Published by :
https://www.ijert.org/
An International Peer-Reviewed Journal

International Journal of Engineering Research & Technology (IJERT)
ISSN: 2278-0181
Vol. 15 Issue 05 , May - 2026

On Some Modification of Simpson Method and Their Application to Solve Some Problems from the Environmental Engineering

Nigar Mammadzada
Lecturer, Department of Cybersecurity, Azerbaijan Technical University, Baku, Azerbaijan.
PhD Candidate, Faculty of Mechanics and Mathematics, Baku State University, Baku, Azerbaijan

Vaqif Ibrahimov
Baku State University, Head of Department of Computational Mathematics
Institute of Control Systems of the Ministry of Science and Education, Baku ,Azerbaijan.

Lamiya Rustamova
Xirdalan Secondary School No. 2, Xirdalan, Azerbaijan .

Abstract. In recent years, many scientists have investigated ordinary differential equations, which are related to a wide range of applications. Among them, the study of ordinary differential equations related to this research occupies a significant place in environmental theory. For solving this problem, scientists often use some numerical methods such as the Runge-Kutta, Adams-Moulton, Adams-Bashforth, Simpson, etc. However, these methods are more exact than the above-mentioned methods. It should be noted that there are numerical methods which are more exact than these methods. For example, they are known as multistep methods. This method has been investigated by many authors. Dahlquist investigated the multistep method in full form. By using the Dahlquist law, one can find the maximum value for the multistep method. Also, one can show that the multistep method can be stable. In this case, the maximum value of p can be found in the form: $p_{max} = 2[k/2] + 2$.By using the Dahlquist result, one can construct methods with the degree $p \le 2k$ presented.

By using the given stable methods, which are more exact than the other methods, we suggest using stable methods. Therefore, some stable methods have been considered here for illustrating the obtained results.

Noted that, for the illustrated reserving some results, here presented specifie methods.

Key words: Initial-value problem, Ordinary Differential Equation, Multistep Methods, Degree and Stability, Runge-Kutta methods.

INTRODUCTION

As is known, one of the popular tasks in natural sciences is the initial-value problem for the ordinary differential equation (ODE) of the first order, which can be presented as follows:

$$y' = f(x, y), y(x_0) = y_0, x_0 \le x \le X. \qquad (1)$$

If we take into account that problem (1) has been studied by scientists for more than three centuries, then it is obvious that research in this direction is difficult. Many known methods have been suggested, and some of these methods have been successfully applied in solving certain environmental problems.[1]-[21]

For the investigation of problem (1), suppose that the right-hand side of equation (1) has continuous partial derivatives up to some order p, inclusively. The problem (1) has the exact solution $y(x)$, which is defined on the segment $[x_0, X]$, and has continuous derivatives up to $p + 1$, inclusively.

To define the numerical solution of problem (1), let us designate by $y(x_i)$ the exact values of the solution of problem (1). We also designate by $f\big(x_i, y(x_i)\big)$ the exact values of the function $f(x, y)$ at the point x_i, and the corresponding approximate values by $f(x_i, y_i)$ at the mesh point x_i.

The mesh points x_{i+1} are defined as:

$$x_{i+1} = x_i + h, i = 0,1, \dots, N - 1.$$

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Here, $h > 0$ is the step size, which divides the segment $[x_0, X]$ into N equal parts.
Let us consider the following famous methods:

$$y_{n+1} = y_n + hf(x_n, y_n),\ y_{n+1} = y_n + hf(x_{n+1}, y_{n+1}), \qquad (2)$$

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

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

$$y_{n+1} = y_n + hf\left(x_n + \frac{h}{2}, y_{n+1/2}\right), \qquad (5)$$

$$y_{n+1} = y_n + \frac{h}{6}[f(x_{n+1}, y_{n+1}) + 4f(x_{n+1/2}, y_{n+1/2}) + f(x_n, y_n)]. \qquad (6)$$

By using that, the method (4) becomes more accurate. Let us consider the investigation of the Simpson method.

These methods are successfully applied to solve the initial-value problem (1) and also to the calculation of definite integrals.

It should be noted that method (4) is implicit and has the maximum order of accuracy for $k = 2$(see, for example, [22]–[34]).

§1. On Some Presentation of the Simpson Method

As is known, there are some methods for solving problem (1), one of which is the multistep methods with constant coefficients, and the other is the explicit Runge–Kutta methods. The explicit Runge–Kutta methods are studied very well. There are many popular methods in the class of explicit Runge–Kutta methods. One of them is called the Runge method and is presented as follows:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \qquad (7)$$

where,

$$k_1 = f(x_n, y_n), k_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{hk_1}{2}\right),$$

$$k_3 = f(x_n + h, y_n + hk_2), k_4 = f(x_{n+1}, y_n + hk_3).$$

Let us suppose that the function $f(x, y)$ is independent of the variable y. In this case, from method (7) it follows that:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 4k_2 + k_4). \qquad (8)$$

If here we replace h by $2h$, then from (8) it follows that:

$$y_{n+2} = y_n + \frac{h}{3}[f(x_n) + 4f(x_{n+1}) + f(x_{n+2})]. \qquad (9)$$

In our case, we obtain that methods (9) and (4) are the same. Thus, a direct link between the classes of Runge–Kutta and multistep methods is established.

The multistep method is usually presented in the following form:

$$\sum_{j=0}^{k}(\alpha_j y_{n+j}) = h\sum_{j=0}^{k}(\beta_j f_{n+i}), n = 0,1,2, \dots, N - k. \qquad (10)$$

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ISSN: 2278-0181
Vol. 15 Issue 05 , May - 2026

As is known, numerical methods are based on the concepts of stability and degree, which can be formulated in the following form.

DEFINITION 1. Method (10) is called as the stable if the roots of the following polynomial

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

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 (10), if the following asymptotic equality holds:

$$\sum_{j=0}^{k} \left(\alpha_j y(x + jh) - h\gamma_j y'(x + jh)\right) = O(h^{p+1}), h \to 0. \qquad (11)$$

Method (4) is stable and has the degree $p = 4$. By the Dahlquist's rule, we obtain that if method (10) is stable, then

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

It follows that, if method (10) 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:

$$y_{n+3} = y_n + \frac{3h}{8}(f_{n+3} + 3f_{n+2} + 3f_{n+1} + f_n),\ R_n = O(h^5). \qquad (12)$$

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:

$$\tilde{y}_{n+1} = y_{n-3} + \frac{4h}{3}(2y'_n - y'_{n-1} + 2y'_{n-2}), \qquad (13)$$

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

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

$$R_n^{(13)} = \frac{28}{90} h^5 y_{n-1}^{(5)} + O(h^6), \quad R_n^{(14)} = -\frac{1}{90} h^5 y_{n-1}^{(5)} + O(h^6). \qquad (15)$$

By the above-described predictor–corrector method, the region of stability for the Simpson method (6) is extended as

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$$-0.84 < h\lambda < -0.3.$$

The method (5) is one of the popular methods with a fractional step size. In its application, some difficulties arise in the calculation of the values of type $y_{n+\alpha}$.
If $\alpha -$ rational number, then no difficulty arises in the calculation of $y_{n+\alpha}$. However, if α- irrational, then difficulties arise in the calculation of values $y(x_n + \alpha h)$.
For simplicity of this, let us consider the case, when α is a rational number. The Simpson method let us write in the following form:

$$y_{n+1} = y_n + \frac{h}{6}\big(f(x_n, y_n) + 4f(x_{n+1/2}, y_{n+1/2}) + f(x_{n+1}, y_{n+1})\big), \qquad (16)$$

here we use the hybrid point.

For obtaining more accurate results, one can use the following predictor–corrector method:

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

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

Note that method (16) is obtained by using the chaining step-size h by the $h/2$ method. From the above description, it is clear that the predictor–corrector approach can be applied to using method (16). In this case, we received the following:

$$y_{n+1} = y_n + \mathrm{h}(f(x_n, y_n) + 4f(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + f(x_{n+1}, \hat{y}_{n+1}))\ /6. \qquad (17)$$

For the computation of the value $\hat{y}_{n+1}$, one may use either method (12) or method (13). Method (12) is implicit, whereas method (13) is explicit. In method (17), if we replace h with $2h$, then one can be presented:

$$y_{n+2} = y_n + \frac{h}{3}(f(x_n, y_n) + 4f(x_{n+1}, y_{n+1}) + f(x_{n+2}, y_{n+2})). \qquad (18)$$

Similar studies have been carried out by many authors (see, for example, [35]–[47]).
To solve certain problems, method (17) is preferable to method (18), since method (17) is a one-step method. If the values y_0 and $y_1$are given, then by using method (18), one can compute the values y_2, y_3, ... However, when using method (17), at each step it is necessary to compute the intermediate values $y_{n+1/2}$ and $\hat{y}_{n+1}$.

As noted above the following method:

$$y_{n+3} = y_n + \frac{3h}{8}(f_n + 3f_{n+1} + 3f_{n+2} + f_{n+3}), \qquad (19)$$

is stable and has order $p = 4$. It can be obtained as a particular case of method (8) for $k = 4$.
In [48], using this and several other methods, L-stable methods of orders $p = 3$ and $p = 4$ were constructed.
One such method can be written as:

$$y_{n+1} = y_n + \frac{h}{8}(f_n + 3\bar{f}_{n+1/3} + 3\bar{f}_{n+2/3} + f_{n+1}), \qquad (20)$$

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here

$$\bar{f}_{n+1/3} = f\left(x_n + \frac{h}{3}, \bar{y}_{n+1/3}\right), \bar{f}_{n+2/3} = f\left(x_n + \frac{2h}{3}, \bar{y}_{n+2/3}\right),$$

$$\bar{y}_{n+1/3} = y_{n+1/3} - \frac{2h^3}{81} y_n''' - \frac{h^4}{81} y_n^{(4)} + O(h^5),$$

$$\bar{y}_{n+2/3} = y_{n+2/3} - \frac{h^3}{81} y_n''' - \frac{2h^4}{243} y_n^{(4)} + O(h^5).$$

2. Construction and investigation of the Advanced methods

By using Dahlquist law, we receive that the exactness for stable multistep methods is bounded (see, for example, [49]–[69]). Therefore, for the construction of stable methods, it is recommended to use stable advanced methods. Advanced methods, in one version, can be written as:

$$\sum_{i=0}^{k-m} \alpha_i \, y_{n+i} = h \sum_{i=0}^{k} \beta_i \, f_{n+i}, n = 0,1, \dots, N-k; m > 0. \qquad (21)$$

In formal form, one can say that method (10) can be received from (21) as a partial case. If in method (21) 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 condition:

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

Usually, the condition $\rho(1) = 0$ is called the necessary condition for the convergence of method (21). This method is sometimes called the forward-jumping method. Numerical methods of type (21) have been constructed by some well-known scientists such as Laplace, Steklov, etc. The advanced methods constructed by these scientists obey the Dahlquist law.
In the work [38], the following method is constructed:

$$y_{n+2} = \frac{11}{19} y_n + \frac{8}{19} y_{n+1} + h(10 f_n + 57 f_{n+1} + 24 f_{n+2} - f_{n+3})/57. \qquad (22)$$

It is proved that method (22) is stable and has order $p = 5$. It follows that if method (21) is stable, then it is more accurate and stable than method (2).
However, method (21) 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 (21). In our case, it is arises the calculation of the value y_{n+3} before calculation y_{n+2}.

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Here, we suggest using an additional method for the calculation of the value y_{n+3}. It should be noted that the properties of the resulting method depend on the properties of the method used for calculating the value $y_{n+k-j}(j \leq m)$.
For illustration of this, let us use the following method:

$$y_{n+3} = y_{n+2} + h(23f_{n+2} - 16f_{n+1} + 5f_n)/12, \qquad (23)$$

with the local truncation error:

$$R_n = \frac{3h^4 y_n^{(4)}}{8}.$$

After using method (21) in method (22), we obtain:

$$y_{n+2} = (11y_n + 8y_{n+1})/19 + h(10f_n + 57f_{n+1} + 24f_{n+2})/57 - hf(x_{n+3,}y_{n+2} + h(23f_{n+2} - 16f_{n+1} + 5f_n)/12)/57. \qquad (24)$$

This method is L-stable and has the degree $p = 5$. Let us consider the following method:

$$y_{n+1} = y_n + h\frac{5f_{n+1} + 8f_{n+1} - f_{n+2}}{12}. \qquad (25)$$

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 (25), we receive:

$$y_{n+1} = y_n + h\frac{8f_{n+1} + 5f_n}{12} - \frac{h}{12}f\left(x_{n+2}, 3y_{n+1} - 2y_n + \frac{hf_n}{12}\right). \qquad (26)$$

This method is not A-stable. However, it is possible to change method (26) to the following method:

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

and by using this in method (25), 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.

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Note that in the construction of methods, one of the main question is the determination of the signs for some members of the used methods. By using this, Dahlquist proved that if method (10) is stable and has the maximum degree, then the condition $\beta_k > 0$ is satisfied. If method (23) is stable and has the maximum degree, then $\beta_{k-m} > 0$ and

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

As is known, for the construction of more accurate methods one can use hybrid methods, which can be written as following, in the section. Consider the construction of hybrid methods with multistep type.

The accuracy of this method depends on the calculation of the value y_{n+k}. By this way receive that using hybrid method one can construct more exact method.

To solve this problem, specialists suggest constructing new methods with order less than $2k + 2$. To construct similar methods, let us consider the following formula:

$$y_{n+1} = y_n + hy'_{n+1/2}, \tag{27}$$

which is called the Midpoint Method. Let us consider the generalization of this method, which can be presented as follows:

$$\sum_{i=0}^{k} \alpha_i\, y_{n+i} = h\sum_{i=0}^{k} \beta_i\, y'_{n+i+\nu_i}, |\ \nu_i\ |< 1, i = 0,1,2,\dots,k, n = 0,1,\dots,N-k. \quad (28)$$

Note that, for the stability of method (28), one can use Definition 1. The definition of the degree for method (28) can be given as follows:

Definition 3. The integer value p is called the degree of method (28) if the following asymptotic equality holds:

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

Let us define the maximum value for the stable and unstable methods of type (28). Note that method (28) is called a hybrid method. Depending on the values $\nu_i(i = 0,1,\dots,k)$, method (28) can be called a hybrid method with rational, irrational, or general irrational nodes. Note that the maximum value of the degree depends on the values of $\nu_i(i = 0,1,\dots,k)$. Here, consider to define the maximum value for the stable methods of type (28). For this purpose, let us consider the following theorem.

Theorem . If method (28) has degree p, then

$$p \leq 3k + 1.$$

If method (28) is stable and has degree p, then

$$p \leq 2k + 2,$$

and there exists a stable method with degree

$$p = 2k + 2.$$

For $k = 1$, from method (28) one can obtain the following method, which has degree $p = 4$:

$$y_{n+1} = y_n + h\big(y'_{n+1/2-\alpha} + y'_{n+1/2+\alpha}\big)/2, \alpha = \sqrt{3}/6. \quad (29)$$

Method (29) belongs to the second type, that is, when all the ν_i −are irrational numbers.

Now let us consider the following hybrid methods of the first order ($k = 1$):

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$$y_{n+1} = y_n + h(y'_{n+1} + 3y'_{n+1/3})/4,$$
$$y_{n+1} = y_n + h(y'_n + 3y'_{n+2/3})/4. \qquad (30)$$

Here the variables ν_i are real numbers. These methods belong to the first type. Methods (30) have degree $p = 3$. By simple comparison, we obtain that the values of α_i −are real numbers. Methods of type (30) have some advantages in applications for solving problem (1).

The maximum value of the degree for method (28) is also equal to $3k + 1$, and is simple. The degree for the stable method of type (28) can be increased by using some modifications. For example, consider the following:

$$\sum_{i=0}^{k} \alpha_i \, y_{n+i} = h \sum_{i=0}^{k} \beta_i \, y'_{n+i} + h \sum_{i=0}^{k} \gamma_i \, y'_{n+i+\nu_i}. \qquad (31)$$

If method (31) is stable and has degree p, then,

$$p \leq 3k + 1.$$

Similar results can be obtained for the method

$$\sum_{i=0}^{k} \bar{\alpha}_i \, y_{n+i} = h^2 \sum_{i=0}^{k} \bar{\beta}_i \, y''_{n+i} + h^2 \sum_{i=0}^{k} \bar{\gamma}_i \, y''_{n+i+\nu_i}. \qquad (32)$$

It is easy to determine that method (31) is the generalization of method (32). It is known that if method (31) is stable, then $p_{\max} = 2k + 2$ for the stable methods of type (31).

CONCLUSION

The price of everything in the world is in order. However, we do not always notice that we are considering the investigation of the initial-value problem for first-order ODEs. For this aim, we have used numerical methods for solving the mentioned problem. As is known, many famous scientists have been involved in the study of this problem. Recent research has shown that there are still some unresolved issues. One of them is to find reliable values for the solution of the problem under study.

To obtain a reliable solution of the investigated problem, it is proposed to use bilateral (two-sided) numerical methods. As is known, analytical bilateral numerical methods were constructed by Chaplygin. Here, these methods have been applied to solve problem (1) and have some generalizations.

Before Chaplygin, bilateral (two-sided) methods were constructed for solving nonlinear algebraic equations. Note that there are several ways to increase the accuracy of calculated values by using numerical methods. For example, Hamming method, Richardson extrapolation, and linear combinations of methods, etc. It is obvious that all methods have their own advantages and disadvantages, and the methods considered here are no exception.

Recently, hybrid methods have been developing successfully. As is known, one of the directions in modern computational mathematics is the construction of A-stable methods. As was noted, for this aim one can use advanced (forward-jumping) methods and also apply some linear combinations of stable methods.

We believe that the methods presented here will be suitable for solving many applied problems.

By the above description, we receive some advantages of advanced method.

ACKNOWLEDGEMENTS

The authors thank Academician T. Aliyev, and Academician A. Abbasov for their helpful valuable advise. Finally, the authors also thank the reviewers for their comments. This work was supported by the Azerbaijan Science Foundation – Grant N AEF-MGC-2025-1 (54)-20/05/1-M-05.

Conflict to interest

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

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