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THE INTEGRATION OF STIFF SYSTEMS OF ODEs USING NDFs AND MEBDFs*

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Abstract

In this paper we modify the MEBDF method using the NDFs as predictors instead of the BDFs. We have done it in three different ways: changing both predictors of the MEBDF, changing only the first predictor and changing only the second one. We have called the new methods MENDF, MENBDF and MEBNDF respectively. The new methods are A-stable up to order 4 and the stability properties of the new methods are better than the MEBDF method.

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Key words: BDF, NDF, MEBDF, Stiff ODEs, Stability.

1. Introduction

In this paper we will consider the initial value problem:

$$y'(x) = f\left(x, y(x)\right), \quad y\left(x_0\right) = y_0, \tag{1.1}$$

on the finite interval $T = [x_0, x_n]$, and being $y : [x_0, x_n] \to \mathbb{R}^m$ and $f : [x_0, x_n] \times \mathbb{R}^m \to \mathbb{R}^m$ continuous functions. When we are solving systems of stiff ordinary differential equations by numerical integration, it is important to use an accurate algorithm which has good stability properties [6]. Many researches have been focused on the generation of efficient algorithms for the numerical integration of stiff systems and some of them have been based on backward differentiation formulae (BDF) [9]. The BDFs give us the possibility to use high order formulae in highly stable schemes, but their biggest drawback is the poor stability properties of the highest orders formulae, when the eigenvalues of the Jacobian matrix lie close to the imaginary axis.

A great effort to derive methods with better accuracy and stability properties than the ones of the BDFs has been made. One of the modifications made to the BDFs in this line are the NDFs (Numerical Differentiation formulae) [17]. It is a computationally cheap modification that consists of anticipating a difference of order $(k+1)$ multiplied by a constant $\kappa\gamma_k$ in the BDF formula of order k. This term makes the NDFs more accurate than the BDFs and not

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much less stable. This modification was proposed only for orders $k = 1, 2, 3, 4$, because it is inefficient for orders greater than 4.

The search of higher order and more stable methods has been followed in two main directions. The first of these two directions consists of using superfuture point schemes and the second one uses higher derivatives of the solutions. In [2, 4] Cash introduces methods using superfuture points to solve stiff IVPs. These methods are known as extended BDF (EBDF) and modified extended BDF (MEBDF). They use two BDF predictors and one implicit multistep corrector. Both methods are A-stable up to order 4 and $A(\alpha)$-stable up to order 9, and the class MEBDF has better stability properties than the class EBDF. In [5] a code based on the MEBDF is described and its performance on a set of stiff problems is discussed. In [13] Matrix free MEBDF (MF-MEBDF) methods are introduced to optimize the computations of the EBDF.

A different variation of the BDFs was introduced by Fredebeul [8], the A-BDF method. In this method the implicit and explicit BDF are used in the same formula, with a free parameter, being $A(\alpha)$-stable up to order 7. And in [11], a modification to the methods A-BDF and EBDF is introduced, the method called A-EBDF, in which larger absolute stability regions than the ones of the A-BDF and the EBDF are obtained.

Among the modifications made to the BDFs by using higher derivatives, we can find [7], where a class of second derivative formulae A-stable for order 4 is developed. In [3], Cash introduces another class of second derivative methods which uses the EBDF scheme. This class is A-stable up to order 6. In more recent researches such as [12, 15], different classes of second derivative multistep methods are derived in which very good stability properties are reached again.

The purpose of this paper is to follow the MEBDF scheme but by substituting the BDF predictors by the NDF formulae [17]. We did this in [1], when we changed the predictors of the EBDFs and we obtained new classes of formulae with smaller local truncation error and better stability properties. We have changed the predictors of the MEBDFs in three different ways: changing only the first predictor, changing only the second one or by changing both predictors. We have called the new methods MENBDF, MEBNDF and MENDF respectively and all of them have better stability properties than the MEBDFs. In Section 2, we give details about the modifications introduced in MEBDF, such as, MENDF, MENBDF and MEBNDF. In Section 3, the stability analysis is developed. Finally in Section 4, some computational aspects are included and results of several problems are reported in Section 5.

2. The Use of NDFs as the Predictors of the MEBDF Class

In order to understand the new methods we have developed, we will start analysing the properties of the NDF and MEBDF, to finally derive the MENDF, MENBDF and MEBNDF algorithms.

2.1. NDF scheme

Among the codes that have been created to solve stiff problems, the most popular and widely used are the backward differentiation formulae, BDFs [9]. These numerical methods are A-stable only up to order 2, but they have good stability properties also when working in high