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Explicit advanced step-point (EAS) methods and the EAS2 multistep scheme for the solution of non-stiff initial value problems

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ABSTRACT

In this work, we comprehensively examine, for the first time in a paper, the EAS2 methods, which are part of the explicit advanced step-point (EAS) family of methods. The EAS formulae comprise three distinct schemes: EAS1, EAS2 and EAS3. In this paper, we consider the EAS2 methods, which are meticulously studied and assessed and their superior regions of absolute stability are presented. Crucially, the computational efficiency of EAS2 is thoroughly examined and comparative numerical results are presented with the use of a variable step, variable order EAS2 code. The efficiency of EAS2 is measured against the established and powerful Adams formulae, as the latter were implemented in the Shampine and Gordon code. The extensive numerical results provide good evidence that EAS2 is competitive (i.e. faster and more accurate on a majority of test problems) with the well-established Adams methods for the numerical solution of non-stiff initial value problems.

1. Introduction

This is part of a series of papers about the EAS schemes: EAS1, EAS2 and EAS3. In [1] we thoroughly investigate the theoretical considerations, characteristics and requirements of explicit advanced step-point (EAS) methods and we examine in detail the EAS1 methods for mildly stiff initial value problems (IVPs). It was expected that [1] would be published prior to the present article; however this appears not to have been materialised. The purpose of this work is to comprehensively study and assess, for the very first time, the EAS2 methods. We will examine in detail the EAS2 choice of coefficients and regions of absolute stability. Most importantly, we will present extensive comparative results where we will examine the EAS2 computational efficiency against the efficiency of Adams formulae (Shampine and Gordon code) for the solution of non-stiff IVPs.

Before the present work and [1], most of the first part of the work on EAS methods and the term "Explicit Advanced Step-point" (EAS) methods had appeared in [2]. Prior to the completion of [2], two short and preliminary works appeared [3,4] and in 2004 paper [5] was published. Interestingly, despite the fact that much work had been done on the EAS methods, until the publication of the present article, effectively only the general form of the EAS schemes was known. With this and subsequent papers, we aim to rectify a major gap in the current literature on the EAS schemes. Although there were reasons beyond the author's control that had postponed the publication of the present research, naturally, the author assumes full responsibility for any delay. The second part of the work on EAS methods started with their trigonometric and exponential fitting for $k = 1$ [6]. Following the same methodology as in [6], the second part of the work continued with the trigonometric fitting to the Adams predictor–corrector methods (also known as Adams–Bashforth–Moulton methods) [7–13]. The particular type of trigonometric fitting that was performed on the Adams methods was "a first" in the literature. As we will see in the following sections the original Adams methods (not the trigonometrically fitted versions) are directly linked to the present research.

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Readers who may be interested in the implicit advanced step-point (IAS) methods are referred to [14–19], as this paper deals solely with explicit advanced step-point (EAS) methods.

This work is organised as follows: In Section 2, we give the EAS methods general form and their local truncation error; in Section 3, we briefly provide our theoretical accuracy and stability requirements; in Section 4, we examine in some detail the EAS2 scheme, where we present the choice of coefficients and 12 graphs of the EAS2 regions of absolute stability; in Section 5, we briefly consider the EAS2 implementation and the general non-stiff case; in Section 6, we present our extensive numerical comparative results and in Section 7 we draw some conclusions for this work.

2. The EAS methods formulae

In [20], Shampine and Gordon presented a very successful implementations of the Adams methods based on the very well-known Adams–Bashforth and Adams–Moulton formulae, used as a Predictor–Corrector (P–C) pair. For the sake of completeness the P–C pair has the form:

$$\begin{aligned} \bar{y}_{n+1} &= y_n + h\sum_{i=1}^{k}\gamma_{i-1}\nabla^{i-1}f_n, \\ y_{n+1} &= \bar{y}_{n+1} + h\gamma_k\nabla^k\bar{f}_{n+1}, \end{aligned} \tag{1}$$

where $\bar{f}_{n+1} = f(x_{n+1}, \bar{y}_{n+1})$.

Explicit advanced step-point (EAS) methods belong to a wider class of numerical multistep methods and in order to obtain their general form we first need to assign specific values to certain coefficients of an even more general form (more details appear in [1]). Finally, we can express the EAS methods in backward difference form as follows:

$$\begin{aligned} y^{(p)}_{n+k} &= y_{n+k-1} + h\sum_{i=0}^{k-1}\gamma_i\nabla^i f_{n+k-1}, \\ y^{(p)}_{n+k+1} &= y^{(p)}_{n+k} + h\sum_{i=0}^{k}\gamma_i\nabla^i f^{(p)}_{n+k} - \gamma_k ha\nabla^k f^{(p)}_{n+k}, \\ y^{(c)}_{n+k} &= y_{n+k-1} + h\sum_{i=0}^{k-1}\gamma_i\nabla^i f_{n+k-1} + \gamma_k h\nabla^k f^{(p)}_{n+k} + h\bar{a}\nabla^{k+1}f^{(p)}_{n+k+1}, \end{aligned} \tag{2}$$

where a and $\bar{a}$ are free coefficients.

The EAS corrector $y^{(c)}_{n+k}$ from (2) has a local truncation error (LTE) given by

$$\mathrm{LTE} \equiv [\bar{a}(1+a) + \gamma_k - (k+1)\bar{a}]\gamma_k h^{k+2}\frac{\vartheta f}{\vartheta y}y^{(k+1)}(x_n) - (\bar{a} - \gamma^*_{k+1})h^{k+2}y^{(k+2)}(x_n) + 0(h^{k+3}), \tag{3}$$

where $\gamma^*_{k+1} = \gamma_{k+1} - \gamma_k$, is the Adams–Moulton coefficient. For a proof of (3) see [1].

We notice that with the EAS predictor–corrector approach we have two free parameters at our disposal, namely a and $(\bar{a})$. We can also see that the Shampine and Gordon code [20] corresponds to $a = \bar{a} = 0$. When a predictor–corrector scheme is applied in a PECE (prediction–evaluation–correction–evaluation) mode, as it is basically the case with EAS, the LTE of the corrector may be "polluted" by that of the predictors. The level of this "pollution" can be shown by the LTE of the corrector (3). If we express (3) in terms of elementary differentials [1] we can **rewrite the LTE (3) in terms of elementary differentials:**

$$\left.\begin{aligned} \mathrm{LTE} &= (B_1 + B_2)h^{k+2}(\mathit{elementarydifferential})_1 + B_2h^{k+2}(\mathit{elementarydifferential})_2 \\ &= E_1h^{k+2}(\mathit{elementarydifferential})_1 + E_2h^{k+2}(\mathit{elementarydifferential})_2, \end{aligned}\right\} \tag{4}$$

where $(\mathit{elementary\ differential})_i$, $i = 1$ or 2, are subsets of all elementary differentials of order $(k+2)$ and B_1, B_2 depend on the free parameters a and $\bar{a}$. Instead of (3) we will be using (4), which is too complicated to estimate in a reliable and economical way. Hence, we adopted the well-known Fehlberg embedding [21] approach where we estimate and control the error in a solution which is asymptotically less accurate than the one we actually accept. To do this we use an **embedded formula** of the form,

$$\breve{y}_{n+k} = y_{n+k-1} + h\sum_{i=0}^{k-1}\gamma_i\nabla^i f_{n+k-1} + h(\tilde{a}_2 + (k+1)\tilde{a}_1)\nabla^k f^{(p)}_{n+k} + h\tilde{a}_1\nabla^{k+1}f^{(p)}_{n+k+1}, \tag{5}$$

where $\tilde{a}_1$ and $\tilde{a}_2$ are free parameters and (5) is of order k. Now we give the local error of EAS methods [1]:

$$\text{Local Error} \approx y^{(c)}_{n+k} - \breve{y}_{n+k} = h(\gamma_k - \tilde{a}_2 - (k+1)\tilde{a}_1)\nabla^k f^{(p)}_{n+k} + h(\bar{a} - \tilde{a}_1)\nabla^{k+1}f^{(p)}_{n+k+1}. \tag{6}$$

3. Accuracy and stability requirements for the EAS methods

The choice of a, $\bar{a}$ and $\tilde{a}_1$, $\tilde{a}_2$ will directly influence the stability and accuracy of our methods, since these same parameters form the coefficients of the LTE and the local error. However, our research has shown that the simultaneous requirements of