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GRID-INDEPENDENT CONSTRUCTION OF MULTISTEP METHODS*

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Abstract

A new polynomial formulation of variable step size linear multistep methods is presented, where each k-step method is characterized by a fixed set of $k-1$ or k parameters. This construction includes all methods of maximal order ($p = k$ for stiff, and $p = k+1$ for nonstiff problems). Supporting time step adaptivity by construction, the new formulation is not based on extending classical fixed step size methods; instead classical methods are obtained as fixed step size restrictions within a unified framework. The methods are implemented in MATLAB, with local error estimation and a wide range of step size controllers. This provides a platform for investigating and comparing different multistep method in realistic operational conditions. Computational experiments show that the new multistep method construction and implementation compares favorably to existing software, although variable order has not yet been included.

Mathematics subject classification: 65L06, 65L05, 65L80
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1. Introduction

Linear multistep methods for solving ordinary differential equations

$$\dot{y} = f(t, y), \qquad y(t_0) = 0, \qquad t \in [t_0, t_f], \tag{1.1}$$

consist of a discretization formula and a pointwise representation of the differential equation,

$$\sum_{i=0}^{k} \alpha_{k-i} x_{n-i} = h \sum_{i=0}^{k} \beta_{k-i} x'_{n-i} \tag{1.2}$$

$$x'_{n-i} = f(t_{n-i}, x_{n-i}). \tag{1.3}$$

Here x_{n-i} approximates $y(t_{n-i})$, k is the step number, and the step size is assumed to be constant, $h = t_n - t_{n-1}$. There is a well established theory for such methods, covering all essential aspects such as order of convergence and stability, [9, 10]. Other classes of problems, such as differential-algebraic equations of the form $F(t, y, \dot{y}) = 0$, can, at least in principle, be treated in a similar manner, by replacing (1.3) by $F(t_{n-i}, x_{n-i}, x'_{n-i}) = 0$. Here, a dot denotes the *time derivative of a function* as in (1.1), while a prime denotes a *sample of the vector*

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field that defines the ODE. This distinction is motivated by the fact that in the computational process, the vector field samples are not located on a single trajectory, whence a dot notation would be misleading in (1.2)–(1.3).

In practice, a multistep method must be adaptive and use *variable step size*. There are several well-known and efficient implementations. Most of these are based on predictor-corrector schemes (Adams-Bashforth, Adams–Moulton) for nonstiff problems, or on backward differentiation formulas (BDF) for stiff problems, e.g. the codes VODE [5] and LSODE [12]. All of these use variable step size as well as variable order.

An established methodology for the construction of variable step size multistep methods, other than extending classical constant step-size formulas case by case, is still missing, [14]. One of the more general approaches is the one by Nordsieck [11], who developed a theory showing the equivalence of k-step methods of higher order to polynomials defined by a vector of dimension k. Although this approach also identifies a set of parameters with each multistep method, these parameters vary with the step sizes. Among other notable extensions we find fixed leading coefficient implementations and divided difference implementations. Some have better stability and computational properties than others, but the theoretical understanding of variable step size multistep methods remains incomplete.

This is a well recognized problem, and different approaches are taken depending on particular preferences. In recent years, there has been an increasing interest in solving this problem in various, demanding special contexts. For example, in [21] the special needs of PDE's are taken into account, when explicit and implicit methods are mixed in a splitting scheme. The approach is to identify an additive decomposition, distinguishing a nonstiff and a stiff part, to be treated with dedicated methods, while incorporating time step adaptivity. The multistep methods are extended to variable step size on a case-by-case basis, deriving step size ratio dependent method coefficients, although the order remains fairly low.

In [8], the special requirements of strong stability preserving schemes are considered. In nonlinear conservation laws in PDE's it is essential that the scheme does not add numerical energy errors; for this reason it is important to maintain interpolation conditions when the step size varies, and methods are again extended to variable step size on a case-by-case basis. This is a tedious approach, and the order is severely restricted. Finally in [6], a general attempt is made to extend multistep methods to variable step size using exponential methods, a technique that, just like splitting methods, has received new attention in recent years.

These examples are by no means exhaustive, but they point to the diversity of difficulties that one encounters when multistep methods are the preferred integration methods and adaptivity is crucial.

The objective of this paper is to develop a new, general methodology for variable step size multistep methods. Our approach addresses several well known problems and opens a new avenue of research in adaptive multistep methods. The main idea is to construct multistep methods that approximate the solution to the ODE by a polynomial, and where specific methods are characterized in terms of a fixed set of interpolation and collocation conditions. This will cover all k-step methods of orders $p = k$ and $p = k + 1$; these methods are of maximal order for stiff and nonstiff problems, respectively.

Our approach is not based on extending classical methods; on the contrary, classical methods are obtained as fixed step size restrictions within a general interpolation representation, which, for each method, can be characterized in terms of a set of *fixed parameters*, even in the presence of varying step size. Further, the approach provides a continuous extension of