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One-leg multistep methods for the numerical integration of periodic second order initial value problems

Solomon A. Okunuga
Department of Mathematics,
University of Lagos, Akoka, Lagos, Nigeria.

e-mail: wordinmn@yahoo.com, Phone: 080232444222

Abstract

The need to develop some efficient schemes that is suitable for second order initial value problems in ordinary differential equations is of interest. We observe that some second order differential equations do exists that will not contain the first derivative of the dependent variable in the equation. Such equations may be highly oscillatory or periodic in nature and require some efficient algorithms in terms of accuracy and stability. This paper discusses some one-leg methods that are suitable for such problems.

***Keywords*:** One-leg, twin- multistep, Periodic, stability

1.0 Introduction

Over the years, attentions of Numerical Analysts have been on the solutions of first order ordinary differential equations (ODE) with an initial value specified. Many numerical methods have been developed to handle the initial value problem (IVP)

$$y' = f(x, y),\ y(a) = \eta \tag{1.1}$$

The problem, be it a single equation or systems of equations (stiff or non-stiff) have the same theories and approaches. Henrici [9] and Fatunla [7] gave a number of ways of handling problem (1.1) which include the one-step and multistep methods of various orders.

In this paper, the focus is to discuss some k-step method for the numerical treatment of the second order differential equation

$$y'' = f(x, y) \tag{1.2}$$

which does not contain y′ explicitly. One way is to turn equation (1.2) to a system of equations. On the other hand, we intend to solve (1.2) as a second order differential equation without introducing the first derivative function y′. One question that may be raised is whether there exists a direct method that will not require the introduction of first derivative explicitly into an equation in which it does not appear. In other words, we intend to examine some methods that could handle equation (1.2) with ease and yet satisfy some required numerical conditions such as stability and convergence. Thus our intention is to consider the second order IVP

$$y'' = f(x, y),\ y(a) = \alpha,\ y'(a) = \beta \tag{1.3}$$

Its solution may sometimes be highly oscillatory or periodic in nature. Although there exists some known Runge-Kutta methods for general second order ODE, however, we shall in this paper consider only the linear k-step method or the multistep method of the form

$$\rho(E)\, y_n = h^2 \sigma(E)\, f_n \tag{1.4}$$

where $\rho(E)=\sum_{j=0}^{k}\alpha_j E^j$, $\sigma(E)=\sum_{j=0}^{k}\beta_j E^j$ and E is a shift operator.

As usual we accept the localizing assumption $\alpha_k = +1$ and not both α_0 and β_0 vanish at the same time. Using a direct k-step method (1.4) for the treatment of equation (1.3) is established by Ash [1] where he studied asymptotic errors of using method (1.4) as against turning equation (1.3) to a system of equations. Dalquist [5] denotes a method of the form

$$\rho y_n = hf(\sigma x_n, \sigma y_n)$$

as a one-leg-twin multistep method for a first order IVP (1.1). A one-leg twin multistep method suitable for the treatment of second order ODE of type (1.3) can also be considered.

2.0 Derivation of methods

To derive a class of methods of for second order ODE as given by (1.4), we give the following definition by Lambert [10].

***Definition* 2.1**

If $y(x)$ is an arbitrary function, which is continuously differentiable many times on interval (a, b), then the linear k-step method (1.4) has the associated linear difference operator

$$L[y(x);h]=\sum_{j=0}^{k}[\alpha_j y(x+jh)-h^2\beta_j y''(x+jh)] \qquad (2.1)$$

And on using Taylor's expansion about the point x, we obtain

$$L[y(x);h]=c_0 y(x)+c_1 hy'(x)+c_2 h^2 y''(x)+\ldots+c_q h^q y^{(q)}(x)+\ldots. \qquad (2.2)$$

Where the c_j are obtained from (2.1) and (2.2) as:

$$\left.\begin{aligned} c_o &= \sum_{r=0}^{k}\alpha_r \\ c_1 &= \sum_{r=1}^{k} r\alpha_r \\ c_2 &= \sum_{r=1}^{k}\tfrac{1}{2!}r^2\alpha_r-\sum_{r=0}^{k}\beta_r \\ c_q &= \sum_{r=1}^{k}\left\{\tfrac{1}{q!}r^q\alpha_r-\tfrac{1}{(q-2)!}r^{q-2}\beta_r\right\} \quad , \qquad q=2,3,\ldots. \end{aligned}\right\} \qquad (2.3)$$

These expressions permit us to define the order of method (1.4) in terms of c_j, as given by Lambert [10]

***Definition* 2.2**

The linear k-step method (1.4) is said to be of order p if in equation (2.2) or (2.3)

$$c_o = c_1 = c_2 = \ldots = c_p = c_{p+1} = 0 \;\; and \;\; c_{p+2} \neq 0$$

c_{p+2} is then said to be the error constant and $c_{p+2}h^{p+2}y^{(p+2)}(x)$ is the principal local truncation error at the point x_n.

***Theorem* 2.3**

The k-step method given by equation (1.4) *is said to be p-stable if*

i) *It is implicit i.e.* $\beta_k \neq 0$

ii) *It is at best of order* $p = 2$

Theorem 2.3 is the barrier theorem given by Lambert & Watson [11] and subsequently by Dalquist [5], however, Cash [2] and Fatunla [7] independently showed that the order barrier imposed by theorem 1 on the attainable order of p-stable method could be crossed by considering certain hybrid 2-step methods. They further showed that orders 4 and 6 p-stable methods exist.

In the same spirit we shall derive some linear multistep methods (LMM) based on the definitions above. It will be observed that y'' can least be approximated by three discrete values of y, thus, it is expected that a method of order k for a second order differential equation requires k to be at least 2.
Thus, to construct the least explicit LMM that satisfy equation (1.4) $k = 2$, $\beta_2 = 0$

We require a method of the form

$$\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} = h^2(\beta_0 f_n + \beta_1 f_{n+1})$$

From equation (2.3) set $c_o = c_1 = c_2 = c_3 = 0$, for the determination of the unknowns. That is,

$$c_0: \ \alpha_0 + \alpha_1 + \alpha_2 = 0$$

$$c_1: \ \alpha_1 + 2\alpha_2 = 0$$

$$c_2: \ \tfrac{1}{2}(\alpha_1 + 2^2\alpha_2) - (\beta_0 + \beta_1) = 0$$

$$c_3: \ \tfrac{1}{6}(\alpha_1 + 2^3\alpha_2) - \beta_1 = 0$$

With localizing assumption $\alpha_k = \alpha_2 = +1$ and solving, we obtain an explicit 2-step method as

$$y_{n+2} - 2y_{n+1} + y_n = h^2 f_{n+1} \tag{2.4}$$

Equation (2.4) is a member of Stormer Cowell method (Lambert [10]).
Since explicit methods are known to be somewhat less accurate than an implicit method, then an implicit scheme of the same or higher order can be derived by ensuring that $\beta_k = \beta_2 \neq 0$. Introducing one free parameter, it will lead to the determination of only four unknowns. Hence we must set $C_0, = C_1 = C_2 = C_3 = 0$
Thus, an implicit 2-step method of the form (1.4) is

$$\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} = h^2(\beta_0 f_n + \beta_1 f_{n+1} + \beta_2 f_{n+2}))$$

If we choose or set β1 = a (a reasonable free parameter), then we have the set of equations

$$c_0: \ \alpha_0 + \alpha_1 + \alpha_2 = 0$$

$$c_1: \ \alpha_1 + 2\alpha_2 = 0$$

$$c_2: \ \tfrac{1}{2}(\alpha_1 + 2^2\alpha_2) - (\beta_0 + \beta_1 + \beta_2) = 0$$

$$c_3: \ \tfrac{1}{6}(\alpha_1 + 2^3\alpha_2) - (\beta_1 + 2\beta_2) = 0$$

Using the localizing assumption and the free parameter we solve the above equations to arrive at

$$y_{n+2} - 2y_{n+1} + y_n = h^2\left[\tfrac{1}{2}(1-a) f_n + a\ f_{n+1} + \tfrac{1}{2}(1-a) f_{n+2}\right] \tag{2.5}$$

This equation has many structure depending on the condition imposed on the free parameter *a*

If *a* = 1, we have the explicit method (2.4) in which case the error constant $c = c_4 = \frac{1}{12}$

Furthermore, if *a* = ½, we have

$$y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{4} h^2\left[f_n + 2\ f_{n+1} + f_{n+2}\right] \tag{2.6}$$

This method has an error constant $c_4 = -\frac{1}{6}$, and it is of order 2.

By definition 2 however, if we set *a* = 5/6, we obtain the optimal 2-step method known as Numerov's method. Thus, with *a* = 5/6 in (2.5) we have

$$y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{12} h^2\left[f_n + 10\ f_{n+1} + f_{n+2}\right] \tag{2.7}$$

which is of order 4 since its error constant is $c_6 = -\frac{1}{240}$. Equation (2.7) is known to be p-stable and unconditionally stable LMM.

Another method that is obtained when a is taken to be ¾ is

$$y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{8}h^2\left[f_n + 6\, f_{n+1} + f_{n+2}\right],\ c_4 = -\tfrac{1}{24} \tag{2.8}$$

And with the choice a = ¼ we get

$$y_{n+2} - 2y_{n+1} + y_n = \tfrac{1}{8}h^2\left[3f_n + 2\, f_{n+1} + 3f_{n+2}\right],\ c_4 = -\tfrac{7}{24} \tag{2.9}$$

All the methods given in (2.6) through (2.9) are implicit and will require an explicit method such as equation (2.4) to serve as the twin-multistep schemes for their implementation. The choice of implementation between PECE and $PE(CE)^m$ modes depends on the level of accuracy achieved. For higher accuracy we implement our methods using the $PE(CE)^m$ mode

By Dalquist [5] methods (2.6) or (2.7) can be regarded as a one-leg multistep method. We define a multistep method for the treatment of second order IVP as a one-leg-twin multistep method for second order ODE, if the method can be written as

$$\rho(E)y_n = h^2 f(\sigma(E)x_n, \sigma(E)y_n)$$

Hence the method (2.7) is a one-leg-twin multistep method for second order ODE.

The LMM of the form (1.4) is said to be zero-stable if no root of the first characteristic polynomial $\rho(\xi)$ has modulus greater than one and if every root of modulus one has multiplicity not greater than two.

The characteristic polynomial is conventionally used to describe the zero stability as well as the consistency of a LMM. Thus, Lambert [10] stated that a method is said to be consistent if it has order of at least one defines the first and second characteristic polynomials as:

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j$$

Indeed method (1.4) is said to be consistent iff

$$\rho(1) = \rho'(1) = 0,\ \rho''(1) = 2\sigma(1)$$

It is easily verified by this definition that our methods (2.4), (2.6) and (2.7) are all consistent and zero stable.

To implement our one-leg twin methods on a second order equation of the type (1.3), we require some starting point in addition to the prescribed initial points. Indeed, an approximation of the Taylor's expansion will do. The other aim of this paper therefore, is to implement and do comparison of accuracy of various orders of schemes of the one-leg methods using $PE(CE)^m$ mode.

3.0 Numerical experiments

***Example* 3.1**

We consider a highly oscillatory test problem

$$y'' + \lambda^2 y = 0, \quad y(x_0) = y_0,\ y'(x_0) = \bar{y}_0 \tag{3.1}$$

Taking λ = 2 to be specific, the problem is solved with given initial conditions

$$y(0) = 1,\ y'(0) = 2$$

Due to the oscillatory nature of the problem, we implement with two different steps. The results obtained with the methods derived above are given in Table3.1 below. The analytical solution of this problem is *y*(*x*) = cos2*x* + sin2*x*

Table 3.1: Solution of problem 3.1

x	Method (2.6)	Method (2.7)	Method (2.8)
0.2	1.3132673267	1.3129568106	1.3130348259
0.3	1.3945240663	1.3935698281	1.3938095592
0.4	1.420552130	1.4186252445	1.4191092851
0.5	1.390320703	1.3871241728	1.3879270495

0.6	1.305027070	1.3003224695	1.3015039363
0.7	1.168049197	1.1616806679	1.1632796714
0.8	0.984811950	0.9767260156	0.9787557180
0.9	0.762572249	0.7528321202	0.7552763132
1.0	0.510131667	0.4989249842	0.5017361597

Table 3.2: Error analysis of numerical experiment 3.1. Step-length h = 0.1

x	Error Method (2.6)	Error Method (2.7)	Error Method (2.8)
0.2	2.79 E-03	2.48 E-03	2.56 E-03
0.3	4.55 E-03	3.59 E-03	3.83 E-03
0.4	6.49 E-03	4.56 E-03	5.05 E-03.
0.5	8.55 E-03	5.35 E-03	6.15 E-03
0.6	1.06 E-02	5.93 E-03	7.11 E-03
0.7	1.26 E-02	6.26 E-03	7.86 E-03
0.8	1.44 E-02	6.35 E-03	8.38 E-03
0.9	1.59 E-02	6.19 E-03	8.63 E-03
1.0	1.70 E-02	5.77 E-03	8.59 E-03

It would be observed that though all the methods have similar accuracy but the integration formula (2.6) performed worst in terms of error, while Method (2.7) has the least error.
The next table gives the error analysis for the first ten values when a step length h = 0.01 is used.

Table 3.3: Error analysis of numerical experiment 3.1. Step-length h = 0.01

x	Error Method (2.6)	Error Method (2.7)	Error Method (2.8)
0.02	2.68E-06	2.65E-06	2.66E-06
0.03	4.06E-06	3.98E-06	4.01E-06
0.04	5.47E-06	5.30E-06	5.39E-06
0.05	6.90E-06	6.62E-06	6.68E-06
0.06	8.36E-06	7.94E-06	7.99E-06
0.07	9.84E-06	9.25E-06	9.65E-06
0.08	1.14E-05	1.06E-05	1.26E-05
0.09	1.29E-05	1.19E-05	1.29E-05
0.1	1.45E-05	1.32E-05	1.41E-05

The result in Table 3.3 shows a very high degree of accuracy. This is achieved by reducing the step length because of the oscillatory nature of the problem.

***Example* 3.2**

We shall also consider the nearly periodic IVP discussed by Lambert and Watson [11].

$$y'' + y = 0.001e^{x},\ y(0) = 1,\ \ y'(0) = 0 \qquad (3.2)$$

Without changing this problem to a first order system of equations, we shall solve the problem using our derived formulas above. The starting point uses the Taylor's approximation on the predictor and the results were corrected by the implicit schemes (2.6) – (2.9), with h = 0.1. The exact solution is

$$y = 0.9995\cos x - 0.0005\sin x + 0.0005e^{x}$$

Petzold [12] described the solution of this problem as highly oscillatory. After implementation of these methods on Problem 3.2, the results with the accuracy obtained are given in the Tables 4 and 5 below.

Ta**ble 3.4**: Solution of problem 3.2

x	Method 10	Method 11	Method 12	Method 13
0.2	0.98009581	0.980079287	0.980083424	0.980108175
0.3	0.95542233	0.955373155	0.955385463	0.955459099
0.4	0.92123194	0.921134745	0.921159074	0.921304627
0.5	0.87786713	0.877707575	0.877747512	0.877986446
0.6	0.82576202	0.825527126	0.825585921	0.825937690
0.7	0.76543811	0.765116500	0.765196998	0.765678635
0.8	0.69749904	0.697081217	0.697185796	0.697811537
0.9	0.62262463	0.622103181	0.622233696	0.623014650
1.0	0.54156410	0.540933890	0.541091623	0.542035488

Table 3.5: Error analysis of Numerical methods on problem 2 Step-length h = 0.1

x	Error Method (10)	Error Method (11)	Error Method (12)	Error Method (13)
0.2	7.90E-06	8.62E-06	4.49E-06	2.03E-05
0.3	3.63E-05	1.28E-05	5.27E-07	7.31E-05
0.4	8.03E-05	1.69E-05	7.41E-06	1.53E-04
0.5	1.39E-04	2.08E-05	1.91E-05	2.58E-04
0.6	2.10E-04	2.46E-05	3.42E-05	3.86E-04
0.7	2.94E-04	2.80E-05	5.25E-05	5.34E-04
0.8	3.87E-04	3.12E-05	7.33E-05	6.99E-04
0.9	4.87E-04	3.41E-05	9.64E-05	8.77E-04
1.0	5.94E-04	3.67E-05	1.21E-04	1.06E-03

The result above shows that the integrating formula (2.7) performs best with least error in computation. This was earlier confirmed with its error constant being the least among the methods. While Lambert and Watson has an error order of 10^{-3} our order 4 formula (2.7) has maximum error to 10^{-5}. Thus some class of second order differential equation could be solved by the scheme given in this paper without the traditional way of converting them firstly to a system of first order differential equations.

4.0 Conclusion

This paper has discussed intelligently the derivation of some new multistep schemes that can be used in solving some highly oscillatory second order ODEs.

The schemes proposed in this paper are seen to be comparable to other known results in terms of accuracy without necessarily reducing the second order equation to a system of first order ODEs. It was also shown that the methods given in this paper are consistent and satisfy the zero stability conditions. This is a sufficient condition that an efficient numerical scheme needs to satisfy. Hence, the methods given in this paper are of great usefulness in the literature.

References

[1] Ash J. H. (1969): 'Analysis of Multistep Methods for special second order differential equations', Ph.D. Thesis. Univ. of Toronto

[2] Cash J. R. (1981) "High Order P-stable Formulae for the Numerical Integration of Periodic Initial Value Problems," Numerische Mathematik 37, 355-370

[3] Chawla M. M. (1981) "Two-step Fourth Order P-stable Methods for Second Order Differential Equations," BIT 21, 190 – 193.

[4] Dalquist G. (1979) "Some properties of Linear Multistep and One-leg Methods for ODEs," Report TRITA-NA-7904, Department of Computer Science, Royal Institute of Technology, Stockholm.

[5] Dalquist G. (1978) "On Accuracy and Unconditional Stability of LMM for SecondOrder Differential Equations," BIT 18, 133 -136

[6] Fatunla, S. O. (1985), "One Leg Hybrid Formula for Second Order IVPs,"Computers and Mathematics with Applications 10, 329 -333

[7] Fatunla, S. O. (1988), *Numerical Methods For Initial Value Problems in Ordinary Differential Equations*, New York, Academic Press

[8] Hairer, E. (1979), "Unconditionally stable methods for second order differential equations". Numer. Math 32, 373 - 379
[9] Henrici P (1962), *Discrete Variable Methods in ODEs*, New York: John Wiley & Sons
[10] Lambert J. D. (1973) *Computational Methods in ODEs*, New York: John Wiley
[11] Lambert J. D. & Watson I. A. (1976), "Symmetric Multistep Methods for Periodic Initial Value Problems," Journal of the Institute of Mathematics and Its Applications 18, 189 – 202
[12.] Petzold L. (1981), "An Efficient Numerical Method for Highly Oscillatory ODEs, "SIAM Journal on Numerical Analysis 18, 455 – 479