Boundary Value Methods for the Numerical Approximation of Ordinary Differential Equations

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Abstract. Many numerical methods for the approximation of ordinary differential equations (ODEs) are obtained by using Linear Multistep Formulae (LMF). Such methods, however, in their usual implementation suffer of heavy theoretical limitations, summarized by the two well known Dahlquist barriers. For this reason, Runge-Kutta schemes have become more popular than LMF, in the last twenty years. This situation has recently changed, with the introduction of Boundary Value Methods (BVMs), which are methods still based on LMF. Their main feature consists in approximating a given continuous initial value problem (IVP) by means of a discrete boundary value problem (BVP). Such use allows to avoid order barriers for stable methods. Moreover, BVMs provide several families of methods, which make them very flexible and computationally efficient. In particular, we shall see that they allow a natural implementation of efficient mesh selection strategies.

1 Introduction

Usually, the solution of an initial value ODE problem,

\[ y' = f(t, y), \quad t \in [t_0, T], \quad y(t_0) = \eta, \quad (1) \]

is obtained by using a \( k \)-step LMF,

\[ \sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}. \quad (2) \]

In the previous equation, \( y_n \) denotes, as usual, the discrete approximation of the solution \( y(t) \) at \( t = t_n = t_0 + nh, \) \( h = (T - t_0)/N, \) and \( f_n \equiv f(t_n, y_n). \) Since (2) is a \( k \)th order difference equation, then \( k \) conditions need to be imposed to obtain the discrete solution. Usually, such conditions are obtained by fixing the first \( k \) values, \( y_0, \ldots, y_{k-1}, \) of the discrete solution. That is, the continuous IVP (1) is approximated by means of a discrete IVP. This approach is very straightforward. However, it suffers of heavy theoretical limitations, summarized by the two Dahlquist barriers.

It is possible to get rid of such limitations by suitably modifying the use of LMF. This is, in fact, the idea on which Boundary Value Methods rely. Early
references on such methods can be found in [4, 12]. However, only in the last three years such methods have been systematically studied, starting from [14]. In particular, a linear stability theory has recently been devised [6], which has made possible the derivation of several families of methods, each containing stable methods of arbitrarily high order. In this paper, a brief review on BVMs is presented, along with a mesh selection strategy which is very efficient for such methods.

In Sect. 2 the main facts about BVMs will be recalled, and in Sect. 3 the principal families of methods are sketched. In Sect. 4 the block version of the methods is presented, along with the mesh selection strategy. Finally, in Sect. 5 some numerical examples on difficult stiff problems are reported, showing the effectiveness of BVMs.

2 Boundary Value Methods

Suppose, when approximating (1) by means of (2), to fix the first $k_1 \leq k$ values of the discrete solution, $y_0, \ldots, y_{k_1-1}$, and the last $k_2 \equiv k - k_1$ ones, $y_{N-k_2+1}, \ldots, y_N$. In this way, the discrete problem becomes

$$
\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i}, \quad n = k_1, \ldots, N - k_2,
$$

$y_0, \ldots, y_{k_1-1}, y_{N-k_2+1}, \ldots, y_N$, fixed.

That is, the continuous IVP (1) is approximated by means of a discrete BVP. This approach defines a BVM with $(k_1, k_2)$-boundary conditions. Observe that, for $k_1 = k$ and, therefore, $k_2 = 0$, problem (3) becomes an IVP, so that BVMs contain as a proper subclass the usual initial value methods for ODEs based on LFM.

In order to completely exploit all the advantages of this new approach, that is, to derive effective BVMs, we need to generalize the known notions of stability. This is done by introducing the following polynomials [6].

Definition 1. Let $p(z)$ be a polynomial of degree $k$, and let $|z_1| \leq \ldots \leq |z_k|$ be its roots. We say that $p(z)$ is a

- $S_{k_1,k_2}$-polynomial if $|z_{k_1}| < 1 < |z_{k_1+1}|$;
- $N_{k_1,k_2}$-polynomial if $|z_{k_1}| \leq 1 < |z_{k_1+1}|$, with simple zeros of unit modulus.

Observe that for $k_1 = k$ and $k_2 = 0$, one obtains the usual Schur polynomials and von Neumann polynomials, respectively.

Now, let us denote by $\rho(z)$ and $\sigma(z)$ the two polynomials associated with the LMF (2), and, as usual, let $\pi(z, q) = \rho(z) - q\sigma(z)$ denote the stability polynomial. The following definitions are then stated [6].

Definition 2. A BVM with $(k_1,k_2)$-boundary conditions is