Some algorithm of step-size control for explicit
pseudo Runge-Kutta Method

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Abstract. We derive some special algorithm of pseudo
Runge-Kutta method which is useful in the step-size control. The
new method is designed to be able to change the step-size without
new functions evaluations, and this formulas can also provide dens
output.

1. Introduction. This paper deals with the numerical method
of the initial value problem;

$$(1.1) \quad \begin{cases} y' = f(x,y) \\ y(x_0) = y_0 . \end{cases}$$

In earlier papers [15] [16] , the author has presented some
pseudo Runge-Kutta (abbr, pseudo R-K) method, which is defined by

$$(1.2) \quad y_{n+1} = v_1 y_{n-1} + v_2 y_n + h \Phi(x_{n+1}, x_n, y_{n-1}, y_n; h),$$

$$\Phi(x_{n-1}, x_n, y_{n-1}, y_n; h) = h \sum_{i=0}^{r} w_i k_i ,$$

$$k_0 = f(x_{n-1}, y_{n-1}), \quad k_1 = f(x_n, y_n),$$

$$k_i = f(x_n + a_i h, y_n + b_i (y_n - y_{n-1}) + h \sum_{j=0}^{i-1} b_{ij} k_j),$$

$$a_i = b_i + \sum_{j=0}^{i-1} b_{ij} , (0 < a_i \leq 1),$$

where y_n is an approximation to the true solution $y(x_n)$ of (1.1)
at the point $x = x_0 + nh$. On using the numerical methods, it is
required convenient procedures for estimating local truncation
error, which is also important from the point of view of
step-size control policy. We may provide some formulas for
estimating the local truncation error of (1.2). However, We
should restrict here our attention to develop some specific

method of (1.2) which is ready to compute the local truncation

error estimate. So the aim of this paper is to present some kind

of pseudo R-K method (1.2) which is useful in step-size control.

2. Specific Integration formulas. The new algorithm

parallel to (1.2) is defined as follow, setting y_{n+h} by $y_{n+\sigma h}$

in (1.2), we have

(2.1) $y_{n+\sigma h} = v_1 y_{n-1} + v_2 y_n + \Phi(x_{n-1}, x_n, y_{n-1}, y_n ; h)$

where the function $\Phi(x_{n-1}, x_n, y_{n-1}, y_n)$ is the same as that in (1.2).

The proposed method (2.1) requires that the constants v_1, v_2 , w_i ,

a_i ,b_i and b_{ij} (i=2,3...,r;j=0,1,2,...,i-1) are chosen so that the

expansion for right hand of the function (2.1) is equivalent

to a Taylor expansion $y(x_n + \sigma h)$ up to p-th powers of h and

moreover the coefficients a_i, b_i and b_{ij} (i=2,3,..r;j=0,1,..,i-1)

are independent of the factor σ . Thus the new algorithm is

designed to compute the value $y_{n+\sigma h}$ at the desired point x = $x_n + \sigma h$

without computing the new functions k_i (i=0,1,..,r) to coincide the

out point. We shall see that what can be achieved in (2.1)

with r=2,3, and we get the following results.

(I) Order 4 (r = 2). On two stage, as we [17] know ,it is not

possible for the method (2.2) to get ordre 5 with two stage. So

we see whether it is possible to get order 4 with r = 2. The method

with r = 2 have order 4 if

(2.2) $(-1)^j \dfrac{v_1}{j} + \sum_{i=0}^{r} (a_i)^{j-1} w_i = \dfrac{\sigma^j}{j}$ (r=2,j=1,2,3,4)

and

(2.3) $a_2^j = (-1)^{j+1} \left\{ b_0 + j b_{20} \right\}$ (j=2,3),

with a_0 = -1 and a_1 = 0, which lead to the following solution:

(2.4) $b_2 = -(3a_2^2 + 2a_2^3)$, $b_{20} = a_2^2 + a_2^3$,

$w_2 = \sigma^2(\sigma+1)^2 / 2a_2(2a_2+1)(a_2+1)$, $w_0 = (3a_2^2 + 4a_2^3)w_2 - (\sigma^3 + \sigma^4)$,

$v_1 = \sigma^2 - 2a_2 w_2 + 2w_0$, $v_2 = 1 - v_1$, $w_1 = \sigma - (-v_1 + w_0 + w_2)$,

(II) Order 4 (r = 3). We check whether it is possible for the method (2.1) with r = 3 to have fifth order. We see that the method (2.1) will have fifth order if ,in addition to (2.2) with (r=3,p=1,..,5),

(2.5) $- \dfrac{v_1}{5} + w_0 + \displaystyle\sum_{i=2}^{3} d_i w_i = \dfrac{1}{5}\sigma^5$,

(2.6) $a_i = (-1)^{j+1} b_i + j \displaystyle\sum_{\ell=0}^{i-1} a_\ell^{j-1} b_{i\ell}$ (i=2,3,j=2,3),

with $d_i = -b_i + 4 \displaystyle\sum_{\ell=0}^{i-1} a_\ell^3 b_{i\ell}$,

if we define,

$$D_1 = \begin{pmatrix} 1 & 3 & 3a_2 & 3a_3 & \sigma^2 \\ 1 & -4 & 4a_2^2 & 4a_3^2 & \sigma^3 \\ -1 & 5 & 5a_2^3 & 5a_3^3 & \sigma^4 \\ -1 & 5 & d_2 & d_3 & \sigma^5 \end{pmatrix}, \quad V = \begin{pmatrix} v_1 \\ w_0 \\ w_1 \\ w_2 \\ -1 \end{pmatrix},$$

then the equations (2.2) with r = 3 and (2.5) can be expressed as

$D_1 V_1 = 0$,

and

$$\det(D_1) = a_2 a_3 (a_2+1)(a_3+1)\sigma^2(\sigma+1)^2 \Big[a_2 a_3 \big\{ (5a_3+3)d_2 - (5a_2+3)d_3 \\ + \big\{ (5a_2^2 - a_2 - 2)d_3 - (5a_3^2 - a_3 - 2)d_2 \big\}\sigma + \big\{ (4a_3 + 2)d_2 - (4a_2 + 2)d_3 \big\}\sigma^2 \Big]$$
$$= 0,$$

which leads to

(2.7) $d_2 = 0$.

The solution of (2.6) and (2.7) implies $a_2 = 0$. However, the equation (2.2) has no solution for the value $a_2 = 0$.

(III) Order 5 (r = 4). Treating r=4 similarly, we now consider the solutions of fifth order conditions only the cases $w_2 = 0$.

We see that the method (2.1) will have fifth order if, in addition to (2.2) with (r = 4,j=1,2,3,4,5),

$$(2.8) \quad -\frac{v_1}{5} + w_0 + \sum_{i=2}^{4} d_i w_i = \frac{1}{5}\sigma^5,$$

$$(2.9) \quad a_i^j = (-1)^{j+1} b_i + j \sum_{\ell=0}^{i-1} a_\ell^{j-1} b_{i\ell} \quad (i=2,3,4, j=2,3).$$

Solving fifth order conditions listed above we have

$$(2.10) \quad w_3 = (R_1 S_2 - Q_2 R_2)/(Q_1 S_2 - Q_2 S_1), \quad w_4 = (Q_1 R_2 - S_1 R_1)/(Q_1 S_2 - Q_2 S_1),$$

$$w_2 = \frac{\sigma^2(\sigma+1)^2 - \sum_{i=3}^{4} 2a_i(2a_i+1)(a_i+1)w_i}{2a_2(2a_2+1)(a_2+1)},$$

$$w_0 = \sigma^2 + \sigma^3 - \sum_{i=2}^{4}(3a_i^2+2a_i)w_i, \quad v_1 = \sigma^2 + 2w_0 - 2\sum_{i=2}^{4} a_i w_i,$$

$$v_2 = 1 - v_1, \quad w_1 = \sigma + v_1 - w_0 - \sum_{i=2}^{4} w_i,$$

$$b_2 = -(3a_2^2 + 2a_2^3), \quad b_{20} = a_2^2 + a_2^3,$$

$$b_i = 6\sum_{j=2}^{i-1}(a_j + a_j^2)b_{ij} - 3a_i^2 - 2a_i^3,$$

$$b_{i0} = -\sum_{j=2}^{i-1}(2a_j + 3a_j^2)b_{ij} + a_i^2 + a_i^3, \quad (i=3,4),$$

with

$$Q_{i-2} = 2a_i(a_i+1)(a_2-a_i)\left\{10a_2 a_i + 5(a_2+a_i) + 3\right\} \quad (i=3,4),$$

$$S_{i-2} = 2a_i(2a_i+1)(a_i+1)a_2(a_2+1)+2(2a_2+1)\left\{ \sum_{j=2}^{i-1} 2a_j(2a_j^2+3a_j+1)b_{ij} - a_i^2(a_i+1)^2 \right\} (i=3,4),$$

$$R_1 = \sigma^2(\sigma+1)^2\left\{a_2(5a_2+3) - 2\sigma(2a_2+1)\right\}, \quad R_2 = \sigma^2(\sigma+1)^2 a_2(a_2+1).$$

Thus, concerning the attainable order of the method (2.1) with 2-,3- and 4 stage, we have the following Theorem.

Theorem. The attainable order is 4 ,4 and 5 for the algorithm (2.2) of 2-,3- and 4 stage respectively.

3. Step-size control. We now turn to the problem of automatic step control. The useful ideas of deriving step-size control method have been proposed by many people. The most commonly used method for the step-size control policy arises from controlling the bound for the local truncation error. The local truncation error at the point (x_n, y_n) for (2.1) is defined by,

(3.1) $y_{n+\sigma h} - u(x_n + \sigma h) = (\sigma h)^{p+1} \sum\limits_{j=1}^{p+1} T_{p+1,j} \; D_{p+1,j} + O(h^{p+2})$,

where $u(x)$ is the solution of the initial value problem:

$$u' = f(x,u), \; u(x_n) = y_n ,$$

$T_{p+1,j}$ is the truncatin error coefficients and $D_{p+1,j}$ is the elementary differential operator which is the functions of $f(x,y)$ and (x_n, y_n). In order to obtain an estimate of the local truncation error, we use the procedure suggested by Shampine and Gordon 22 . Subtracting $y_{n+1}(4)$ and $y_{n+1}(5)$ which are the numerical solutions of order 4 and 5 respectively, we obtain,

$$TE = y_{n+1}(4) - y_{n+1}(5)$$
$$= O(h^5),$$

which is an estimate of the local truncation error of $y_{n+1}(4)$, and it is the error which we will control. Thus the formulas are developed on the assumption that the integration is advanced with the approximation $y_{n+1}(4)$, we, however, may expect to get better numerical results if we continue the integration with higher order result $y_{n+1}(5)$. This is called the local exterpolation method which is the most popular code tody. For this reason, we use the code.

We now outline a simple version of the overall procedure, denoting the local accuracy and minimum step-size by $\widetilde{E}$ and $\widetilde{h}$ respectively, which are pre-assigned toerance, the way is as follow:

1   If $TE > \widetilde{E}$ set $\sigma = 0.6$ and recompute the numerical solution at the point $x = x_n + \sigma h$.

2   If $h \leqslant \widetilde{h}$, accpet the solution, setting $y_{n+1} = y_{n+1}(5)$

  $x = x_n + \sigma h$, $h = \sigma h$ and $\sigma = 1$

3   If $TE \leqslant \widetilde{E}$, accpet the solution, setting $y_{n+1} = y_{n+1}(5)$,

  $x_{n+1} = x_n + \sigma h$ and $h = \sigma h$. Moreover,

(1) If $TE \geq \tilde{E}/2$, we set $\sigma = 1$.

(2) If $TE \leq \tilde{E}/2$, we set $\sigma = 1.2$.

Let us consider briefly the above process. The difficulty in the process is that, when the step-size is changed, we have to comput the weights w_i $(i=0,1,..,r)$, v_1 and v_2 for the given σ, however we usually take the factor σ in the form $\sigma = 2^I$, where the number I is finite integer, then the weights $w_i(i=0,1,..,r)$, v_1 and v_2 can be given previously. It means that, on changing the step-size and recomputing y_{n+1} .our's method (2.1) requires only the linear conbimation of w_i , k_i $(i=0,1,..,r)$, v_1 and v_2 without new function evaluations k_i, w_i $(i=0,1,..r)$, v_1 and v_2.

4. Determination of free parameters. The most important task to which free parameters can be applied is the reduction of the the local truncation error and the providing for the available step-size control.

The parameters involved in the formula (2.10) are a_2 ,a_3 ,a_4 ,b_{32} ,b_{42} and b_{43} , we set the constant b_{32} to satisfy the following fifth order condition:

(3.1) $\qquad a_3^4 = - b_4 - 4 \sum_{\ell=0}^{2} a_\ell^3 b_{3\ell}$,

which leads to the following solution,

(3.2) $\qquad b_{32} = \dfrac{a_3^2 (a_3 + 1)^2}{4a_2^3 + 6a_2^2 + 2a_2}$,

and the other parameters a_2,a_3 ,a_4 ,b_{42} and b_{43} are chosen so that the method (2.1) with (2.10),(3.2) and $\sigma = 1$ have the minimum error bound and the effective step police. In order to get the appropriate step-control it is necessary that the bound for the **truncation error decreases as the parameter** approch to zero.

Denoting the local truncation error of (2.1) by $T(\sigma,p)$, where p is the order.

If we take

(3.3) $a_2 = 0.1$, $a_3 = 0.9$, $a_4 = 0.4$, $b_{42} = -0.2$, $b_{43} = 0.055$,

then, we find that the bound for the local truncation error $T(1,5)$ of (2.10) and (3.2) is

$$|T(1,5)| \leq 0.800 \, M \, L^5 \, h^6.$$

With those values, the bound $T(1,4)$ for the fourth order method with (2.9) is

$$|T(1,4)| \leq 4.502 \, M \, L^4 \, h^5,$$

the constants L and M listed above satisfy

$$\left| f(x,y) \right| \leq M, \quad \left| \frac{\partial^{i+j} f(x,y)}{\partial x^i \, \partial y^j} \right| \leq \frac{L^{i+j}}{M^{j-1}}.$$

From (2.9),(2.13),(3.2)and (3.3) we obtain the following formulae:

(3.4)

a_i	b_i, b_{ij}				
	v_i, w_i				
	$\tilde{v}_i$, $\tilde{w}_i$				
$\dfrac{1}{10}$	$-\dfrac{4}{125}$	$\dfrac{11}{1000}$	$\dfrac{121}{1000}$		
$\dfrac{9}{10}$	$\dfrac{13689}{4000}$	$-\dfrac{88749}{88000}$	$-\dfrac{100719}{8000}$	$\dfrac{9747}{880}$	
$\dfrac{4}{10}$	$-\dfrac{1757}{10000}$	$\dfrac{747}{20000}$	$\dfrac{13667}{20000}$	$-\dfrac{1}{5}$	$\dfrac{11}{200}$
	v_1 v_2 w_0 w_1 w_2				
	$\tilde{v}_1$ $\tilde{v}_2$ $\tilde{w}_0$ $\tilde{w}_1$ $\tilde{w}_2$ $\tilde{w}_3$ $\tilde{w}_4$				

where

(3.5) $v_1 = \sigma^2(1 - 6\sigma - 5\sigma^2)/2$, $v_2 = 1 - v_1$,

$w_0 = \sigma^2(17 - 78\sigma - 115\sigma^2)/132$,

$w_1 = \sigma(12 - 41\sigma - 118\sigma^2 - 65\sigma^3)/12$,

$$w_2 = 125\sigma^2(\sigma + 1)^2 / 33,$$

and

(3.6) $$\widetilde{v}_1 = \sigma^2(47142 - 202272\,\sigma - 9625\,\sigma^2 + 132520\sigma^3)/107269,$$

$$\widetilde{w}_0 = \frac{\sigma^2(6794073 - 27944497\sigma - 9553550\,\sigma^2 + 25365020\sigma^3)}{67257663},$$

$$\widetilde{w}_1 = \frac{\sigma(11585052 - 35383731\,\sigma - 64000538\,\sigma^2 + 24490325\sigma^3 + 41522080\sigma^4)}{11585052}$$

$$\widetilde{w}_2 = \frac{\sigma^2(67618125 + 79138250\,\sigma - 44577875\,\sigma^2 - 56098000\sigma^3)}{21239262},$$

$$\widetilde{w}_3 = \frac{\sigma^2(-3735375 + 5163250\,\sigma + 21532625\,\sigma^2 + 126340000\sigma^3)}{110057994},$$

$$\widetilde{w}_4 = \frac{\sigma^2(928125 + 1086250\,\sigma - 611875\,\sigma^2 - 770000\sigma^3)}{3861684},$$

$$\widetilde{v}_2 = 1 - \widetilde{v}_1.$$

here we note that (3.5) and (3.6) are the fourth- and fifth order

method respectively.

We have discussed the policy for changing the step-size. How

such a change can be effected in practice is important. That

is, when the step-size is changed from h to $h = \sigma h$, how does

the accuracy of this result at the point $x = x_n + \sigma h$ compared to

that at the point $x = x_n + h$. In general it would be unable

to get out the answer, we may say, however ,that the comparison

of truncation error bound provides some detail and reliable

conclusions. Thus the ratio $T(\sigma, p)/T(1, p)$ measures the accuracy

of the result at $x = x_n + \sigma h$ compared to that at $x = x_n + h$.

Figure(1) and Figure (2) show the magnitute of the ratio of

the truncation errors of (3.5) and (3.6) for $0 \leq \sigma \leq 1$ respectively.

5. Numerical Examples. The described method is programmed

in FORTRAN and run on the Personal Computer pc-9801(NEC). The

computations are done in duble precision. The three test

problems considered are the following:

(1) $\begin{cases} y' = -z, \quad y(0) = 2 \\ z' = -3y - z, \quad z(0) = 2, \end{cases}$

(2) $\begin{cases} y' = -y + 95z, & y(0) = 1, \\ z' = -y - 95z, & z(0) = 1. \end{cases}$

The true solutions to the problems (1) and (2) are

$\begin{cases} y(x) = \exp(x) + \exp(-3x) \\ z(x) = \exp(-3x) - \exp(x), \end{cases}$

$\begin{cases} y(x) = (95\exp(-2x) - 48\exp(-96x))/47 \\ z(x) = (48\exp(-96x) - \exp(-2x))/47, \end{cases}$

respectively.

The value y_1 necessary for the evaluation, when we use the method (2.1), is computed by Nystrom's sixth order method. The results obtained in computations are given in TABLE 1 to TABLE 11.

Here A-B(5)4 denotes the imbeding formula of the methods (2.4),(2.10) with (3.2) and (3.3), F-L(5)4 is the formula due to Felberg 5(4), the formula A-B(5) and F-L(5) are the (2.10) with (3.2),(3.3) and Felberg fifth order methods respectively. $\widehat{E}$ and $\widetilde{h}$ represent the local accuracy and the minimum step-size requirement respectively, we define the average of the absolute value of the error in each component by

$$ERR(x_{NS}) = \left(\sum_{i=1}^{NS} \left| Error(yz_i) \right| / NS \right),$$

where NS is the number of integration step and yz_i is the numerical solution in each componet. The results of the computation show that our's scheme is efficient than the R-K process and is quite efficients in the step-size control.

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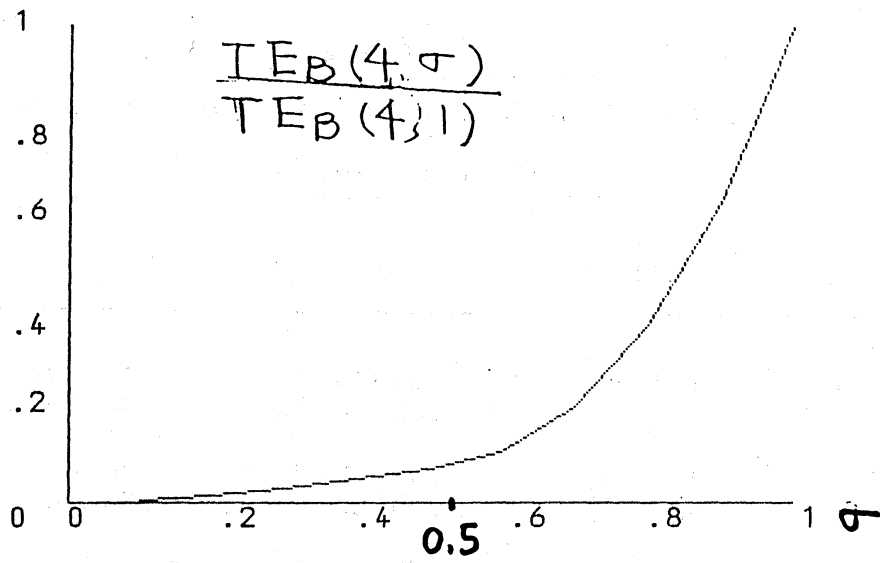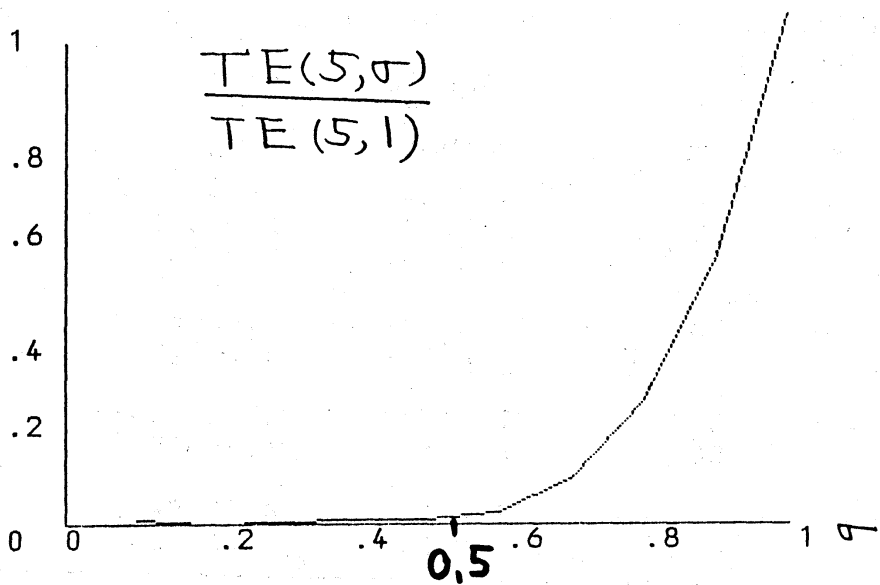
Figure(1)

Figure(2)

The ratio $T(p,\sigma)/T(p,1)$ of thr truncation error bound for $0 \leq \sigma \leq 1$.

TABLE 1

Results for the Problem 1 with the constant step-size $h = 1 / 2^4$

Absolute Error.

x	Method	$y(x_n) - y_n$	$z(x_n) - z_n$
0.5	F-L(5)	9.9338D-8	1.6528D-7
	A-B(5)	6.2380D-7	1.8427D-6
1.5	F-L(5)	2.8047D-7	2.4094D-7
	A-B(5)	1.5453D-7	2.1950D-7
4.0	F-L(5)	8.7906D-6	8.7905D-6
	A-B(5)	2.0081D-6	2.0076D-6
ERR(4)	F-L(5)	1.7174D-6	1.7108D-6
	A-B(5)	5.4575D-7	7.9672D-7

Results using the step-size control with $\widetilde{E} = 1,0D-4$ and $\widetilde{h} = 1/2^8$.

Absolute error.

x	Function evaluations	Method	$y(x_n) - y_n$	$z(x_n) - z_n$
0.15	3 · 6	F-L(5)4	1.1695D-7	3.2516D-7
	3 · 4	A-B(5)4	1.0885D-8	3.2561D-8
1.2	13 · 6	F-L(5)4	7.1545D-7	1.3099D-6
	21 · 4	A-B(5)4	2.3307D-7	5.7725D-7
4.5	31 · 6	F-L(5)4	6.1881D-5	6.1877D-5
	56 · 4	A-B(5)4	1.7661D-5	1.7659D-5
ERR(4.5)		F-L(5)4	4.1769D-5	4.1769D-5
		A-B(5)4	2.6376D-6	2.6948D-6

TABLE 2

Results for the Problem 3 with the constant step-size $h = 1/2^7$.

Absolute Error.

x	Method	$y(x_n) - y_n$	$z(x_n) - z_n$
0.25	F-L(5)	2.5609D-8	2.8564D-10
	A-B(5)	3.2005D-7	3.2004D-7
0.5	F-L(5)	3.1046D-8	3.2680D-10
	A-B(5)	3.1449D-10	3.0808D-10
1.0	F-L(5)	2.2636D-8	2.3828D-10
	A-B(5)	4.7762D-12	5.0558D-14
ERR(1.)	F-L(5)	4.2013D-6	4.2014D-6
	A-B(5)	9.8820D-6	9.8801D-6

Results using the step-size control with $\widetilde{E} = 1,0D-4$ and $\widetilde{h} = 1/2^9$.

Absolute error.

x	Function evaluations	Method	$y(x_n) - y_n$	$z(x_n) - z_n$
0.019	9 · 6	F-L(5)4	5.5687D-6	5.1354D-6
	4 · 4	A-B(5)4	7.9060D-7	7.9060D-7
0.48	28 · 6	F-L(5)4	2.6617D-5	6.2768D-5
	68 · 4	A-B(5)4	8.5731D-7	8.5732D-7
0.89	42 · 6	F-L(5)4	1.0919D-5	1.0901D-5
	74 · 4	A-B(5)4	2.3345D-6	2.3342D-6
ERR(0.89)		F-L(5)4	3.8565D-5	3.7960D-5
		A-B(5)4	1.6726D-6	1.6726D-6