PAMM · Proc. Appl. Math. Mech. **11**, 757 – 758 (2011) / **DOI** 10.1002/pamm.201110368

Rational multistep methods via modified φ_j - functions

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A class of rational multistep methods, in particular of Adams-Padé type, is designed via rational modification of the φ_j - functions inherent in exponential integrators. Convergence properties and implementation issues are discussed.

1 Exponential and rational Adams schemes

Exponential integrators (see [5]) are well-suited for the numerical solution of stiff systems

$$u'(t) = A\,u(t) + g(t, u(t)), \quad u(0) = u_0. \tag{1}$$

Here we assume that $A \in \mathbf{R}^{d\times d}$ is negative semidefinite ($A \leq 0$), and $g(t,u)$ is Lipschitz continuous in a neighborhood of the solution $u(t) \in \mathbf{R}^d$.

1.1 φ_j - functions and their approximation

First we consider the so-called ‘φ_j - functions’, which are are the basic building blocks in exponential integrators. They are defined as $\varphi_j(Z) = \dfrac{1}{(j-1)!}\displaystyle\int_0^1 \mathrm{e}^{(1-\theta)Z}\,\theta^{\,j-1}\,\mathrm{d}\theta,\ j \geq 1$, and satisfy the recursion (see [5])

$$\varphi_0(Z) = \mathrm{e}^Z, \qquad \varphi_j(Z) = Z^{-1}\big(\varphi_{j-1}(Z) - \frac{1}{(j-1)!}\,I\big), \quad j \geq 1. \tag{2}$$

Here, $Z \in \mathbf{R}^{d\times d}$ is to be identified with hA, where h is the step size used in the exponential method.

Replacing $\varphi_0(Z) = \mathrm{e}^Z$ by some (typically rational) well-defined approximation $\tilde\varphi_0(Z) = R(Z)$ in starting the recursion (2), natural lower order approximations $\tilde\varphi_j(Z) \approx \varphi_j(Z)$ are obtained: We have

$$(\tilde\varphi_j - \varphi_j)(Z) = Z^{-j}(R(Z) - \mathrm{e}^Z), \quad j \geq 0. \tag{3}$$

Thus, the $\tilde\varphi_j(Z)$ are well-defined for $j \leq q$ and the asymptotic order of approximation is $q-j$, provided $R(Z)$ approximates e^Z with order q, i.e., if $R(z) - \mathrm{e}^z = \mathcal{O}(|z|^{q+1})$ for $|z| \to 0$.

For the analysis of rational modifications of exponential integrators, uniform stability of the error $(\tilde\varphi_j - \varphi_j)(Z)$ is required. Universal bounds valid for arbitrary $Z \leq 0$ can be obtained for the case of A-stable Padé (μ,ν) - approximations to e^Z, To this end we generalize the classical Perron representation for the Padé error $R(z) - \mathrm{e}^z$ (valid for arbitrary $\mu,\nu \geq 0$, see [3, p. 241]) in the following way: If $Z \in \mathbf{C}^{d\times d}$ and $R(Z) = \frac{P(Z)}{Q(Z)}$ is well-defined, i.e., if $Q(Z)$ is invertible, then [1]

$$(\tilde\varphi_j - \varphi_j)(Z) = \frac{(-1)^{\nu+1-\ell}}{(\mu+\nu)!}\,Q(Z)^{-1}\,Z^{\,\mu+\nu+1-j-\ell}\int_0^1 K_\ell(\theta)\,\mathrm{e}^{\theta Z}\,\mathrm{d}\theta, \tag{4}$$

for $0 \leq \ell \leq \min\{\mu,\nu\}$, with kernel polynomial $K_\ell(\theta) = \frac{\mathrm{d}^\ell}{\mathrm{d}\theta^\ell}\big((1-\theta)^\mu\,\theta^\nu\big)$, see [1]. For the case of A-stable approximations ($\nu-2 \leq \mu \leq \nu$), $\|Q^{-1}(Z)\|$ is uniformly bounded. With an appropriate choice $\ell = \ell(j)$ in (4), application of the maximum principle yields uniform estimates with universal constants C_j (see [1]),

$$\|(\tilde\varphi_j - \varphi_j)(Z)\| \leq C_j \quad \text{for} \quad 0 \leq j \leq q+1, \tag{5}$$

where $q = \mu + \nu$ is the asymptotic order of the Padé approximation error.

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[1] Here, $P(0) = Q(0) = 1$ is assumed.

1.2 Coefficient matrices for exponential and rational Adams schemes. Adams-Padé methods.

Exponential Adams schemes are particular class of exponential integrators (see [2,5,6]). On a grid $\{t_n = nh,\ n = 0,1,2,\ldots\}$ and given p starting values $u_0,\ldots,u_{p-1}$, the basic version of a p-step exponential Adams method admits the Newton-type representation (a generalization of the analogous formulation of classical Adams-Bashforth schemes),

$$u_{n+1} = \mathrm{e}^Z u_n + h \sum_{k=0}^{p-1} \gamma_k(Z)(\nabla^k G_n)_n, \tag{6}$$

where $G_n(t) \in \mathbf{P}_{p-1}$ interpolates $g(t_{n-p+1}, u_{n-p+1}),\ldots,g(t_n,u_n)$, and $\nabla^k(\cdot)_n$ denotes the k-th backward difference over $t_n,\ldots,t_{n-k}$, defined in the usual recursive way. Convergence results for (6) are given in [6].

The coefficient matrices $\gamma_k(Z)$ in (6) are certain linear combinations of the $\varphi_j(Z)$ and satisfy the recursion (see [2])

$$\gamma_0(Z) = Z^{-1}(\mathrm{e}^Z - I) = \varphi_1(Z), \qquad \gamma_k(Z) = Z^{-1}\Big(\sum_{\ell=0}^{k-1} \frac{\gamma_\ell(Z)}{k-\ell} - I \Big), \quad k \geq 1. \tag{7}$$

Analogously as in & 1.1, replacing e^Z by $R(Z)$ in starting the recursion (7) gives rise to rational versions $\tilde\gamma_k(Z) \approx \gamma_k(Z)$, which are linear combinations of the $\tilde\varphi_j(Z)$. Using an A-stable Padé approximation $R(Z) = \frac{P(Z)}{Q(Z)}$ we end up with a p-step *Adams-Padé method*,

$$\tilde u_{n+1} = R(Z)\tilde u_n + h \sum_{k=0}^{p-1} \tilde\gamma_k(Z)(\nabla^k \tilde G_n)_n, \tag{8}$$

which is a rational version of (6). The coefficients can be written in the form $\tilde\gamma_k(Z) = \frac{P_k(Z)}{Q(Z)}$ with certain polynomials P_k.

2 Convergence and implementation of Adams-Padé methods

2.1 An a priori error bound

Rational multistep schemes equivalent or closely related to (8) were constructed in an *ad hoc* manner by several authors, cf. e.g. [7], but a convergence analysis for stiff problems was not given so far. Our interpretation as modified exponential schemes enables a precise convergence theory. The following result – compared with [6] – shows that the convergence order of an Adams-Padé scheme is the same as for the corresponding exponential Adams scheme. This result is formulated for subdiagonal Padé schemes; diagonal Padé versions may also be used.

Theorem 2.1 *Choose $R(z) = \text{Padé}\,(p-2,p-1)\ p \geq 3$, or $R(z) = \text{Padé}\,(p-1,p)$, $p \geq 2$. Let $f(t) = g(t,u(t)) \in C^p([0,T])$. Then, for $\|\tilde u_n - u(t_n)\| \leq C_0\, h^p$, $n = 0\ldots p-1$, the following error bound holds uniformly for $0 \leq t_n \leq T$, with constants C_1, C_2 depending only on the length T of the integration interval:*

$$\|\tilde u_n - u(t_n)\| \leq C_1\, h^p + C_2\, h^p \sup_{0\leq t\leq t_n} (\,\|u^{(p+1)}(t)\| + \|f^{(p)}(t)\|\,). \tag{9}$$

Proof: See [1]. Basically, the proof is organized in a similar way as in [6] for the exponential version; in addition, we make use of (5) and apply a nontrivial reformulation of the scheme (8) in terms of derivatives of the interpolant $\tilde G_n(t)$.

2.2 Discussion

For numerical evidence, see [1]. In contrast to the $\gamma_k(Z)$, for which a careful implementation is required, the coefficients of the $\tilde\gamma_k(Z)$ are easily computed a priori. In typical PDE applications a direct implementation of (8) would involve the solution of a large, highly ill-conditioned system with coefficient matrix $Q(Z)$. Therefore, spectral methods (in special cases), or (in general) Krylov subspace techniques are the method of choice, similarly as in e.g. [4] for the exponential case. In the Krylov context, due to the above results it appears natural to directly approximate the action of $R(Z)$ (or $Q^{-1}(Z)$), instead of e^Z, on the projected level. Moreover, special Krylov techniques have been suggested for rational matrix functions. Pros and cons of such rational Krylov versions compared to the exponential case are subject to further investigation.

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