667578383D−1*r**9
−0.2570594861585*r**8+0.4539720546295*r**2+0.1794981597713D2*r−0.14914445270198D1*r**7
−0.2632219798427D2*r**4−0.21778760814159D2*r**3+0.14090927883535D2)/temp(4)

$b_{5,5,5}$ = (0.5127210007646*r**6+0.13799426606459D1*r**5+0.17841056408476D−2*r**9
+0.24278956119399D−1*r**8−0.40665220774155D−1*r**2−0.18972098980445D1*r
+0.1401535952098*r**7+0.23587849968429D1*r**4+0.19738291212813D1*r**3
−0.16577562215924D1)/temp(5)

$b_{5,6,1}$ = (−0.91996206757024D−2*r**7+0.98937493588733D−1*r**6−0.65145913009008D−3*r**9
+0.8564085069086*r**3+0.2993272451331*r**2−0.64104692233464D−2*r**8+0.4841153456184*r**5
+0.938818503222*r**4)/temp(1)

$b_{5,6,2}$ = (−0.547743971 6478*r**6−0.28062699019037D1*r**5+0.40224458213594D−2*r**9
+0.40356152322922D−1*r**8−0.6974490236012*r**2+0.17104058810176D1*r
+0.67999676872212D−1*r**7−0.54663343538901D1*r**4−0.4728962681265D1*r**3
+0.1121986365099D1)/temp(2)

$b_{5,6,3}$ = (0.9888734650303*r**6+0.52921849334994D1*r**5−0.7995359209682D−2*r**9
−0.81440410315547D−1*r**8−0.62515735689244D−1*r**2−0.58343290985147D1*r
−0.1528695703571*r**7+0.10386229324735D2*r**4+0.87094838149471D1*r**3
−0.40391509143564D1)/temp(3)

$b_{5,6,4}$ = (−0.43572293394483D1*r**6−0.24155680779586D2*r**5+0.37857264695096D−1*r**9
+0.3895991144966*r**8+0.27528470222855D1*r**2+0.3469181840886D2*r+0.7814462666736*r**7
−0.47951802486165D2*r**4−0.40376138338365D2*r**3+0.26254480943317D2)/temp(4)

$b_{5,6,5}$ = (0.3758469467226*r**6+0.21381001819364D1*r**5−0.34266652828597D−2*r**9
−0.35492254322095D−1*r**8−0.2262108767639*r**2−0.36182813622925D1*r
−0.74021853394855D−1*r**7+0.43063953859336D1*r**4+0.37408449784956D1*r**3
−0.30518029130693D1)/temp(5)

$b_{5,7,1}$ = (−0.61891863177109D−1*r**7−0.46882159831774D−1*r**6−0.14824398365774D−2*r**9
+0.441952376279*r**3+0.1500970334534*r**2−0.1704805812064D−1*r**8+0.1819694899398*r**5
+0.474380747704*r**4)/temp(1)

$b_{5,7,2}$ = (0.2760742130672*r**6−0.10715607795727D1*r**5+0.87296193855231D−2*r**9
+0.1003906229335*r**8−0.1528876251524*r**2+0.11102323850917D1*r+0.3644616093455*r**7
−0.27768080474346D1*r**4−0.24124780016804D1*r**3+0.6751413152584)/temp(2)

$b_{5,7,3}$ = (−0.5275555077675*r**6+0.2052111416921D1*r**5−0.16681597083554D−1*r**9
−0.1918383664608*r**8−0.4025371929304*r**2−0.34307180908689D1*r−0.696456678238*r**7
+0.53336656918212D1*r**4+0.45431111074805D1*r**3−0.22504710508616D1)/temp(3)

$b_{5,7,4}$ = (0.24289584084882D1*r**6−0.94878274116888D1*r**5+0.76805008964033D−1*r**9
+0.8832576030863*r**8+0.29157308573742D1*r**2+0.1966911698453D2*r

+0.32066091242484D1*r**7−0.24917674049506D2*r**4−0.21652232649256D2*r**3
+0.14177967620428D2)/temp(4)

$b_{5,7,5}$ = (−0.2159217610431*r**6+0.8487525730943*r**5−0.68275655665813D−2*r**9
−0.78517004015684D−1*r**8−0.234902849982*r**2−0.2016422061572D1*r−0.2850508624047*r**7
+0.22675049547299D1*r**4+0.20674746839268D1*r**3−0.16203391566204D1)/temp(5)

$b_{5,8,1}$ = (0.53403318049054D−1*r**7−0.70376465645967D−1*r**6+0.16559168387301D−2*r**9
−0.22196474637359D1*r**3−0.1563126860727D1*r**2+0.18215085226032D−1*r**8
−0.7127703716743*r**5−0.17519143624927D1*r**4−0.95875643162407D−1−0.5857196462796*r)/
temp(1)

$b_{5,8,2}$ = (0.4144247500836*r**6+0.41957474901517D1*r**5−0.97511705902121D−2*r**9
−0.1072628764923*r**8+0.77801883944574D1*r**2+0.9787235740767*r−0.3144752515343*r**7
+0.10272679072237D2*r**4+0.12688923128958D2*r**3−0.5555551142046/r−0.14965526449442D1)/
temp(2)

$b_{5,8,3}$ = (−0.7919322019712*r**6−0.80205110917152D1*r**5+0.18633698869928D−1*r**9
+0.2049706875692*r**8−0.13010431606705D2*r**2+0.19323523792002D1*r+0.6009367885552*r**7
−0.19622453271235D2*r**4−0.23893511873568D2*r**3+0.22222204568187D1/r
+0.65605105965638D1)/temp(3)

$b_{5,8,4}$ = (0.36461952393797D1*r**6+0.3697229832276D2*r**5−0.85792829161952D−1*r**9
−0.9437211207814*r**8+0.55047501903563D2*r**2−0.23377894892112D2*r
−0.27668187404733D1*r**7+0.90708749358367D2*r**4+0.11020465689001D3*r**3
−0.1666665342614D2/r−0.47783008901104D2)/temp(4)

$b_{5,8,5}$ = (−0.3241277802217*r**6−0.32945756744904D1*r**5+0.76265360052238D−2*r**9
+0.83891896057463D−1*r**8−0.48616915117463D1*r**2+0.31052460274972D1*r
+0.245955786168*r**7−0.81447770690625D1*r**4−0.10028006375675D2*r**3
+0.22222204568187D1/r+0.59857150673588D1)/temp(5)

$b_{5,10,1}$ = (0.10579680585657D−1*r**5+0.1249008479024*r**4+0.5069651199235*r**3
+0.8377221850470*r**2+0.5760763397176*r+0.1309981072774)/temp(1)

$b_{5,10,2}$ = (−0.62120846407946D−1*r**6−0.732987938937*r**5−0.33306452960439D1*r**2
−0.5652706222263*r−0.29720259164997D1*r**4−0.48994608842577D1*r**3
+0.422902552998)/(r*temp(2))

$b_{5,10,3}$ = (0.118410174234*r**6+0.1396512314747D1*r**5+0.62533034804558D1*r**2+0.6573833364571*r
+0.56571939424415D1*r**4+0.93067214918065D1*r**3−0.16916102119953D1)/(r*temp(3))

$b_{5,10,4}$ = (−0.5441734550835*r**6−0.6415678900805D1*r**5−0.28320374575695D2*r**2
−0.7475080707441*r−0.2597188539557D2*r**4−0.42661068048888D2*r**3
+0.12687076589965D2)/(r*temp(4))

$b_{5,10,5}$ = (0.48315031580767D−1*r**6+0.5694922739037*r**5+0.24762488720869D1*r**2
−0.1901156265281*r+0.23043730761482D1*r**4+0.37812698783188D1*r**3
−0.16916102119953D1)/(r*temp(5))

$b_{5,11,1}$ = (0.29816644062775D−2*r**5+0.1996885936980*r**2+0.1340071243685*r**3+0.104142419530*r
+0.69811010688267D−2+0.34461513538093D−1*r**4)/temp(1)

$b_{5,11,2}$ = (−0.17818788763407D−1*r**6−0.2065828950923*r**5−0.6659573795835*r**2
−0.85496908120525D−2*r−0.8084832945383*r**4−0.12247209268749D1*r**3+0.1326525612058)/
(r*temp(2))

$b_{5,11,3}$ = (0.34482600449558D−1*r**6+0.4008159099812*r**5+0.13571538924929D1*r**2
−0.63053580619243D−1*r+0.15770471276289D1*r**4+0.24212974907852D1*r**3−0.5306102448234)/
(r*temp(3))

$b_{5,11,4}$ = (−0.1602273721644*r**6−0.18659147436037D1*r**5−0.65052562589208D1*r**2
+0.825052285741*r−0.73696607828234D1*r**4−0.11422103452866D2*r**3
+0.39795768361757D1)/(r*temp(4))

$b_{5,11,5}$ = (0.14329277279519D−1*r**6+0.1670726787108*r**5+0.5890705345255*r**2−0.1432441806246*r
+0.6615023995751*r**4+0.10314499128699D1*r**3−0.5306102448234)/(r*temp(5))
$b_{5,12,1}$ = 0.27474919934264 1D−1
$b_{5,12,2}$ = −0.26567908068999
$b_{5,12,3}$ = 0.679968625106813
$b_{5,12,4}$ = −0.618972746597041
$b_{5,12,5}$ = 0.182184683748008
$b_{5,13,1}$ = 0.112098509531683
$b_{5,13,2}$ = −0.597612727437998
$b_{5,13,3}$ = 0.1038345985682242D1
$b_{5,13,4}$ = −0.738317431540081
$b_{5,13,5}$ = 0.186601602902871