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A family of three-stage third order AMF-W-methods for the time integration of advection diffusion reaction PDEs.

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ABSTRACT

In this paper new three-stage W-methods for the time integration of semi-discretized advection diffusion reaction Partial Differential Equations (PDEs) are provided. In particular, two three-parametric families of W-methods of order three are obtained under a realistic assumption regarding the commutator of the exact Jacobian and the approximation of the Jacobian which defines the corresponding W-method. Specific methods are selected by minimizing error coefficients, enlarging stability regions or increasing monotonicity factors, and embedded methods of order two for an adaptive time integration are derived by further assuming first order approximations to the Jacobian. The relevance of the newly proposed methods in connection with the Approximate Matrix Factorization technique is discussed and numerical illustration on practical PDE problems revealing that the new methods are good competitors over existing integrators in the literature is provided.

1. Introduction

We consider numerical methods for the time integration of a family of initial value problems (IVPs) in ordinary differential equations (ODEs)

$$y_h'(t) = f_h(t, y_h(t)), \quad y_h(0) = u_{0,h}^*, \quad 0 \le t \le t^*, \quad y_h, f_h \in \mathbb{R}^{m(h)}, \quad h \to 0^+, \tag{1}$$

coming from the spatial semi-discretization -by means of the *method of lines* (MOL)- of an $l-$dimensional advection diffusion reaction problem in time dependent partial differential equations (PDEs) with prescribed boundary conditions and an initial condition. Here h denotes a small positive parameter associated with the spatial resolution and usually $l = 2, 3, \ldots$ We denote by $u_h(t)$ the solution of the PDE problem confined to the spatial grid (or to the related h-space). It will be tacitly assumed that the PDE problem admits a smooth solution $u(x, t)$ in the sense that continuous partial derivatives in all variables up to some order p exist and are continuous and uniformly bounded on $\Omega \times [0, t^*]$ and that $u(x, t)$ is continuous on $\bar{\Omega} \times [0, t^*]$ ($\bar{\Omega} = \Omega \bigcup \partial\Omega$). It is also assumed that the spatial discretization errors

$$\sigma_h(t) := u_h'(t) - f_h(t, u_h(t))$$

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satisfy in the norm considered

$$\|\sigma_h(t)\| \le C\,h^r, \quad C \ge 0,\ r > 0, \quad 0 \le t \le t^*, \quad h \to 0^+.$$

Regarding the right-hand side f_h in (1), some natural splitting (directional or not)

$$f_h(t,y) = \sum_{j=0}^{d} f_{j,h}(t,y) \tag{2}$$

is considered, in such a way that it also provides a natural splitting for the Jacobian matrix at the current point (t_n, y_n)

$$J_h = \sum_{j=0}^{d} J_{j,h}, \quad J_h := \frac{\partial f_h(t_n,y_n)}{\partial y}, \quad J_{j,h} := \frac{\partial f_{j,h}(t_n,y_n)}{\partial y}. \tag{3}$$

The ODE system (1) is usually stiff and implicit integration methods must be applied. However, due to the high dimension of the problem at hand, special approaches for the solution of the algebraic equations are necessary. One possibility is the use of Krylov techniques. Krylov methods have been applied successfully in the codes VODPK [3], ROWMAP [27] and EXP4 [13]. Another strategy is to make use of the special splitting (2) and to exploit the special structure of the matrices $J_{j,h}$. This leads to the so-called *Approximate Matrix Factorization* (AMF). For a survey regarding AMF methods see [14]. Numerical comparisons of AMF versus Krylov in Beck et al. [1] show the efficiency of AMF especially for low accuracy solutions.

In this paper we will consider the application of AMF in W-methods. W-methods belong to the class of linearly-implicit Runge–Kutta methods, which avoid the solution of non-linear algebraic equations arising in implicit Runge–Kutta methods by incorporating an approximation of the Jacobian directly into the formulation of the method. They can be interpreted as performing only one step in the Newton iteration. The most popular methods of this class are the so-called ROW-methods, see [16,20], which are very efficient for the solution of stiff systems for moderate tolerances [12]. ROW-methods use the exact Jacobian $f_y(y_n)$ and are usually considered for autonomous problems. Non-autonomous ROW-methods can be formulated by using in addition $f_t(t_n, y_n)$, [12]. The advantage of ROW-methods is a relatively small number of order conditions allowing the construction of higher order methods with small numbers of stages. To avoid exact Jacobians, Steihaug and Wolfbrandt [25] consider an arbitrary matrix T instead of the exact Jacobian. This reduces the costs but leads to an increase of the number of order conditions and makes the construction of higher order methods rather difficult. A compromise is the use of an approximation $T = f_y + \mathcal{O}(\tau)$ of the Jacobian. For an overview about linearly-implicit Runge–Kutta methods and the order conditions for the different cases see [26].

In the AMF-context the use of exact Jacobians is not possible. For this reason, we will therefore consider AMF-W-methods. In detail we study 3-stage methods. By assuming a special relation between the exact Jacobian and the approximation T we will reduce the number of order conditions. This allows to construct a family of 3-stage methods of order 3 for special problems. We show that this relation is satisfied for the problem (2) if the splitting matrices $J_{j,\,h}$ in (3) commute pairwise, which often holds for MOL problems. In numerical experiments the advantage of the new methods over existing W-methods is shown.

The reminder of this paper is organized as follows. Section 2 considers the order conditions of W-methods and formulates a special relation reducing the number of order conditions for order 3, allowing the construction of a family of 3-stage methods of order 3. In Section 3 free parameters of the methods are determined with respect to accuracy, linear stability and monotonicity. In Section 4 embedded methods are constructed allowing an efficient error estimation and step size control. In Section 5 the constructed methods are applied with AMF for the solution of MOL problems (2). Here, both exact and inexact AMF are discussed. Numerical tests on non-trivial MOL problems are presented in Section 6. Here we compare the new methods with AMF implementations of various W-methods from literature and with VODPK [3].

2. A family of 3-stage W-methods

We initially assume that the ODE system is autonomous

$$y'(t) = f(y(t)), \quad y(0) = y_0, \quad t \in [0, t^*]. \tag{4}$$

For the integration of (4) we deal with an s-stage W-method given by the formula

$$(I - \theta\tau T)K_i = \tau f\left(y_n + \sum_{j=1}^{i-1} a_{ij}K_j\right) + \sum_{j=1}^{i-1} \ell_{ij}K_j, \quad i = 1, 2, \ldots, s,$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i K_i, \tag{5}$$

where T is an arbitrary matrix. The matrix T is expected to be a rough approximation to $f'(y_n) = \dfrac{\partial f}{\partial y}(y_n)$, but by the moment we assume that it is arbitrary. By defining the super-vectors $K^T = (K_1^T, \ldots, K_s^T)$ and $F(K)^T = (f(K_1)^T, \ldots, f(K_s)^T)$, the strictly lower