

J. S. CHOMICZ, A. OLEJNICZAK and M. SZYSZKOWICZ (Wroclaw)

A METHOD FOR FINDING THE STEP SIZE OF INTEGRATION OF A SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS

In this paper we give a method for finding the step size of integration of an initial value problem. This method can be used with a slight modification in other numerical problems (see [1]). Some numerical results are presented which show the advantages of the method.

1. Method of choice of the step size. The initial value problem which we wish to solve numerically is

$$(1.1) \quad y' = f(x, y), \quad y(a) = y_0, \quad x \in [a, b], \quad y, f \in R^n.$$

Let (1.1) have a unique solution. For the numerical solution of this problem we apply a one-step method of rank p ($p \geq 1$) and of the form

$$(1.2) \quad \begin{cases} \eta_k^0 = y_{0k} \\ \eta_k^{i+1} = \eta_k^i + h_i \Phi(x, \eta_1^i, \eta_2^i, \dots, \eta_n^i, h_i) \quad (i = 0, 1, \dots). \end{cases} \quad (k = 1, 2, \dots, n).$$

In the case of one equation ($n = 1$), one of the possible methods for finding the step size h_i was given by Krylov ([2], p. 103-107) and Stoer ([3], p. 114-118). In this paper we apply this method to the general case of a system of ordinary differential equations. Let $\eta_k(x_0 + h, h)$ denote the approximation of the solution of problem (1.1) at the point $x_0 + h$ obtained from (1.2) with step size h and let $\eta_k(x_0 + h, h/2)$ denote the approximation of this solution by twofold application of (1.2) with step size $h/2$.

For one-step methods of rank p we have (see [2])

$$y_k(x_0 + h) = \eta_k(x_0 + h, h) + C_k^0(x_0) h^{p+1} + C_k^1(x_{0k}) h^{p+2} \quad (k = 1, 2, \dots, n),$$

where x_{0k} are the points from $[x_0, x_0+h]$, $y_k(x)$ is the exact solution of (1.1), and $C_k^i(x)$ are any continuous functions independent of h . Since we are interested only in the rank of the error, we can write

$$(1.3) \quad y_k(x_0+h) - \eta_k(x_0+h, h) \doteq C_k(x_0)h^{p+1}$$

and

$$(1.4) \quad y_k(x_0+h) - \eta_k(x_0+h, h/2) \doteq 2C_k(x_0)(h/2)^{p+1}$$

for $k = 1, 2, \dots, n$, where $C_k(x_0) = C_k^0(x_0)$.

The derivation of formula (1.4) is as follows:

From (1.3) with step size $h/2$ at the point x_0 we have

$$(1.5) \quad y_k(x_0+h/2) - \eta_k(x_0+h/2, h/2) \doteq C_k(x_0)(h/2)^{p+1}.$$

Applying this formula twice at the points $x_0, x_0+h/2$ with $h/2$ we have

$$\begin{aligned} y_k(x_0+h) &\doteq y_k(x_0) + \frac{h}{2} \Phi\left(x_0, y_1(x_0), y_2(x_0), \dots, y_n(x_0), \frac{h}{2}\right) + \\ &+ C_k(x_0)\left(\frac{h}{2}\right)^{p+1} + \frac{h}{2} \Phi\left(x_0 + \frac{h}{2}, y_1\left(x_0 + \frac{h}{2}\right), y_2\left(x_0 + \frac{h}{2}\right), \dots, y_n\left(x_0 + \frac{h}{2}\right), \frac{h}{2}\right) + \\ &+ C_k\left(x_0 + \frac{h}{2}\right)\left(\frac{h}{2}\right)^{p+1}. \end{aligned}$$

Since we omit elements with the exponent h greater than $p+1$, we can write

$$C_k(x_0+h/2)(h/2)^{p+1} \doteq C_k(x_0)(h/2)^{p+1}.$$

Using this formula and replacing $y_1(x_0+h/2), \dots, y_n(x_0+h/2)$ by suitable values from (1.5) and omitting elements with the exponent h greater than $p+1$ in the Taylor series Φ , we have

$$y_k(x_0+h) \doteq \eta_k(x_0+h, h/2) + 2C_k(x_0)(h/2)^{p+1} \quad (k = 1, 2, \dots, n).$$

From (1.3) and (1.4) we obtain

$$(1.6) \quad \Delta_k = \eta_k\left(x_0+h, \frac{h}{2}\right) - \eta_k(x_0+h, h) \doteq C_k(x_0)h^{p+1} \frac{2^p - 1}{2^p} \quad (k = 1, 2, \dots, n).$$

Let H denote the integration step which gives an approximation of the solution with given error and let ε denote the error vector. We want to obtain

$$(1.7) \quad \varepsilon_k \geq |y_k(x_0+H) - \eta_k(x_0+H, H)| \doteq |C_k(x_0)H^{p+1}| \quad (k = 1, 2, \dots, n).$$

Let $H = h/\omega$. By (1.7) we can write

$$\varepsilon_k \geq |C_k(x_0)H^{p+1}| = |C_k(x_0)(h/\omega)^{p+1}|,$$

and using (1.6) we have

$$\varepsilon_k \geq \frac{|\Delta_k|2^p}{\omega^{p+1}(2^p - 1)} \quad (k = 1, 2, \dots, n).$$

Finally, for finding ω which designates H we have

$$(1.8) \quad \omega = a \sqrt[p+1]{\frac{2^p}{2^p - 1} \max_{1 \leq k \leq n} \frac{|\Delta_k|}{|\varepsilon_k|}},$$

where the constant $a > 1$ is introduced for the algorithm to work.

It is clear from (1.3) that the error of the obtained solution is $O(H^{p+1})$. Applying Richardson's extrapolation we obtain

$$(1.9) \quad \eta_k^*(x_0 + H) = \eta_k\left(x_0 + H, \frac{H}{2}\right) + \frac{\eta_k(x_0 + H, H/2) - \eta_k(x_0 + H, H)}{2^p - 1} \quad (k = 1, 2, \dots, n),$$

where $\eta_k^*(x_0 + H)$ is a solution with error $O(H^{p+2})$.

We may accept this value as the exact value to the next step of method (1.2).

The numerical realization of this method is shown in Fig. 1.

2. The procedure *diffsysrunkut4*. The procedure *diffsysrunkut4* calculates the approximate values $y_1(x)$, $y_2(x)$, ..., $y_n(x)$ of the solutions of the system of differential equations

$$(2.1) \quad y'_k = f_k(x, y_1, y_2, \dots, y_n),$$

$$(2.2) \quad y_k(x_0) = y_{0k}$$

for $k = 1, 2, \dots, n$ ($n \geq 1$) using the standard Runge-Kutta method of fourth order.

Data:

$x0$ — parameter in (2.2);

$x1$ — value of x for which we want to obtain a solution of (2.1);

eps , eta — positive parameters ε , η characterizing the precision of the solutions;

$hmin$ — the minimum admissible absolute value of the step size h ;

n — number of equations;

$y0[1:n]$ — values of y_{0k} in (2.2).

Results:

$x0$ — given value of $x1$;

$y0[1:n]$ — approximate values of $y_k(x_1)$ ($k = 1, 2, \dots, n$).

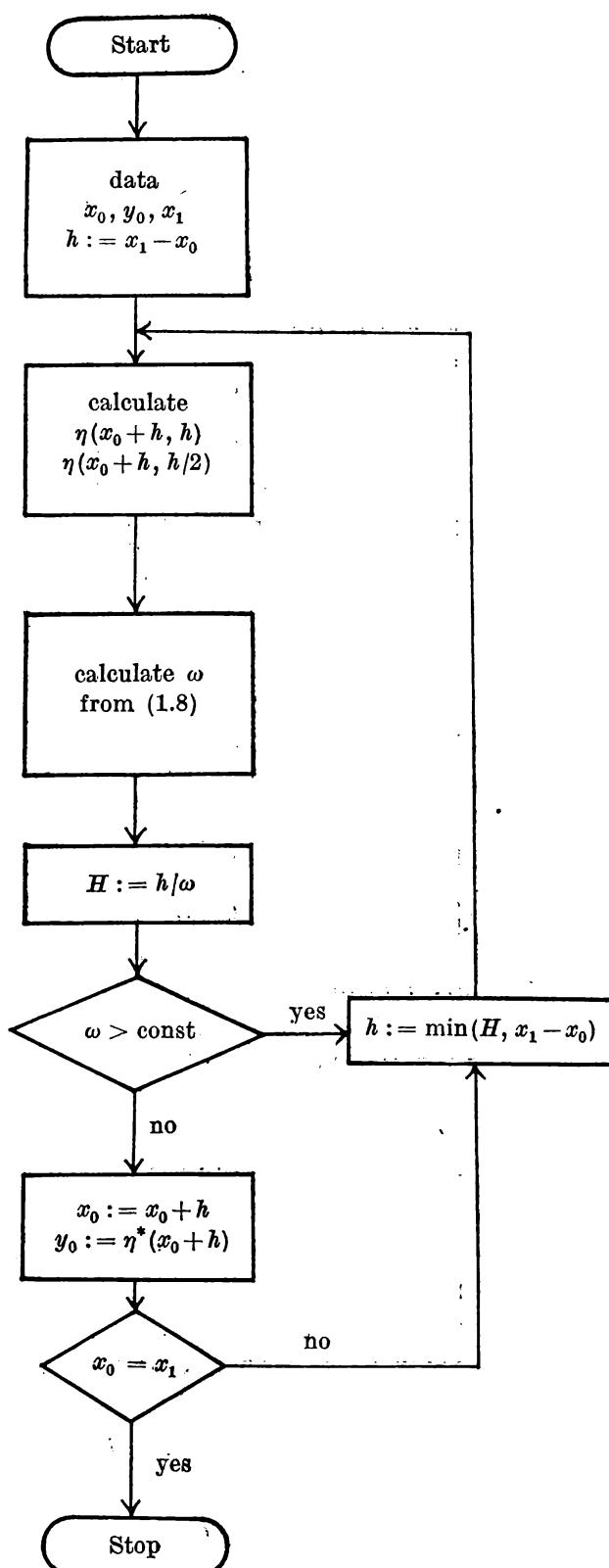


Fig. 1. Flow diagram of the method

```

procedure diffsysstrunkut4(x0,x1,eps,eta,hmin,n,y0,notacc,f);
  value x1,eps,eta,hmin,n;
  real x0,x1,eps,eta,hmin;
  integer n;
  array y0;
  label notacc;
  procedure f;
  begin
    real h,hh,ww,w1,w2,w3,w4;
    integer i;
    Boolean last;
    array k1,yh,y1,y2,y3[1:n];
    procedure steprunkut(h,x,y,df);
      value h,x;
      real h,x;
      array y,df;
      begin
        w1:=w4:=.5*h;
        w2:=x;
        for i:=1 step 1 until n do
          begin
            yh[i]:=y[i];
            df[i]:=.0
          end i;
        for w3:=w4,h,h,w4 do
          begin
            f(w2,n,yh,k1);
            for i:=1 step 1 until n do
              begin
                w2:=k1[i];
              end i;
            w2:=w3;
          end w3;
        end w4;
      end steprunkut;
      begin
        notacc:=.0;
        for i:=1 step 1 until n do
          begin
            if abs(yh[i]-y0[i])>eps then
              begin
                notacc:=.1;
                exit;
              end;
            y0[i]:=yh[i];
          end i;
      end;
    end notacc;
  end;
end;

```

```

df[i]:=df[i]+w3×w2;
yh[i]:=y[i]+w1×w2
end i;
w2:=x+w1;
w1:=w3
end w3;
for i:=1 step 1 until n do
  df[i]:=y[i]+.33333333333×df[i]
end steprunkut;
eps:=.033333333333/eps;
h:=x1-x0;
last:=true;
cont h:
hh:=.5×h;
steprunkut(h,x0,y0,y1);
steprunkut(hh,x0,y0,y2);
steprunkut(hh,x0+hh,y2,y3);
ww:=.0;
for i:=1 step 1 until n do
begin
  w3:=y3[i];
  w1:=w3-y1[i];
  w3:=y3[i]:=w3+.06666666666×w1;
  w1:=abs(w1);
  w3:=abs(w3);
  if w3<eta
    then w3:=eta;
  w1:=w1/w3;
  if w1>ww
    then ww:=w1

```

```

end i;

ww:=if ww=0 then eta else (eps>ww)? .2*1.25;
hh:=h/ww;
if ww>1.25
    then
        begin
            if abs(hh)<hmin
                then go to notacc;
            last:=false
        end ww>1.25
    else
        begin
            x0:=x0+h;
            for i:=1 step 1 until n do
                y0[i]:=y3[i];
            if last
                then go to end;
            w1:=x1-x0;
            if (w1-hh)*h<0
                then
                    begin
                        hh:=w1;
                        last:=true
                    end (w1-hh)*h<0
            end ww<1.25;
            h:=hh;
            go to conth;
        end:
        end diffsysstrunkut4

```

Other parameters:

notacc — label (outside of the body of the procedure *difsysstrunkut4*) to which an exit is made if the computed step size *h* is smaller than *hmin*.

Remark. After a jump to *notacc* the variable *x0* has the value of *x* ($x \in [x0, x1]$) for which a correct solution was obtained and the array *y0* contains this solution.

f — identifier of the procedure with the head

```
procedure f(x, n, y, d);
  value x, n, y;
  real x;
  integer n;
  array y, d;
```

which for given *n*, *x*, and *y[1 : n]* computes the values of *d[1 : n]* of the right-hand side of (2.1).

3. Examples of the use of the procedure. We give three examples of the use of the procedure *difsysstrunkut4*.

As the first example we take a problem which was given by Stoer ([3], p. 117-118):

$$y' = -200xy^2, \quad y(-3) = 1/901$$

with the exact solution $y(x) = 1/(1+100x^2)$. We obtained the following results:

$(\eta - y(0))/y(0)$	Number of evaluations of the right-hand side	$\text{eps} = \text{eta}$
$-7.246325 \cdot 10^{-3}$	276	10^{-5}
$-5.561725 \cdot 10^{-4}$	456	10^{-6}
$-5.636424 \cdot 10^{-5}$	732	10^{-7}
$-4.719455 \cdot 10^{-6}$	1152	10^{-8}
$-5.210094 \cdot 10^{-7}$	1848	10^{-9}

The remaining two examples are the following:

Example A.

$$\begin{cases} y'_1 = 1/y_2, & y_1(0) = 1, \\ y'_2 = -1/y_1, & y_2(0) = 1, \end{cases} \quad \text{with the solution} \quad \begin{cases} y_1(x) = e^x, \\ y_2(x) = e^{-x}. \end{cases}$$

Example B.

$$\begin{cases} y'_1 = y_2, & y_1(0) = 0, \\ y'_2 = -y_1, & y_2(0) = 1, \end{cases} \quad \text{with the solution} \quad \begin{cases} y_1(x) = \sin x, \\ y_2(x) = \cos x. \end{cases}$$

For these examples we obtained results which are given in Tables A and B, respectively. For comparison Table A presents also results obtained with the library procedure *RungeKutta4* [4].

TABLE A

x	<i>diffsystrunkut4</i>		<i>RungeKutta4</i>	
	Errors for $\text{eps} = \text{eta} = 10^{-9}$	Number of evaluations of the right- hand side	Errors for $\text{eps} = \text{eta} = 10^{-9}$	Number of evaluations of the right- hand side
0.5	$3.53 \cdot 10^{-11}$ $0.00 \cdot 10^0$	132	$-7.06 \cdot 10^{-11}$ $2.39 \cdot 10^{-11}$	224
1.0	$-4.28 \cdot 10^{-11}$ $1.58 \cdot 10^{-10}$	132	$-1.07 \cdot 10^{-10}$ $7.91 \cdot 10^{-11}$	224
1.5	$-1.29 \cdot 10^{-10}$ $2.44 \cdot 10^{-10}$	132	$-7.79 \cdot 10^{-11}$ $8.15 \cdot 10^{-11}$	224
2.0	$-2.52 \cdot 10^{-10}$ $3.49 \cdot 10^{-10}$	132	$-1.57 \cdot 10^{-10}$ $1.07 \cdot 10^{-10}$	224
4.0	$-5.79 \cdot 10^{-10}$ $9.18 \cdot 10^{-10}$	492	$-1.87 \cdot 10^{-10}$ $2.48 \cdot 10^{-11}$	816
10.0	$-4.61 \cdot 10^{-9}$ $5.86 \cdot 10^{-9}$	1416	$1.51 \cdot 10^{-9}$ $-1.58 \cdot 10^{-9}$	3136

TABLE B

x	Errors for $\text{eps} = \text{eta} = 10^{-3}$	Number of evaluations of the right-hand side	Errors for $\text{eps} = \text{eta} = 10^{-6}$	Number of evaluations of the right-hand side
0.5	$1.33 \cdot 10^{-6}$ $4.04 \cdot 10^{-6}$	12	$3.27 \cdot 10^{-8}$ $4.75 \cdot 10^{-8}$	48
1.0	$5.37 \cdot 10^{-6}$ $1.03 \cdot 10^{-5}$	12	$1.43 \cdot 10^{-7}$ $1.99 \cdot 10^{-7}$	36
1.5	$1.00 \cdot 10^{-5}$ $5.85 \cdot 10^{-5}$	12	$1.92 \cdot 10^{-7}$ $6.21 \cdot 10^{-7}$	48
2.0	$1.57 \cdot 10^{-5}$ $3.72 \cdot 10^{-6}$	12	$2.45 \cdot 10^{-7}$ $1.53 \cdot 10^{-7}$	48
2.5	$2.47 \cdot 10^{-5}$ $1.28 \cdot 10^{-5}$	12	$4.14 \cdot 10^{-7}$ $3.02 \cdot 10^{-7}$	36
3.0	$6.84 \cdot 10^{-5}$ $1.95 \cdot 10^{-5}$	12	$8.09 \cdot 10^{-7}$ $3.79 \cdot 10^{-7}$	48
3.5	$2.66 \cdot 10^{-6}$ $2.69 \cdot 10^{-5}$	12	$2.32 \cdot 10^{-7}$ $4.17 \cdot 10^{-7}$	84

In all presented examples h_{\min} was equal to 10^{-6} .

The procedure *diffsystrunkut4* has been verified on the Odra 1204 computer (with 38-bit mantissa) in the Institute of Computer Science of the University of Wrocław.

References

- [1] J. S. Chomicz, *Rozwiązań liniowego zagadnienia brzegowego metodą kollokacji*, Report no. N-65, Institute of Computer Science, University of Wrocław, 1979.
- [2] V. I. Krylov, V. V. Bobkov and P. I. Monastyrnyi (B. И. Крылов, В. В. Бобков и П. И. Монастырный), *Вычислительные методы высшей математики, том 2*, Минск 1975.
- [3] J. Stoer and R. Bulirsch, *Einführung in die numerische Mathematik, II*, Berlin 1973.
- [4] *Systemy programowania maszyny cyfrowej Odra 1204*, Zeszyt 1204-VIII-11, Mera-Elwro, Wrocław 1974.

INSTITUTE OF COMPUTER SCIENCE
UNIVERSITY OF WROCŁAW
51-151 WROCŁAW

*Received on 7. 3. 1978;
revised version on 4. 4. 1979*

J. S. CHOMICZ, A. OLEJNICZAK i M. SZYSZKOWICZ (Wrocław)

**METODA ZNAJDOWANIA KROKU CAŁKOWANIA
UKŁADU RÓWNAŃ RÓŻNICZKOWYCH ZWYCZAJNYCH**

STRESZCZENIE

W pracy podana jest metoda znajdowania kroku całkowania zagadnienia początkowego (1.1). Jest to uogólnienie na przypadek układu równań różniczkowych pierwszego rzędu metod podanych przez Kryłowa ([2], str. 103-107) oraz Stoera ([3], str. 114-118). Po prostych modyfikacjach metodę można stosować także do niektórych innych zagadnień [1].

W pracy zamieszczono procedurę realizującą przedstawioną metodę oraz wyniki testów wykonanych na m.c. Odra 1204 w Instytucie Informatyki Uniwersytetu Wrocławskiego.
