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On Some Comparison of Explicit Runge-Kutta and Multistep Methods

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Abstract - As is known, one of the popular methods for investigation of the numerical solution of ordinary differential equations is the Runge–Kutta method. At present, some modifications and variants of Runge–Kutta methods have been developed to solve various ordinary differential equations. The Runge–Kutta method is a one-step method. Therefore, it is easy to apply for the solution of many problems. As is known, every numerical method has its advantages and disadvantages. One of the main disadvantages of the Runge–Kutta methods is the repeated calculation of the function located on the right-hand side of the differential equation under consideration. Let us note that another popular numerical method for solving initial value problems for ordinary differential equations is represented by multistep methods with constant coefficients. As was noted above, these methods also have their own advantages and disadvantages. One of the main advantages of multistep methods is the use of information obtained at previous mesh points. Some authors suggested using forward jumping or advanced methods. It should be noted that advanced methods can be constructed based on multistep methods. In many cases, advanced methods are more exact than multistep methods. For the sake of objectivity, let us note that advanced methods are more exact than both Runge–Kutta and multistep methods. However, some difficulties arise in their implementation when solving some classes of problems. Here, we investigate two known methods (Runge–Kutta and Multistep Methods), and less known methos so called as the advanced method. The results obtained are illustrated with the help of specific examples.

Keywords - Runge–Kutta methods, Ordinary Differential Equations, Multistep Methods with Constant Coefficients, Initial Value Problems, Stability and Degree, Advanced Methods.

I. INTRODUCTION

As is known, one of the first numerical methods was constructed by Euler and later developed by many scientists.
One of the popular methods was constructed by Runge and by Kutta at the end of the 19th century and the beginning of the 20th century. It should be noted that these methods are some families. These methods were adopted by Professor Butcher and his followers. Butcher constructed a new family of implicit nonlinear methods (see for example [1]–[13]).
As is known, one of the main disadvantages of the classical Runge–Kutta methods is the repeated calculation of the value of the function which is on the right-hand side of the differential equation.

Let us consider the following problem:

$$y' = f(x,y), y(x_0) = y_0, \quad x_0 \le x \le X, \tag{1}$$

which is called the initial value problem for ordinary differential equations (ODEs).
To find the numerical solution of problem (1), the segment is divided into (N) equal parts with the constant step size (h>0), and the mesh points are defined as
$x_i = x_0 + ih \quad (i = 0,1,2, \dots . N)$. The exact and approximate values of the solution at the points (x_i) are denoted by (y (x_i)) and (y_i), respectively.
Let us denote the value $f(x_i, y_i)$ or f_i, the value of the function at the point (x_i), and suppose that problem (1) has the unique solution, which has continuous derivatives (p+1) inclusively. The function (f(x,y)) is defined in some closed set in which it has continuous partial derivatives up to some order inclusively.
As is known, some scientists consider Euler's method to be a special case of the Runge–Kutta method, which is not correct. However, some connection can be established between these methods.
Let us consider the following method:

$$y_{n+1} = y_n + \frac{h}{2}\Big(f(x_n, y_n) + f\big(x_{n+1}, y_n + hf(x_n, y_n)\big)\Big) \tag{2}$$

This method can be obtained from the following method:

$$y_{n+1} = y_n + \frac{h}{2}\big(f(x_n, y_n) + f(x_{n+1}, y_{n+1})\big) \tag{3}$$

Note that the accuracy of these methods is the same. But one of them is explicit, and the other is implicit. Here, considering the investigation of explicit methods, we study the Runge–Kutta methods. By simple comparison, we receive that method (2) is from the class of Runge–Kutta methods. It is not difficult to construct methods which differ from methods (2) or (3). For this, let us consider the following midpoint method in the class of Runge–Kutta methods.
This method is presented as follows:

$$y_{n+1} = y_n + hf\left(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}\right). \tag{4}$$

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By this way, here two methods from the class of Runge–Kutta methods are constructed.

As is known, one of the popular methods is the multistep method with constant coefficients. One of the well-known representatives of these methods is the trapezoidal method, which can be received as a partial case from the multistep method as the special case. Note that, in the application of the trapezoidal method, there arise some difficulties with the calculation of the value . For this aim, one can use the following method (2), which is not identical with method (3). Note that the trapezoidal method has accuracy which is equal to for the local truncation error.

And now let us consider the following method:

$$y_{n+1} = y_n + h(5f_n + 8f_{n+1} - f_{n+2})/12. \tag{5}$$

This method differs from known methods in that here the value , which needs to be determined, is used. Along with this, such a property is often called forward jumping or advanced method. Method (5) is the first method constructed with this property. There are some designs for using above present method.

Most scientists conducting research in the field of ecology work in the field of biological sciences. Usually, the concepts of ecosystem and biosystem are studied within biological sciences. Recently, representatives of other sciences have often encountered ecological problems. Mathematical methods are used to investigate ecological problems. Similar studies concerning Volterra-type equations, finite-difference methods, Simpson-type modifications, and related numerical models have also been carried out by many authors. Taking this into account, this paper studies some well-known numerical methods and considers some of their properties.

II. COMPARISON OF SOME NUMERICAL METHODS FOR SOLVING THE INITIAL VALUE PROBLEM FOR ODES

In the introduction, some information is given about the problems which are studied here. For this aim, some classes of methods are suggested, and comparisons are made of the studied problems.

As is known, here, considering the comparison of some families, let us consider the methods and for this study, the following general Runge–Kutta method is used:

$$y_{n+1} = y_n + h\sum_{i=1}^{s} p_i k_i, \tag{6}$$

where,

$$k_1 = f(x_n, y_n),$$
$$k_2 = f(x_n + c_2 h,\ y_n + (a_{21}k_1)h),$$
$$k_3 = f(x_n + c_3 h,\ y_n + (a_{31}k_1 + a_{32}k_2)h),$$
$$\ldots\ldots\ldots..$$
$$k_s = f\big(x_n + c_s h,\ y_n + \big(a_{s1}k_1 + a_{s2}k_2 + \cdots + a_{s,s-1}k_{s-1}\big)h\big).$$

Let us consider the following Runge–Kutta method of third order:

$$y_{n+1} = y_n + h(k_1 + 4k_2 + k_3)/6\,, \tag{7}$$

where,

$$k_1 = f(x_n, y_n),$$
$$k_2 = f\left(x_n + \frac{h}{2},\ y_n + \frac{k_1}{2}\right),$$
$$k_3 = f(x_n + h,\ y_n + 2k_2 - k_1).$$

The method presented here has accuracy $p = 3$. Here, p is the order of the presented method. It is not difficult to demonstrate a constructed more exact method with accuracy $p = 3$. For this, let us consider the following:

$$k_1 = f(y_n),$$
$$k_2 = f\left(y_n + hb_{21}k_1 + c_{21}f_y h^2 + \tfrac{1}{2}c_{22}h^3(f^2 y_{yy} + ff_y^2)\right),$$
$$k_3 = f\left(y_n + hb_{31}k_1 + hb_{32}k_2 + c_{31}fh^2 f_y + \frac{1}{2}c_{32}h^3(f^2 f_{yy} + ff_y^2)\right).$$

By using the above-presented equations, one can con\struct the Runge–Kutta method with the degree $p = 3$. In our case, one can construct the following method:

$$y_{n+1} = y_n + h(k_1 + k_2 + 4k_3)/6, \tag{8}$$

here ,

$$k_2 = f\left(y_n + hk_1 + \frac{2}{5}h^2 ff_y + \frac{1}{10}h^3(f^2 f_{yy} + ff_y^2)\right),$$
$$k_3 = f\left(y_n + \frac{3}{8}hk_1 + \frac{1}{8}hk_2 + \frac{1}{40}h^2 ff_y - \frac{1}{80}h^3(f^2 f_{yy} + ff_y^2)\right).$$

Note that here, three methods are constructed which have the degree $p = 3$. All the methods have the same degree $p = 3$. But methods (8) and (7) are independent from x in other words, the function $f(y)$is independent from the argument x.

And now let us consider the following Runge–Kutta method with the degree

$p = 4$, which can be represented in the following form:

$$y_{n+1} = y_n + \frac{h(k_1 + 2k_2 + 2k_3 + k_4)}{6}\,. \tag{9}$$

Here,

$$k_1 = f(x_n, y_n), \qquad k_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{hk_1}{2}\right),$$
$$k_3 = f\left(x_n + hk_2, y_n + \tfrac{hk_2}{2}\right), \qquad k_4 = f(x_{n+1}, y_n + hk_3).$$

Let us consider the case when the following function $f(x)$can be presented as follows:

$$k_1 = f(x_n), \qquad k_2 = f\left(x_n + \tfrac{h}{2}\right),$$
$$k_3 = f\left(x_n + \tfrac{h}{2}\right), \qquad k_4 = f(x_n + h).$$

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From here, we receive the following:

$$y_{n+1} = y_n + h\big(f(x_n) + 4f(x_{n+1/2}) + f(x_{n+1})\big)/3, \qquad (10)$$

which is identical with the Simpson method.
Here, some methods with the degree $p = 3$ and with the degree $p = 4$ are constructed.
One popular technique that uses this inequality for error control is the Runge–Kutta–Fehlberg method. This technique uses a Runge–Kutta method with local truncation error of order five:

$$\tilde{w}_{i+1} = w_i + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6,$$

to estimate the local error in a Runge–Kutta method of order four, given by

$$w_{i+1} = w_i + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5,$$

where,

$$k_1 = hf(t_i, w_i),$$

$$k_2 = hf\left(t_i + \frac{h}{4}, w_i + \frac{1}{4}k_1\right),$$

$$k_3 = hf\left(t_i + \frac{3h}{8}, w_i + \frac{3}{32}k_1 + \frac{9}{32}k_2\right),$$

$$k_4 = hf\left(t_i + \frac{12h}{13}, w_i + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3\right),$$

$$k_5 = hf\left(t_i + h, w_i + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4\right).$$

$$k_6 = hf\left(t_i + \frac{h}{2}, w_i - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5\right).$$

An advantage to this method is that only six evaluations of are required per step. Arbitrary Runge–Kutta methods of orders four and five used together require at least four evaluations of for the fourth-order method and an additional six for the fifth-order method, for a total of at least ten functional evaluations.
And now, let us consider the comparison of some methods which are recommended here to solve some ordinary differential equations. For this, let us consider the following orders of exactness, which are applied for comparison of methods of Runge-Kutta type. Note that the first method has the degree $p = 3$, and the other methods also have the degree $p = 3$. The next method which is used here has a degree $p = 4$. Thus, we find that when moving from one method to another, accuracy increases depending on the quantity.

For the methods (7) and (8), k_s, in our case, $s = 1 - 4$. From method (9), it is received that method (9) has the degree $p = 4$. As is known, the following method has the degree $p = 5$, and the amount of k_i is equal to $6(six)$.
By this way, we prove the following theorem:
Theorem. Let $p \epsilon N$ be the degree of accuracy of an explicit Runge–Kutta type method and let s denote the number of quantities k_i. For p=1,2,3,4, it is possible to take s=p. However, for p>4, the number of quantities k_i becomes greater than p.

Indeed, each quantity k_i corresponds to one evaluation of the function f (x, y) at a given step. Thus, the number of quantities k_i is the number of stages of the method. For the first four degrees, this number coincides with the degree of accuracy. Beginning from the fifth degree, this relation changes. In the Runge–Kutta–Fehlberg method, fourth and fifth-degree approximations are obtained by using six evaluations of f. Therefore, for p=5, one has $k_1, k_2, \dots, k_6$.
For higher degrees, the number of stages increases further. For single explicit Runge–Kutta methods, known constructions give s=7 for p=6, s=9 for p=7, and s=11 for p=8. In embedded pairs, this number may be larger; for example, a 5,6 pair usually use eight stages. For p=9, known constructions use more than nine stages; in particular, Khashin constructed a ninth-order method with thirteen stages (Khashin, 2009), while Butcher's lower bound gives $s_9 \geq 12$ (Verner, 2013).
Thus, after p=4, increasing the degree of accuracy requires increasing the number of quantities k_i. This explains why high-degree explicit Runge–Kutta methods are more accurate, but also more expensive computationally. Recent Runge–Kutta pairs of orders 8,9 also confirm the practical use of such high-order explicit pairs in high-precision computations (Kovalnogov et al., 2024).

III. MULTISTEP METHOD

As is known, one of the popular methods is the multistep method with constant coefficients. This method has been studied by many famous scientists. Thus, the method is usually presented as follows (see for example [14]– [43]):

$$\sum_{i=0}^{k} \alpha_i \, y_{n+i} = h \sum_{i=0}^{k} \beta_i \, f_{n+i}, n = 0,1,2, \dots, N - k. \qquad (11)$$

It is known that numerical methods are usually based on the concepts of stability and degree, which can be formulated in the following form:
DEFINITION 1. Method (11) is called stable if the roots of the following polynomial

$$\rho(\lambda) = \alpha_k\lambda^k + \alpha_{k-1}\lambda^{k-1} + \dots + \alpha_1\lambda + \alpha_0$$

are located in the unit circle, on the boundary of which there are no multiple roots.
DEFINITION 2. The integer value p is called as the degree of method (11), if the following asymptotic equality holds:

$$\sum_{i=0}^{k} (\alpha_i y(x + ih) - h\gamma_i y'(x + ih)) = O(h^{p+1}), h \to 0. \qquad (12)$$

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Method (4) is stable and has the degree as By Dahlquist's rule, we obtain that if method (11) is stable, then

$$p \leq 2\left[\frac{k}{2}\right] + 2.$$

It follows that, if method (11) is stable, then there exists a stable method with degree $p = 4$ for $k = 2$ and $k = 3$. Note that the values of $p_{\max}$ for $k = 2$ and $k = 3$ do not match.
The stable method with degree $p_{\max} = 4$ for $k = 2$ is the Simpson method, and the method with degree $p_{\max} = 4$ for $k = 3$ can be presented as:

$$y_{n+3} = y_n + \frac{3h}{8}(f_{n+3}+3f_{n+2}+3f_{n+1}+f_n),\ R_n = O(h^5). \quad (13)$$

Some authors call this method Simpson's rule. As was noted, the region of stability for the Simpson method consists of one point, which is called the origin of the coordinate system.
By using the predictor-corrector method, one can expand the region of stability. For example, let us consider the following predictor-corrector method:

$$\tilde{y}_{n+1} = y_{n-3} + \frac{4h}{3}(2y'_n - y'_{n-1} + 2y'_{n-2}). \quad (14)$$

$$y_{n+1} = y_{n-1} + \frac{h}{3}(\tilde{y}'_{n+1}+4y'_n+y'_{n-1}). \quad (15)$$

Note that the local truncation errors for these methods can be presented as follows:

$$R_n^{(13)} = \frac{28}{90}h^5 y_{n-1}^{(5)} + O(h^6), R_n^{(14)} = -\frac{1}{90}h^5 y_{n-1}^{(5)} + O(h^6). \quad (16)$$

Simpson method let us write in the following form:

$$y_{n+1} = y_n + \frac{h}{6}\left(f(x_n, y_n) + 4f\left(x_{n+1/2}, y_{n+1/2}\right) + f(x_{n+1}, y_{n+1})\right) \quad (17)$$

here we use the hybrid point.
For obtaining more accurate results, one can use the following predictor-corrector method:

$$\tilde{y}_{n+1/2} = y_n + \frac{h}{2}f(x_n, y_n),$$
$$y_{n+1/2} = y_n + \frac{h}{2}\left(f(x_n, y_n) + f(x_{n+1/2}, y_{n+1/2})\right)$$

Note that method (17) is obtained by changing the step size by method. From the above description, it is clear that the predictor-corrector approach can be applied to using method (17). In this case, we recieved the following:

$$y_{n+1} = y_n + \frac{h}{6}\left(f(x_n, y_n) + 4f(x_{n+1/2}, y_{n+1/2}) + f(x_{n+1}, \hat{y}_{n+1})\right). \quad (18)$$

For the computation of the value $\hat{y}_{n+1}$, one may use either method (13) or method (14). Method (13) is implicit, whereas method (14) is explicit. In method (18), if we replace h with $2h$, then one can be presented:

$$y_{n+2} = y_n + \frac{h}{3}\left(f(x_n, y_n) + 4f(x_{n+1}, y_{n+1}) + f(x_{n+2}, y_{n+2})\right). \quad (19)$$

Similar studies have been carried out by many authors. To solve certain problems, method (18) is preferable to method (19), since method (18) is a one-step method. If the values are given, then by using method (18), one can compute the values. However, when using method (17), at each step it is necessary to compute the intermediate values and.

IV. ADVANCED METHODS AND THEIR INVESTIGATION

And know let us consider the construction the multistep methods of advanced type. Advanced methods have been investigated by the well-known scientist Cowell in the 19th century, or as the forward-jumping method.
Cowell, by using the so-named method, calculated the orbit of Halley's comet.
Let us note that the advanced methods, or forward-jumping methods, have been investigated by the well-known scientist Cowell in the 19th century. Advanced methods, in one version, can be written as:

$$\sum_{i=0}^{k-m} \alpha_i y_{n+i} = h\sum_{i=0}^{k} \beta_i f_{n+i}, \qquad \mathrm{n} = 0,1,\dots,N-k; m > 0. \quad (20)$$

In formal form, one can say that method (10) can be received from (20) as a partial case. If in method (20) we put $m = 0$, in this case we receive the known multistep method. For the case of objectivity, let us note that the main properties of these methods differ in that the condition $k - m < k$, which is satisfied because $m > 0$.

A.The coefficients $\alpha_i (i = 0,1,\dots,k-m)$,$\beta_i (i = 0,1,\dots,k)$ are real numbers, and $\alpha_{k-m} \neq 0$.

B. The polynomials

$$\rho(\lambda) = \sum_{i=0}^{k-m} \alpha_i \lambda^i, \delta(\lambda) = \sum_{i=0}^{k} \beta_i \lambda^i$$

have no common factor different from a constant.

C. The polynomials $\rho(\lambda)$and $\delta(\lambda)$satisfy the conditions:

$$\rho(1) = 0, \rho'(1) = \delta(1) \neq 0, p \geq 1.$$

Usually, the condition is called the necessary condition for the convergence of method (20). Numerical methods of type (20) have been constructed by some well-known scientists such as Laplace, Steklov, etc. The advanced methods constructed by these scientists may or may not obey the Dahlquist law.
The following method has been constructed in the related literature:

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$$y_{n+2} = \frac{11}{19}y_n + \frac{8}{19}y_{n+1} + \frac{h(10f_n + 57f_{n+1} + 24f_{n+2} - f_{n+3})}{57} \quad (21)$$

It is proved that method (21) is stable and has order. It follows that if method (20) is stable, then it is more accurate than method (2).

However, method (20) has some disadvantages. For example, in the application of this method to solve a problem, it is necessary to calculate the value $y_{n+j}(j \geq k-m)$,which participates in method (20). In our case, it arises the calculation of the value y_{n+3} before calculation y_{n+2}.

Let us consider the following theorem.

Theorem. Suppose that method (20) is stable and has degree p. Then, in the class of methods (20), there are stable methods with degree $p \leq k+m+1$, for the case,$k \geq 3m+1$.

It should be noted that the properties of the resulting method depend on the properties of the method used for calculating the value $y_{n+k-r}(j \leq m)$.

For the illustration,

$$y_{n+1} = y_n + h\frac{5f_n + 8f_{n+1} - f_{n+2}}{12}. \quad (22)$$

The local truncation error for this method is:

$$R_n = \frac{h^4 y_n^{(4)}}{24} + O(h^5).$$

For the calculation of the value y_{n+2}, let us use the following method:

$$y_{n+2} = 3y_{n+1} - 2y_n + \frac{hf_n}{12}.$$

By using this method in (22), we receive:

$$y_{n+1} = y_n + h\frac{8f_{n+1}+5f_n}{12} - \frac{h}{12}f\left(x_{n+2}, 3y_{n+1} - 2y_n + \frac{hf_n}{12}\right)$$
(23)

This method is not A-stable. However, it is possible to change method (23) to the following method:

$$y_{n+2} = y_{n+1} + h\frac{3f_{n+1} - f_n}{2},$$

and by using this in method (22), we receive an A-stable method. By the above, we have shown some advantages of the predictor-corrector method.

Very often, the question arises about the reliability of the obtained values by some numerical methods. For solving this problem, it is recommended to use bilateral methods. It is easy to construct that the bilateral method has some relation with the predictor–corrector methods. As is known, in predictor–corrector methods, one can use methods for which the remainder terms are the same. However, in the construction of the bilateral method, the signs of the main terms of the local truncation errors should be different.

Note that in the construction of methods, one of the main questions is the determination of the signs for some members of the used methods. By using this, Dahlquist proved that if method (1) is stable and has the maximum degree, then the condition is satisfied. If method (22) is stable and has the maximum degree, then and

$\beta_{k-m+j-1}\beta_{k-m+j} < 0$,if $\beta_{k-m+1} \neq 0 (j = 1,2,\dots,m,$
$1 \leq j \leq m)$.

V. NUMERICAL RESULTS

And now, for the illustration of the above-obtained results, let us consider the following example problem:

$y' = \cos x,\ y(0) = 0, \qquad 0 \leq x \leq 1$

with the exact solution:

$y(x) = \sin x$. (24)

For solving this problem, let us apply Simpson's method and its modification, presented in the following form:

$$y_{n+1} = y_n + \frac{h}{6}\left(y'_{n+1} + 4y'_{n+\frac{1}{2}} + y'_n\right). \quad (25)$$

The results of the solution are given in the following table.

Table 1. Solution of problem (24) by Simpson's method and its modification.

x_n	**Modified method,** $h = 0.1$	**Simpson,** $h = 0.1$	**Modified method,** $h = 0.05$	**Simpson,** $h = 0.05$	**Modified method,** $h = 0.01$	**Simpson,** $h = 0.01$
0.2	$6.5E-9$	$1.0E-7$	$4.3E-10$	$6.8E-9$	$6.8E-13$	$1.1E-11$
0.6	$1.8E-8$	$3.0E-7$	$1.2E-9$	$1.5E-8$	$1.8E-12$	$3.1E-11$
1.0	$2.5E-8$	$4.4E-7$	$1.8E-9$	$2.8E-8$	$2.8E-11$	$4.6E-11$

The numerical results correspond to the theoretical results.

VI. CONCLUSION

As is known, in solving many problems, there appears the need for the construction of more exact numerical methods for solving some applied problems. Therefore, many famous scientists began to study the construction of numerical methods for solving various problems (see for example [44]–[71]). The first approximate numerical method was constructed by Euler, which made it possible to solve initial value problems for ordinary differential equations numerically. The theory of Euler was developed by Adams, Runge, Kutta, and others.

At the beginning of the 19th century, they began to construct a new numerical method, which was called the finite difference method. In the middle of the twentieth century, new constructions of multistep methods with constant coefficients were developed. New works written by some scientists appeared in the mid-twentieth century. Among them, one can note the works written by well-known scientists such as Shura-Bura, Bakhvalov, G. Dahlquist, and Butcher. Butcher developed the theory of Runge–Kutta methods, as a result of which new directions emerged, which are called Butcher theory.

For the sake of objectivity, let us note that some well-known scientists developed the theory of explicit Runge–Kutta methods and constructed methods with an order of accuracy of 14 or more. Note that here it is suggested to investigate the following method, which has not been investigated at a high enough level. This method is called the forward jumping or advanced method. Let us note that the advanced methods are more exact than the multistep methods. But these methods have some disadvantages, which are connected with the construction of more complex methods.

$$y_{n+1} = y_n + \frac{h(5f_n + 8f_{n+1} - f_{n+2})}{12}.$$

Here, the given method is presented, by using which one can show the way for using the above-given method. We hope that this direction will find its followers.

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CONFLICT OF INTEREST

The authors state express that there is no conflict-of-interest misunderstanding between them. We hereby confirm that all the methods in this manuscript are ours

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