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Local and global error estimation and control within explicit two-step peer triples

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ABSTRACT

This paper elaborates a global error estimation and control mechanism in explicit two-step peer methods. These recently designed methods exhibit their high efficiency even in comparison to the best explicit Runge–Kutta pairs. More precisely, we form here triples of the so-called superconvergent explicit peer schemes and show that they are cheap and able to achieve preassigned accuracy conditions in automatic mode. For comparison, we present also numerical data derived by built-in explicit Matlab ODE solvers implemented with only local error control. Especially, we point out that a scaled global error is computed and regulated in this paper in contrast to the earlier published results where the absolute values of the global error have been utilized.

1. Introduction

Numerical schemes for ordinary differential equations (ODEs) of the form

$$x'(t) = g\big(t, x(t)\big), \quad t \in [t_0, t_{end}], \qquad x(t_0) = x^0, \tag{1}$$

where $x(t) \in \mathbb{R}^m$ and $g : D \subset \mathbb{R}^{m+1} \to \mathbb{R}^m$ is a sufficiently smooth function, constitute an important topic in computational mathematics (see [1–9]). This is because problem (1) is not only widely used in simulation and modeling in various areas of science and technology, but it also arises as a subproblem in a variety of more complex computational techniques such as the method of lines or the extended Kalman filtering algorithm [10,11]. ODE (1) assumes that its unique solution $x(t)$ exists on the interval $[t_0, t_{end}]$.

When solving numerically ODE (1) we take care of two aspects of the integration, namely, of its speed and its accuracy. These two features of adaptive ODE solvers may not be equally important in this or that situation and demand different numerical algorithms to be implemented. Therefore, a huge variety of numerical schemes have been developed for nonstiff, stiff, reversible, Hamiltonian and large-scale differential equations in the last century. Many of them are nicely presented in the above-cited literature. However, the accuracy of numerical solution depends not only on the integration method itself but also on the grid generated in the course of computation. This implies that two tasks related to the automatic error control

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have to be solved in order to provide practitioners with a robust and reliable computational technology for efficient treating of ODEs of the form (1). They are

1. accurate global error evaluation method;
2. automatic stepsize selection aiming to ensure the required accuracy of computation.

The first task has been on the list for a long time and resulted in high quality global error estimation techniques for many classes of numerical schemes, as presented, for instance, in [12–39]. The second task is less popular and more difficult for effective solution because of the need for multiple integration of ODE (1) over the integration interval $[t_0, t_{end}]$. A detailed discussion of this difficulty can be found in [21,36,37]. However, modern results show that the global error estimation and control can be performed within a single integration (see [25,39]). Unfortunately, this opportunity follows from the property of double quasi-consistency, which is a rare option nowadays and has been discovered only in explicit parallel two-step peer methods for the moment (see further explanation in [23,24]). Nevertheless, many researchers have contributed to the field of automatic accuracy control and succeeded in developing efficient algorithms for various classes of numerical methods (see, for example, [13–15,18,20,23–29,32,35,37,39]).

Recently, Weiner et al. [40–43] presented a new family of numerical schemes that are not only efficient for treating nonstiff, stiff and MOL-systems of differential equations, but also competitive to the best Runge–Kutta formulas. In addition, the mentioned methods possess an evident applied potential, as shown, for instance, in [44,45]. The main feature of all those schemes is that they produce a set of numerical solutions which share the same stability and accuracy properties in each step. The present paper also contributes to the realm of peer numerical schemes and develops efficient local and global error estimation and automatic error control algorithms within explicit two-step peer triples, namely, in the family of superconvergent explicit methods discovered in [43]. We point out that utilization of triples of numerical schemes is not new and has been implemented effectively in Runge–Kutta formulas in [17,46]. Here, we extend that idea to the class of explicit peer schemes.

2. Explicit two-step peer methods: order conditions, stability and quasi-consistency

Weiner et al. [42] have presented a family of explicit two-step peer numerical techniques that being applied to ODE (1) read

$$x_{ki} = \sum_{j=1}^{s} b_{ij}(k)x_{k-1,j} + \tau_k \sum_{j=1}^{s} a_{ij}(k)g(t_{k-1,j}, x_{k-1,j}) + \tau_k \sum_{j=1}^{i-1} r_{ij}(k)g(t_{kj}, x_{kj}), \quad k = 1, 2, \ldots, K-1, \tag{2}$$

where $t_{ki} := t_k + c_i\tau_k$, $i = 1, 2, \ldots, s$. Notice that, in general, the coefficients $a_{ij}(k)$, $b_{ij}(k)$ and $r_{ij}(k)$ may change in the course of numerical integration. More precisely, they may depend on the current stepsize ratio $\theta_k := \tau_k/\tau_{k-1}$. The extra nodes t_{ki} of the variable mesh

$$w_\tau = \{t_{k+1} = t_k + \tau_k,\ k = 0, 1, \ldots, K-1,\ t_K = t_{end}\}$$

with the diameter $\tau = \max_{0\le k\le K-1}\{\tau_k\}$ introduced in the integration interval $[t_0, t_{end}]$ are fixed by the constants c_i. Without loss of generality, we consider further that these constants are distinct and ordered as follows: $-1 \le c_1 < c_2 < \cdots < c_s = 1$. It is also worthwhile to mention here that numerical schemes defined by formula (2) demand a starting procedure to calculate the starting numerical solution x_{0i}, $i = 1, 2, \ldots, s$, and its accuracy may influence the accuracy of the output numerical solution derived by the peer method.

Method (2) can easily be represented in the matrix form as follows:

$$X_k = (B(k) \otimes I_m)X_{k-1} + \tau_k(A(k) \otimes I_m)g(T_{k-1}, X_{k-1}) + \tau_k(R(k) \otimes I_m)g(T_k, X_k) \tag{3}$$

where I_m is the identity matrix of dimension m and $\otimes$ denotes the Kronecker tensor product (see, for example, [47] for the definition and properties of this product). Here, we have also utilized the following notation:

$$T_k := (t_{ki})_{i=1}^{s}, \qquad X_k := (x_{ki})_{i=1}^{s}, \qquad g(T_k, X_k) := g(t_{ki}, x_{ki})_{i=1}^{s}, \qquad A(k) := \big(a_{ij}(k)\big)_{i,j=1}^{s},$$
$$B(k) := \big(b_{ij}(k)\big)_{i,j=1}^{s}, \qquad R(k) := \big(r_{ij}(k)\big)_{i,j=1}^{s}.$$

Since only explicit methods are considered in this paper the matrix $R(k)$ is strictly lower triangular in formula (3). The described methods are further referred to as variable-stepsize s-stage *explicit two-step peer* methods or, briefly, ETSP-methods.

To investigate the approximation property of ETSP-methods (2) (or (3) in the matrix form) we introduce the notion of defect at first.

Definition 1. The vector-function $L(T_k, x(t), \tau_k) := \big(L_i(t_{ki}, x(t), \tau_k)\big)_{i=1}^{s}$ with the entries satisfying the formula

$$L_i(t_{ki}, x(t), \tau_k) := x(t_{ki}) - \sum_{j=1}^{s} b_{ij}(k)x(t_{k-1,j}) - \tau_k \sum_{j=1}^{s} a_{ij}(k)g\big(t_{k-1,j}, x(t_{k-1,j})\big) - \tau_k \sum_{j=1}^{i-1} r_{ij}(k)g\big(t_{kj}, x(t_{kj})\big) \tag{4}$$

is referred to as the defect of the ETSP-method (2).