AIAA-2000-4029

OBRECHKOFF VERSUS SUPER-IMPLICIT METHODS FOR THE INTEGRATION OF KEPLERIAN ORBITS

Beny Neta
Naval Postgraduate School
Department of Mathematics
Monterey, CA 93943

Toshio Fukushima
National Astronomical Observatory
2-21-1, Ohsawa, Mitaka
Tokyo 181-8588, Japan

This paper discusses the numerical solution of first order initial value problems and a special class of second order ones (those not containing first derivative). Two classes of methods are discussed, super-implicit and Obrechkoff. We will show equivalence of super-implicit and Obrechkoff schemes. The advantage of Obrechkoff methods is that they are high order one-step methods and thus will not require additional starting values. On the other hand they will require higher derivatives of the right hand side. In case the right hand side is complex, we may prefer super-implicit methods. The super-implicit methods may in general have a larger error constant, but one can get the same error constant for the cost of an extra future value.

Introduction

In this paper* we discuss the numerical solution of first order initial value problems (IVPs)

$$\begin{aligned} y'(x) &= f(x, y(x)), \\ y(0) &= y_0 \end{aligned} \tag{1}$$

and a special class (for which y' is missing) of second order IVPs

$$\begin{aligned} y''(x) &= f(x, y(x)), \\ y(0) &= y_0,\ y'(0) = y'_0. \end{aligned} \tag{2}$$

There is a vast literature for the numerical solution of these problems as well as for the general second order IVPs

$$\begin{aligned} y''(x) &= f(x, y(x), y'(x)), \\ y(0) &= y_0,\ y'(0) = y'_0 \end{aligned} \tag{3}$$

See for example the excellent book by Lambert[6]. Here we are interested specifically in two classes of methods. The first class, called super-implicit, was developed recently by the second author[3] for the first order IVPs (1) and for the special second order IVPs (2). The methods are called super-implicit because they require the knowledge of functions not only at past and present but also at future time steps. Fukushima developed Cowell and Adams type super-implicit methods of arbitrary degree and auxiliary formulas to be used in the starting procedure. The resulting methods work as a one-step methods integrating a large time interval (on the order of tens of orbital periods). Symmetric Cowell type methods of order up to 12 are given. The integration error grows linearly with respect to time as in symmetric multistep methods.

The second one is due to Obrechkoff†[10]. These methods for the solution of **first** order IVPs (1) are given by (see e.g. Lambert[6], pp. 199-204, or Lambert and Mitchell[7])

$$\begin{aligned} \sum_{j=0}^{k} \alpha_j y_{n+j} &= \sum_{i=1}^{\ell} h^i \sum_{j=0}^{k} \beta_{ij} y_{n+j}^{(i)}, \\ \alpha_k &= 1 \end{aligned} \tag{4}$$

According to Lambert and Mitchell[7], the error constant decreases more rapidly with increasing ℓ rather than the step k. It is difficult to satisfy the zero stability for large k. The weak stability interval appears to be small. The advantage of Obrechkoff methods is the fact that these are one-step high order methods and as such do not require additional starting values. A list of Obrechkoff methods for

*This paper is declared a work of the U.S. Government and is not subject to copyright protection in the United States

†Bulgarian mathematician Academician Nikola Obrechkoff (1896-1963, born in Varna) who did pioneering work in such diverse fields as analysis, algebra, number theory, numerical analysis, summation of divergent series, probability and statistics.

$\ell = 1, 2, \ldots, 5-k,\ k = 1, 2, 3, 4$ is given in Lambert and Mitchell[7]. For example for $k = 1$ and $\ell = 2$ we get an implicit method of order 4 with an error constant

$$C_5 = \frac{1}{720}$$

and the method is

$$\begin{aligned} y_{n+1} - y_n &= \frac{h}{2}\left(y'_{n+1} + y'_n\right) \\ &- \frac{h^2}{12}\left(y''_{n+1} - y''_n\right) \end{aligned} \tag{5}$$

For $k = 1$ and $\ell = 3$ we get an implicit method of order 6 with an error constant

$$C_7 = -\frac{1}{100800}$$

and the method is

$$\begin{aligned} y_{n+1} - y_n &= \frac{h}{2}\left(y'_{n+1} + y'_n\right) \\ &- \frac{h^2}{10}\left(y''_{n+1} - y''_n\right) \\ &+ \frac{h^3}{120}\left(y'''_{n+1} + y'''_n\right) \end{aligned} \tag{6}$$

Obrechkoff methods for the solution of **second order** IVPs (2) can be found in Ananthakrishnaiah[1]. Here P-Stable Obrechkoff methods with minimal phase-lag for periodic initial-value problems are discussed. Also Simos[13] presents P-stable Obrechkoff method. In Rai and Ananthakrishnaiah[11] Obrechkoff methods for general second-order differential equations (3) are developed.

Before we continue, we need several definitions. For the multistep method to solve the first order IVP

$$\sum_{i=0}^{k} a_i y_{n+i} = h \sum_{i=0}^{k} b_i f_{n+i} \tag{7}$$

we define the characteristic polynomials

$$\rho(\omega) = \sum_{i=0}^{k} a_i \omega^i \tag{8}$$

and

$$\sigma(\omega) = \sum_{i=0}^{k} b_i \omega^i \tag{9}$$

The order of the method is defined to be p if for an adequately smooth arbitrary test function $\zeta(x)$,

$$\sum_{i=0}^{k} a_i \zeta(x+ih) - h \sum_{i=0}^{k} b_i \zeta'(x+ih) =$$

$$C_{p+1} h^{p+1} \zeta^{(p+1)}(x) + O(h^{p+2})$$

where C_{p+1} is the error constant. The method is assumed to satisfy the following:

1. $a_k = 1,\ |a_0| + |b_0| \neq 0,$
2. ρ and σ have no common factor,
3. $\rho(1) = 0,\ \rho'(1) = \sigma(1)$ (consistency)
4. The method is zero-stable (relates to the magnitude of the roots of ρ)

For the multistep method to solve the second order IVP

$$\sum_{i=0}^{k} a_i y_{n+i} = h^2 \sum_{i=0}^{k} b_i f_{n+i} \tag{10}$$

we define the characteristic polynomials ρ and σ as before.

The order of the method is defined to be p if for an adequately smooth arbitrary test function $\zeta(x)$,

$$\sum_{i=0}^{k} a_i \zeta(x+ih) - h^2 \sum_{i=0}^{k} b_i \zeta''(x+ih) =$$

$$C_{p+2} h^{p+2} \zeta^{(p+2)}(x) + O(h^{p+3})$$

where C_{p+2} is the error constant. The method is assumed to satisfy the following:

1. $a_k = 1,\ |a_0| + |b_0| \neq 0,\ \sum_{i=0}^{k} |b_i| \neq 0,$
2. ρ and σ have no common factor,
3. $\rho(1) = \rho'(1) = 0,\ \rho''(1) = 2\sigma(1)$ (consistency)
4. The method is zero-stable

The method is called symmetric if

$$a_i = a_{k-i},\ b_i = b_{k-i} \quad \text{for } i = 0, 1, \ldots, k.$$

Definition (Lambert and Watson[8]) The method described by the characteristic polynomials ρ, σ is said to have *interval of periodicity* $(0, H_0^2)$ if for all H^2 in the interval the roots of

$$V(\omega, H^2) = \rho(\omega) + H^2\sigma(\omega) = 0, \ H = \omega h$$

satisfy:

$$\omega_1 = e^{i\theta(H)}, \ \omega_2 = e^{-i\theta(H)},$$

$$|\omega_s| \leq 1, \ s = 3, 4, \ldots, k,$$

where $\theta(H)$ is a real function.

Definition (Lambert and Watson[8]) The method described by the characteristic polynomials ρ, σ is said to be *P-stable* if its interval of periodicity is $(0, \infty)$.

Lambert and Watson proved that a method described by ρ, σ has a nonvanishing interval of periodicity only if it is symmetric and for P-stability the order cannot exceed 2. Fukushima[4] has proved that the condition is also sufficient. However higher order P-stable methods were developed by introducing off-step points or higher derivatives of $f(x, y)$.

Definition (Brusa and Nigro[2]) Phase-lag is the leading coefficient in the expansion of $|(\theta(H) - H)/H|$.

Symmetric two-step Obrechkoff methods involving higher order derivatives were developed by Ananthakrishnaiah[1].

First Order IVPs

To show the similarity between Obrechkoff and super implicit methods, let us consider the method given by (5). Now if we approximate the higher order derivatives (in this case y'') by some finite differences we get super implicit methods (see Fukushima[3]). Clearly the approximation must be of high enough order so as to preserve the order of Obrechkoff method. If this is **not** done, we may get a super implicit method of a lower order. For example, suppose we use centered differences for the second derivatives, then

$$y''_n = \frac{y'_{n+1} - y'_{n-1}}{2h} \tag{11}$$

$$y''_{n+1} = \frac{y'_{n+2} - y'_n}{2h}$$

Substituting these in (5), we get a second order approximation:

$$\begin{aligned} y_{n+1} - y_n &= -\frac{h}{24}\left(y'_{n+2} - y'_{n-1}\right) \\ &+ \frac{13h}{24}\left(y'_{n+1} + y'_n\right) \end{aligned} \tag{12}$$

Using MAPLE[12], we find that the truncation error is

$$\frac{11}{720}h^5 y^{(5)} + O(h^6)$$

so the method is actually fourth order. Notice that the error constant is 11 times larger than the original Obrechkoff method (5). We had to pay a price for not requiring y'' and it comes in the form of larger error constant **and** requiring a future value (y_{n+2}).

If we take a forward approximation of order three

$$\begin{aligned} y''_n &= \frac{1}{2h}\left(y'_{n+1} - y'_{n-1}\right) \\ &-\frac{1}{12h}\left(y'_{n+2} - 2y'_{n+1} + 2y'_{n-1} - y'_{n-2}\right) \end{aligned} \tag{13}$$

we get a third order approximation:

$$\begin{aligned} y_{n+1} - y_n &= \frac{h}{144}y'_{n+3} - \frac{h}{16}y'_{n+2} + \frac{5h}{9}y'_{n+1} \\ &+ \frac{5h}{9}y'_n - \frac{h}{16}y'_{n-1} + \frac{h}{144}y'_{n-2} \end{aligned} \tag{14}$$

Again using MAPLE[12], we find that the truncation error is

$$\frac{1}{720}h^5 y^{(5)} + O(h^6)$$

so the method is actually fourth order. This time we have the same error constant as Obrechkoff method (5), but require more future values than before. It doesn't seem to be worthwhile. The price now is 2 future values to get the same error constant. For this price, we can get a higher order super-implicit method.

Second Order IVPs

The numerical integration methods for (2) can be divided into two distinct classes: (a) problems for which the solution period is known (even approximately) in advance; (b) problems for which the period is not known[1].

For the first class, see Gautschi[5] and Neta[9] and references there. Here we consider the second class only.

In this section we take the P-stable method of order six given by Ananthakrishnaiah[1]

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} = \\ \frac{h^2}{20}\left(y''_{n+1} + 18y''_n + y''_{n-1}\right) \\ -\frac{h^4}{600}\left(y^{(4)}_{n+1} - 22y^{(4)}_n + y^{(4)}_{n-1}\right) \\ +\frac{h^6}{14400}\left(y^{(6)}_{n+1} + 2y^{(6)}_n + y^{(6)}_{n-1}\right) \end{aligned} \tag{15}$$

and show how to get a super-implicit method equivalent to it. This method has a truncation error

$$-\frac{1}{50400}h^8 y^{(8)} + O\left(h^{10}\right)$$

and it's of minimal phase-lag. In order to get a super-implicit, we expand $y^{(6)}_{n+1} + 18y^{(6)}_n + y^{(6)}_{n-1}$ in terms of y'' at n and neighboring points, i.e.

$$\begin{aligned} y^{(6)}_{n+1} + 2y^{(6)}_n + y^{(6)}_{n-1} = Ay''_n + By''_{n+1} \\ +Cy''_{n-1} + Dy''_{n+2} + Ey''_{n-2} \end{aligned} \tag{16}$$

where the undetermined coefficients can be found by comparing coefficients of the Taylor series expansion on both sides. The resulting system of equations is

$$\begin{array}{rlcl} A+ & B + C + D + E & = & 0 \\ & B - C + 2(D - E) & = & 0 \\ & B + C + 4(D + E) & = & 0 \\ & B - C + 8(D - E) & = & 0 \\ & B + C + 16(D + E) & = & 4\dfrac{24}{h^4} \\ & B - C + 32(D - E) & = & 0 \end{array} \tag{17}$$

With 5 unknowns we can satisfy the first 5 equations, but it turns out that the symmetric property of the solution satisfies also the sixth automatically. It is easy to see that

$$\begin{aligned} A &= \frac{24}{h^4} \\ B = C &= -\frac{16}{h^4} \\ D = E &= \frac{4}{h^4} \end{aligned} \tag{18}$$

Thus

$$\begin{aligned} y^{(6)}_{n+1} + 2y^{(6)}_n + y^{(6)}_{n-1} = \\ \frac{24y''_n - 16(y''_{n+1} + y''_{n-1}) + 4(y''_{n+2} + y''_{n-2})}{h^4} \end{aligned} \tag{19}$$

Now we do the same for the 4^{th} order derivatives

$$\begin{aligned} y^{(4)}_{n+1} - 22y^{(4)}_n + y^{(4)}_{n-1} = ay''_n + by''_{n+1} \\ +cy''_{n-1} + dy''_{n+2} + ey''_{n-2} \end{aligned} \tag{20}$$

where the undetermined coefficients can be found in a similar fashion. It is easy to see that

$$\begin{aligned} a &= \frac{168}{3h^2} \\ b = c &= -\frac{92}{3h^2} \\ d = e &= \frac{8}{3h^2} \end{aligned} \tag{21}$$

Thus

$$\begin{aligned} y^{(4)}_{n+1} - 22y^{(4)}_n + y^{(4)}_{n-1} = \\ \frac{168y''_n - 92(y''_{n+1} + y''_{n-1}) + 8(y''_{n+2} + y''_{n-2})}{3h^2} \end{aligned} \tag{22}$$

Substituting (19) and (22) into (15) we have after collecting terms,

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} = h^2\left\{\frac{97}{120}y''_n\right. \\ \left. +\frac{1}{10}\left(y''_{n+1} + y''_{n-1}\right) - \frac{1}{240}\left(y''_{n+2} + y''_{n-2}\right)\right\} \end{aligned} \tag{23}$$

which is the sixth order method given as equation (3) in Fukushima[3]. The error constant of this sixth order method is

$$C_8 = \frac{31}{60480}$$

which is larger than the error constant for the P-stable sixth order method (15) of Ananthakrishnaiah by a factor of more than 25. Are super implicit methods always giving larger error constant? In first order IVPs we showed that we can get the same error constant if we allow an extra future value (two instead of one). We now get a super-implicit method of the same order **and** error constant. The price is an extra future value. It can be shown that

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \frac{1723}{2160} y_n'' \right.$$

$$+ \frac{311}{2880} \left(y_{n+1}'' + y_{n-1}'' \right)$$

$$\left. - \frac{53}{7200} \left(y_{n+2}'' + y_{n-2}'' \right) + \frac{23}{43200} \left(y_{n+3}'' + y_{n-3}'' \right) \right\} \tag{24}$$

has an error constant of

$$C_8 = -\frac{1}{50400}$$

exactly as (15). For this price, Fukushima[3] has obtained an eighth order method.

We try the eighth order super-implicit

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \frac{12067}{15120} y_n'' \right.$$

$$+ \frac{2171}{20160} \left(y_{n+1}'' + y_{n-1}'' \right) - \frac{73}{10080} \left(y_{n+2}'' + y_{n-2}'' \right)$$

$$\left. + \frac{31}{60480} \left(y_{n+3}'' + y_{n-3}'' \right) \right\} \tag{25}$$

Again using MAPLE, we find the error constant

$$C_{10} = -\frac{289}{3628800}$$

Compare this to the eighth order Obrechkoff method of Ananthakrishnaiah[1] with an error constant

$$C_{10} = -\frac{2}{7 \cdot 10!}$$

The super implicit has an error constant more than 1012 times larger. We can create super implicit method of the same error constant but requiring more future values than the ones in Fukushima[3]. These additional future values can be used to increase the order. We must remark here that future values require more starting steps. For example the eighth order super-implicit of Fukushima requires three steps before actually using it. Formulas for these steps are also given by Fukushima.

Numerical Implementation Issues

To demonstarte how to implement the super-implicit methods, we consider the sixth order one as an example. In order to start the method, we need y_0, the initial value, as well as y_1 and y_2. These two values were obtained by special super implicit methods of the same order given in Fukushima[3]:

$$y_1 = y_0 + hy_0' + h^2 \left\{ \frac{367}{1440} y_0'' + \frac{3}{8} y_1'' - \frac{47}{240} y_2'' + \frac{29}{360} y_3'' - \frac{7}{480} y_4'' \right\} \tag{26}$$

$$y_2 = 2y_1 - y_0 + h^2 \left\{ \frac{19}{240} y_0'' + \frac{17}{20} y_1'' + \frac{7}{120} y_2'' + \frac{1}{60} y_3'' - \frac{1}{240} y_4'' \right\} \tag{27}$$

For linear problems, this leads to a banded system of $N \times N$ equations with a bandwidth of 5. But in general, we get a nonlinear system of N equations. This system requires an initial guess. If we want to continue after N steps, we need the velocity at that point, which can be approximated by

$$y_N' = \frac{y_N - y_{N-1}}{h} + h \left\{ \frac{7}{480} y_{N-4}'' - \frac{29}{360} y_{N-3}'' + \frac{47}{240} y_{N-2}'' - \frac{3}{8} y_{N-1}'' - \frac{367}{1440} y_N'' \right\} \tag{28}$$

Fukushima[3] asserts that the super-implicit methods are less practical for scalar computers but lends themselves quite easily to parallelism.

The Obrechkoff methods require additional formulas. For example y' is needed in calculating the higher derivatives.

Conclusion

In this paper we showed the equivalence of super-implicit and Obrechkoff methods. The advantage of Obrechkoff methods is that they are high order one-step methods and thus will not require additional starting values. On the other hand they will require higher derivatives of the right hand side. In case the right hand side is complex, we may prefer super-implicit methods. One can use super-implicit methods given by Fukushima. In general, these methods have larger error constants. We have found here that one can develop super-implicit methods having the same error constants as Obrechkoff but requiring an extra future value.

This extra future value can be used instead to increase the order of the method.

References

1. Ananthakrishnaiah, U., "P-Stable Obrechkoff methods with minimal phase-lag for periodic initial-value problems," Math. Comput., Vol. 49, 1987, 553-559.

2. Brusa, L., and Nigro, L., "A one-step method for direct integration of structural dynamic equations," Int. J. Numer. Meth. Engng., Vol. 15, 1980, 685-699.

3. Fukushima, T., "Super implicit multistep methods," Proc. of the 31^{st} Symp. on Celestial Mechanics, 3-5 March 1999, Kashima Space Research Center, Ibaraki, Japan, H. Umehara (ed.), pp. 343-366.

4. Fukushima, T., "Symmetric multistep methods revisited," Proc. of the 30^{th} Symp. on Celestial Mechanics, 4-6 March 1998, Hayama, Kanagawa, Japan, T. Fukushima, T. Ito, T. Fuse, and H. Umehara (eds), pp. 229-247.

5. Gautschi, W., "Numerical integration of ordinary differential equations based on trigonometric polynomials," Numer. Math., Vol. 3, 1961, 381-397.

6. Lambert, J. D., "Computational Methods in Ordinary Differential Equations," John Wiley& Sons, London, 1973.

7. Lambert, J. D., and Mitchell, A. R., "On the solution of $y' = f(x, y)$ by a class of high accuracy difference formulae of low order," Z. Angew. Math. Phys., Vol. 13, 1962, 223-232.

8. Lambert, J. D., and Watson, I. A., "Symmetric multistep methods for periodic initial value problems," J. Inst. Math. Appl., Vol. 18, 1976, 189-202.

9. Neta, B., "Trajectory Propagation Using Information on Periodicity," Proc. AIAA/AAS Astrodynamics Specialist Conference, Boston, MA, August 10-12, 1998, Paper Number AIAA 98-4577.

10. Obrechkoff, N., "On mechanical quadrature" (Bulgarina, French summary), Spisanie Bulgar. Akad. Nauk., Vol. 65, 1942, 191-289.

11. Rai, A. S., Ananthakrishnaiah, U., "Obrechkoff methods having additional parameters for general second-order differential equations," J. Comput. Appl. Math., Vol. 79, 1997, 167-182,

12. Redfern, D., 'The Maple Handbook', Springer-Verlag, New York, 1994.

13. Simos, T. E., "A P-stable complete in phase Obrechkoff trigonometric fitted method for periodic initial-value problems," Proc. Royal Soc. London A, Vol. 441, 1993, 283-289.