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The efficiency of second derivative multistep methods for the numerical integration of stiff systems

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Abstract

A substantial increase in efficiency is achieved by the numerical integration methods which take advantage of the second derivative terms of the differential equation to be solved. The second-derivative of high order accuracy methods are stable, convergent and hence suitable for the numerical integration of stiff systems of initial value problems in ordinary differential equations. The unique feature of the paper is the idea of using all the set of collocation points as additional interpolation points. This desirable feature of the proposed approach actually widens the applicability of the methods, to include many other types of numerical integration methods and has many advantages, including didactic advantages. Furthermore, in this formulation symmetry is retained naturally by the integration identities as equal areas under the various segments of the solution curves over the integration interval. In this way the problem of overlap of solution models usually associated with multistep finite difference methods is overcome. The applications of the second derivative multistep integration methods on a significant class of problems found in the literature produce accurate solutions with low computational cost. Comparison of the efficiency curves obtained seems to be in better agreement with the exact solutions.

Keywords: Block method; Continuous scheme; Second-derivative method; Stiff systems

1. Introduction

We discuss the design principles that lead us to develop efficient methods of high order accuracy with less number of stages and, consequently, reduced computational cost for a given problem, particularly stiff systems of initial value problem in ordinary differential equations given by

$$\frac{dy}{dx} = f(x, y(x)), \qquad y(x_0) = y_0, \quad a \le x \le b, \tag{1.1}$$

where $y : [a, b] \to R^m$ and $f : [a, b] \times R^m \to R^m$ is continuous and differentiable. An equidistant set of points is defined on the integration interval $\Omega : a = x_0 < x_{n+1} < x_{n+2} < \cdots < x_{n+4} = b$, $x_n : x_n = x_0 + nh$,

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$n = 0, 1, \ldots, N-1, h = x_{n+1} - x_n$, $N = (b-a)/h$. The step size h can either be a variable or constant, it is assumed in this paper as a constant on the partition Ω, N is a positive integer. Many of the existing numerical integration methods considered for the numerical solution of (1.1) are of low orders and not suitable for large stiff systems of initial value problems in ordinary differential equations. Some were derived on the basis that the required function evaluations are to be done only at the grid points as well as at the first derivative of the differential equation. This is because we are familiar with solution at the grid-points, which is typically of discrete variable methods (Euler method, Runge–Kutta methods, Picard method, etc.) Henrici [1]. Earlier, some authors considered the introduction of off-grid points in between the familiar grid points (see [2–5]), with the hope of generalizing the two traditional numerical integration methods (Runge–Kutta methods and linear multistep methods) as a consequence of the barrier theorem of Dahlquist [6]. Similarly, many authors had introduced the second derivative terms in their methods for example, see [7–15]. In this report, we consider methods that are suitable for generating the solution of stiff systems of initial value problems at both grid and off-grid points simultaneously within the integration interval. These methods are derived by using all the set of collocation points as additional interpolation points in the numerical schemes.

Like traditional Runge–Kutta methods, second-derivative block multistep collocation integrators admit the addition of extra stages, which introduce extra degrees of freedom that can be used to increase the order of accuracy or modify the region of absolute stability. Second-derivative block multistep integrators permit the evaluation of higher derivatives of the unknown in order to decrease the memory footprint and communication overhead. Block methods generally, preserve the traditional advantages of one-step methods (Runge–Kutta methods, Taylor series method, Picard method etc.) of being self-starting and of permitting easy change of step length during integration (see Lambert [16]). Their advantage over Runge–Kutta methods lies in the fact that they are less expensive in terms of number of function evaluations per step. In this paper, we derive a new class of second-derivative block multistep methods with high order of accuracy, very low error constants, large regions of absolute stability, which behave essentially like one-step methods and converge rapidly to the required solution.

Definition 1.1. A numerical method is said to be A-stable if its region of absolute stability contains the whole of the complex left hand-half plane $\mathrm{Re}\, h\lambda < 0$ (see, Dahlquist [6]). Alternatively, a numerical method is called A-stable if all the solution of (1.1) tend to zero as $n \to \infty$, when the method is applied with fixed positive h to any differential equation of the form $dy/dx = \lambda y$, where λ is a complex constant with negative real part.

Definition 1.2. A numerical method is said to be $A(\alpha)$-stable, $\alpha \in (0, \pi/2)$ if its region of absolute stability contains the infinite wedge $W_\alpha = \{\lambda h : -\alpha < \pi - \arg(\lambda h) < \alpha\}$.

Definition 1.3. A solution $y(x)$ of (1.1) is said to be stable if given any $\epsilon > 0$ there is $\delta > 0$ such that any other solution $\hat{y}(x)$ of (1.1) which satisfies

$$\left|y(a) - \hat{y}(a)\right| \leq \delta \tag{1.2a}$$

also satisfies

$$\left|y(x) - \hat{y}(x)\right| \leq \epsilon \tag{1.2b}$$

for all $x > a$.

The solution $y(x)$ is asymptotically stable if in addition to (1.2b) $\left|y(x) - \hat{y}(x)\right| \to 0$ as $x \to \infty$.

Definition 1.4. Let Y_m and F_m be defined by $Y_m = (y_n, y_{n+1}, \ldots, y_{n+r-1})^T$, $F_m = (f_n, f_{n+1}, \ldots, f_{n+r-1})^T$. Then a general k-block, r-point block method is a matrix of finite difference equation of the form

$$Y_m = \sum_{j=1}^{k} A_i Y_{m-i} + h \sum_{i=0}^{k} B_i F_{m-i}, \tag{1.3}$$

where all the A_i's and B_i's are properly chosen $r \times r$ matrix coefficients and $m = 0, 1, 2, \ldots$, represents the block number, $n = mr$ is the first step number of the mth block and r is the proposed block size [17].