NUMERICAL METHODS AND THEIR PHASE-LAG ANALYSIS FOR SECOND ORDER PERIODIC INITIAL-VALUE PROBLEMS

BY
P. SRINIVASA RAO

A THESIS SUBMITTED TO THE
INDIAN INSTITUTE OF TECHNOLOGY, DELHI
FOR THE AWARD OF THE DEGREE OF
DOCTOR OF PHILOSOPHY

DEPARTMENT OF MATHEMATICS
INDIAN INSTITUTE OF TECHNOLOGY, DELHI
APRIL, 1986

Dedicated to
MY MOTHER
AND
UNCLE R.H. RAO

CERTIFICATE

This is to certify that the thesis entitled "NUMERICAL METHODS AND THEIR PHASE-LAG ANALYSIS FOR SECOND ORDER PERIODIC INITIAL-VALUE PROBLEMS" which is being submitted by Mr.P.Srinivasa Rao to the Indian Institute of Technology, New Delhi, for the award of the degree of Doctor of Philosophy in Mathematics, is a record of bonafide research work carried out by him under my guidance and supervision.

The thesis has reached the standard, fulfilling the requirements of the regulations relating to the degree. The results obtained in the thesis have not been submitted to any other University or Institute for the award of any degree or diploma.

M. M. Chawla

(M.M. CHAWLA)
Professor
Department of Mathematics
Indian Institute of Technology
Hauz Khas, New Delhi-110 016.

ACKNOWLEDGEMENTS

It gives me great pleasure to express my profound sense of gratitude to Professor M.M. Chawla, F.I.M.A., Department of Mathematics, Indian Institute of Technology, New Delhi, under whose supervision and able guidance I had the privilege to carry out my research work. I am indebted to him for his invaluable suggestions and constant encouragement without which this work would not have been possible. His ever willingness and kindness gave me the needed inspiration to persue my work in this field.

I express my deep sense of gratitude to Professor O.P. Bhutani, Head, Department of Mathematics, and Professor M.K. Jain, Deputy Director, I.I.T., New Delhi, for their constant encouragement throughout the preparation of this research work. I also thank all the faculty members of the Department of Mathematics, I.I.T., Delhi, for the fruitful discussions I had with them on several occasions especially Professor P.K. Bhattacharyya.

My thanks are also due to the authorities of the Indian Institute of Technology, Delhi for providing me with research facilities and financial support during the course of my research. I also thank Professor R.K. Arora, Head of the Computer Service Center, I.I.T., Delhi for providing computer facilities.

I sincerely thank my brother and sisters for their inspiration and encouragement throughout my studies.

My best friends Mr. G. Giridhar, Mr. V.R. Subramanyam, Mr. B.Ramadas Naidu, Mrs and Mr. D.Anil Kumar, Mr. D.V. Prabhakar, Miss T.Sharada and Miss D.Lakshmi made my stay in the hostel very pleasant and memorable. I owe a deep sense of gratitude not only to these friends but also to my colleagues Mrs. Lalita Dixit, Mrs. Sarada Nagarajan,Mr. R.Subramanian and other numerous friends and well wishers in Vindhyachal Hostel who made my stay in the campus enjoyable. My special thanks are due to my colleague and friend Mr. S.Gopalsamy with whom I had many fruitful discussions and also for the help he rendered during the course of preparation of this thesis work.

Finally, Ms Neelam Dhody deserves special praise for her accurate typing of the manuscript.

P. Srinivasa Rao

P. SRINIVASA RAO

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SYNOPSIS

In 1976, Lambert and Watson [1] introduced the idea of intervals of periodicity (orbital stability, in the terminology of Stiefel and Bettis [2]) for linear multistep methods for the numerical integration of second order periodic initial-value problems:

$$y'' = f(t,y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0 . \qquad (1)$$

In case the problem (1) has periodic solutions, oscillations corresponding to the natural modes of (1) can be modelled using the test equation:

$$y'' + \lambda^2 y = 0, \qquad \lambda > 0. \qquad (2)$$

Consider a (convergent) linear multistep method:

$$\sum_{j=0}^{k} \alpha_j \, y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j \, f_{n+j} , \quad k \geq 2 , \qquad (3)$$

applied to the test equation (2). As usual, we set

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \, \zeta^j , \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \, \zeta^j . \qquad (4)$$

Let r_s, $s = 1(1)k$, denote the roots (assumed distinct) of the polynomial

$$\Omega(r,H) = \rho(r) + H^2 \sigma(r), \tag{5}$$

where we have set

$$H = \lambda h, \quad h \text{ is the step size} \tag{6}$$

and let $r_{1,2}$ correspond to the perturbations of the principal roots $\zeta_1 = \zeta_2 = +1$.

DEFINITION 1.

A linear multistep method (3) is said to have an interval of periodicity $(0,H_p)$ if, for all $H \varepsilon (0,H_p)$, the roots r_s of $\Omega(r,H)$ satisfy

$$r_1 = e^{i\theta(H)}, \quad r_2 = e^{-i\theta(H)}, \quad \theta(H) \text{ real}, \tag{7}$$

$$|r_s| \leq 1, \quad s = 3(1)k.$$

DEFINITION 2.

A linear multistep method is said to be P-stable if its interval of periodicity is $(0,\infty)$.

Lambert and Watson [1] showed in particular that P-stable methods must be implicit and that P-stability forced an "order-barrier", namely that P-stable linear multistep methods can not have order greater than two. Chawla [3] and Cash [4] independently showed that this order-barrier could be crossed over by considering certain hybrid two-step methods and they presented P-stable methods of orders four and six. Jeltsch [5] has given a characterization for linear multistep methods possessing non-vanishing intervals of periodicity by applying these to the test equation (2). It may be noted here that the classical fourth order method of Noumerov possesses an interval of periodicity $(0,\sqrt{6})$; the classical fourth order method of Nyström possesses no interval of periodicity, and consequently, the numerical solutions provided by it for the test equation (2) are orbitally unstable or "spiral inwards". Intervals of periodicity of explicit Nyström methods of orders two, three, four and five involving respectively one, two, three and four-stages have been examined by Chawla and Sharma [6,7]; and it is the second order method for which the scaled interval of periodicity is of length of two. On the other hand if Nyström methods with large number of stages is considered, keeping the order of the method low, can the extra free parameters in the method help to push up the length of scaled interval of periodicity? In Chawla [8] m-stage explicit Nyström methods are considered which are at least order one and it is shown that the length of the interval of periodicity scaled by dividing by m can not exceed two.

Two well known two-step methods for the numerical integration of the initial-value problem (1) are the second order trapezoidal method:

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{4} (f_{n+1} + 2f_n + f_{n-1})$$

and the fourth order method of Noumerov:

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12} (f_{n+1} + 10f_n + f_{n+1}).$$

When applied to the test equation (2), the trapezoidal method reproduces the amplitude of these oscillations for all $H \varepsilon (0,\infty)$ since it is a P-stable method, whereas Noumerov's method reproduces the amplitude provided $H \varepsilon (0,\sqrt{6})$. However, for the test equation (2), both the trapezoidal method and Noumerov's method are out of phase of these oscillations. Brusa and Nigro [9] were the first to investigate this phenomenon of frequency distortion and introduced a measure for the phase-lag of a method.

DEFINITION 3.

Since $\theta(H)$ is supposed to be an approximation for H, as in Brusa and Nigro [9] we define the phase-lag of a numerical method as the absolute value of the leading coefficient in the expansion of $\frac{\theta(H)-H}{H}$.

In this thesis we are concerned with the construction of numerical methods for the initial-value problem (1) and with the study of stability and phase-lag analysis of these methods. The thesis consists of six Chapters and a brief description of each Chapter follows.

Noumerov's method has a phase-lag of size $\frac{1}{480} H^4$ and an interval of periodicity of size 2.449. In Chapter 1 we consider a one-parameter family $M_4(\alpha)$ of Noumerov-type methods for the integration of second order periodic initial-value problems (1). By applying these methods to the test equation (2), we determine the free parameter of the family so that the phase-lag (frequency distortion) for the method is minimal. The resulting method has a very small phase-lag of size $\frac{1}{12096} H^6$; interestingly, this method also possesses an interval of periodicity of size 2.71. The superiority of our method over Noumerov's method is illustrated computationally by numerical examples.

In Chapter 1 we described a Noumerov-type method with minimal phase-lag; however, the method given there is implicit. In Chapter 2 we show the interesting result that if the Noumerov-type methods of Chapter 1 are made explicit with the help of classical second order method, now called $M_4^*(\alpha)$, there exists a selection of the free parameter α for which the resulting method has a considerably smaller frequency distortion of size $\frac{1}{40320} H^6$ and a (slightly) larger interval of periodicity of size 2.75 than phase-lag of size $\frac{1}{12096} H^6$ and interval of periodicity of size 2.71 for the implicit method of Chapter 1. More interestingly, it turns out that Noumerov made explicit of Chawla [10] also has less frequency distortion than the (implicit) Noumerov method.

In Chapters 1 and 2 we described two-step methods for the initial-value problems (1) which when applied to the test equation (2) have higher order phase-lag than the order of the method. Recently, Thomas [11] has also given fourth order and sixth order methods having respectively phase-lags of order six and eight. But high order phase-lag of these methods was achieved by sacrificing P-stability since the resulting methods possesses only a finite interval of periodicity. It is therefore natural to ask if we can obtain methods which are at once P-stable and have a phase-lag order higher than the order of the method. While no such methods can be found from the families of methods in Thomas [11] and Chawla and Neta [12], we show the interesting result that by a suitable modification of Noumerov's method we obtain a new family of methods which are at once P-stable and have phase-lag of order six. However, in comparison with the methods proposed in Chapters 1 and 2, the present methods can be useful in cases where a large step-size is to be used; that is, where a modest accuracy is sufficient or in case of problems where the solution consists of slowly varying oscillations with high frequency super-imposed having a small amplitude.

In Chapter 4 we obtain a one-parameter family $M_6(\alpha)$ of sixth order P-stable methods for the numerical integration of second order periodic initial-value problems (1). The methods presented are symmetric and they are based on three function evaluations per step (per iteration, in case f(t,y) is non-linear in y). For non-linear problems, we also consider the implementational details for a method of $M_6(\alpha)$ and discuss how a method of the family can be implemented by modified Newton's iteration process to provide $O(h^6)$-convergent approximations. We also propose suitable initial approximations $y_{n+1}^{(0)}$ for use with the modified Newton's method; and at each step, I iteration of modified

Newton's method involves 3I+6 function evaluations (3I+3 f-evaluations and 3 f^y-evaluations). Further for non-linear problems and for a proposed initial approximation, we obtain sufficient conditions under which the modified Newton's method giving y_{n+1} will be convergent.

Recently, Thomas [11] gave a sixth order method with phase-lag order eight for the numerical integration of periodic initial-value problems (1). However, Thomas's method is implicit, it possesses an interval of periodicity of size 2.77 and her method requires 6I+1 function evaluations for I iterations of her version of modified Newton's method for the solution of the resulting implicit equations. In Chapter 5 we present the sixth order method of Chapter 4 made explicit which also has a phase-lag or order eight but with a smaller phase-lag constant. In contrast with Thomas's method our present method is explicit and possesses a larger interval of periodicity of size 4.67 and it is more economical since it involves only seven function evaluations per step.

In Chapter 6 we examine the phase-lag of two-parameter family $M_4(\alpha_1,\alpha_3)$ of fourth order explicit Nystrom methods of Chawla and Sharma [6]. While the method $M_4(\frac{1}{6}, \frac{5}{6})$ possessing the largest interval of periodicity of size 3.46 has a phase-lag of $\frac{1}{4320} H^4$, we show that there exist two-fourth order methods for which the phase-lag is minimal and of size $\frac{1}{40320} H^6$; interestingly, both these methods also possesses a sizable interval of periodicity of size 2.75 each. We also include the phase-lag analysis of the uniquely determined four-stage fifth order explicit Nyström method of Chawla and Sharma [7] possessing a non-vanishing interval of periodicity. The single-step explicit methods of this chapter can be used to compute the numerical solution $\tilde{y}_1$ at step number one for starting the two-step methods from step number two onwards studied in Chapters 1 through 5. In Chapter 2, we have briefly examined the effect of the "initial" phase-lag in the computation of y_1 on the subsequent values for the computed solution sequence y_n, $n \geq 2$.

The thesis is based on the following five published/ accepted papers.

1. "A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems", J.Comput. Appl. Math., 11 (1984), 277-281. (With M.M. Chawla)

2. "A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems II. Explicit method", J.Comput. Appl. Math., to appear (1986). (With M.M.Chawla)

3. "Two-step fourth order P-stable methods with phase-lag of order six for y" = f(t,y)", J.Comput. Appl.Math., to appear (1986). (With M.M.Chawla) & B.Neta

4. "High-accuracy P-stable methods for $y'' = f(t,y)$", IMA. J.Numer. Anal., 5 (1985), 215-220. (With M.M. Chawla)

5. "Phase-lag analysis of explicit Nyström methods for $y'' = f(x,y)$", BIT, 26(1986), 64-70. (with M.M. Chawla)

CONTENTS

NOTE: EQUATION NUMBERED n IN CHAPTER m WILL BE REFERRED TO AS EQUATION (m.n); SIMILARLY FOR DEFINITIONS, THEOREMS ETC.