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A POSTERIORI ERROR ESTIMATES FOR THE BDF2 METHOD FOR PARABOLIC EQUATIONS

GEORGIOS AKRIVIS*‡ AND PANAGIOTIS CHATZIPANTELIDIS†

Abstract. We derive optimal order, residual-based a posteriori error estimates for time discretizations by the two–step BDF method for linear parabolic equations. Appropriate reconstructions of the approximate solution play a key role in the analysis. To utilize the BDF method we employ one step by both the trapezoidal method or the backward Euler scheme. Our a posteriori error estimates are of optimal order for the former choice and suboptimal for the latter. Simple numerical experiments illustrate this behaviour.

Key words. Parabolic equations, BDF2 method, residual, BDF2 reconstruction, a posteriori error analysis.

AMS subject classifications. Primary 65M15, 65M50; Secondary 65L70

1. Introduction. In this paper we establish optimal order a posteriori error estimates for time discretizations by the two–step BDF method (BDF2) for linear parabolic partial differential equations (p.d.e's).

We consider initial value problems of the form: Find $u : [0, T] \to D(A)$ satisfying

$$\begin{cases} u'(t) + Au(t) = f(t), \quad 0 \le t \le T, \\ u(0) = u^0, \end{cases} \tag{1.1}$$

with $A : D(A) \to H$ a positive definite, selfadjoint, linear operator on a Hilbert space $(H, \langle \cdot, \cdot \rangle)$ with domain $D(A)$ dense in H, forcing term $f : [0, T] \to H$, and initial value $u^0 \in H$. We denote by $|\cdot|$ the norm of H.

Let $N \in \mathbb{N}, N \ge 2, k := T/N$ be the constant time step, $t^n := nk, n = 0, \dots, N$, be a uniform partition of $[0, T]$, and $J_n := (t^{n-1}, t^n]$. We define nodal approximations $U^m \in D(A)$ to the values $u^m := u(t^m)$ of the solution u of (1.1) as follows: We set $U^0 := u^0$, perform one step with the trapezoidal method to get U^1 and then apply the BDF2 method to obtain $U^2, \dots, U^N$, i.e., the approximations $U^1, \dots, U^N$ are recursively defined by

$$\begin{cases} \dfrac{k}{2}\bar\partial^2 U^n + \bar\partial U^n + AU^n = f^n, \quad n = 2, \dots, N, \\ \bar\partial U^1 + AU^{1/2} = f^{1/2}, \\ U^0 = u^0, \end{cases} \tag{1.2}$$

with $f^m := f(t^m)$. Here we have used the notation

$$\bar\partial v^n := \frac{1}{k}(v^n - v^{n-1}),\ \bar\partial^2 v^n := \bar\partial\bar\partial v^n = \frac{1}{k^2}(v^n - 2v^{n-1} + v^{n-2}),\ v^{n-\frac12} := \frac{v^{n-1} + v^n}{2},$$

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for given $v^0,\dots,v^N$.

Our goal is to derive optimal order residual based a posteriori error estimates. To define the residual, we need to introduce an approximation $U(t)$ to $u(t)$, for all $t\in[0,T]$. Since the error u^m-U^m at the nodes is of second order, a natural choice for a second order BDF2 approximation $U:[0,T]\to D(A)$ to u is the piecewise linear interpolant at the nodal values U^m,

$$U(t)=U^n+(t-t^n)\bar\partial U^n,\quad t\in J_n,\quad n=1,\dots,N. \tag{1.3}$$

Although $U(t)$ is a second order approximation to $u(t)$, its *residual* $R(t)\in H$,

$$R(t):=U'(t)+AU(t)-f(t),\quad t\in J_n, \tag{1.4}$$

i.e., the amount by which the approximate solution U misses being an exact solution of the differential equation in (1.1), is of first order; see §2. The error e, $e:=u-U$, satisfies the error equation $e'+Ae=-R$. Since $R(t)$ is of suboptimal order, applying energy techniques to this error equation leads inevitably to a posteriori estimators of suboptimal order. To recover the optimal order, we shall reconstruct the approximate solution U in an appropriate way.

Next, we modify U to construct appropriate reconstructions $\hat U$. As we will see later on, several continuous approximations $\hat U$ are appropriate for our purposes, in the sense that they lead to optimal order residuals. To motivate the construction of $\hat U$, let us note that U satisfies the relation

$$U'(t)+AU(t)=(t-t^{n-\frac12})A\bar\partial U^n+\bar\partial U^n+AU^{n-\frac12},\quad t\in J_n, \tag{1.5}$$

as we see by writing U in the form

$$U(t)=U^{n-\frac12}+(t-t^{n-\frac12})\bar\partial U^n,\quad t\in J_n.$$

We will be lead to $\hat U$ by replacing the coefficient $A\bar\partial U^n$ on the right-hand side of (1.5) by appropriate quantities.

We first choose a piecewise linear approximation φ to f,

$$\varphi(t)=\alpha_n\cdot(t-t^{n-\frac12})+\beta_n,\quad t\in J_n, \tag{1.6}$$

and introduce the corresponding BDF2 *reconstruction* $\hat U$ of U, namely a piecewise quadratic polynomial in time $\hat U:[0,T]\to D(A)$ defined in $[t^{n-1},t^n]$ by

$$\begin{cases}\hat U'(t)+AU(t)=\varphi(t)\quad\text{in }\ J_n,\\ \hat U(t^{n-1})=U^{n-1}.\end{cases} \tag{1.7}$$

Now, obviously,

$$\hat U(t^n)=U^{n-1}-A\int_{t^{n-1}}^{t^n}U(t)\,dt+\int_{t^{n-1}}^{t^n}\varphi(t)\,dt,$$

and, evaluating the integrals by the mid-point rule, we obtain

$$\hat U(t^n)=U^{n-1}+k\big(\beta_n-AU^{n-\frac12}\big);$$

therefore, the continuity requirement $\hat U(t^n)=U^n$ of $\hat U$ is satisfied, if and only if

$$\beta_n=\bar\partial U^n+AU^{n-\frac12}. \tag{1.8}$$

As we already mentioned, there are several appropriate choices for α_n; see (1.6). (We recall that $\alpha_n := A\bar\partial U^n$ corresponds to U; cf. (1.5).) In the sequel we will consider two particular choices: The first choice is $\alpha_n := \bar\partial f^n$, $n = 1,\dots,N$, and the second $\alpha_1 := \bar\partial^2 U^2 + A\bar\partial U^1$, $\alpha_2 := \bar\partial^2 U^2 + A\bar\partial U^2$, and $\alpha_n := \bar\partial f^n - \frac{k}{2}\bar\partial^3 U^n$, $n = 3,\dots,N$. As we will see later on, the second choice corresponds to the "three–point reconstruction", i.e., the reconstruction is, for $t \in [0, t^2]$, the quadratic interpolant of U^2, U^1 and U^0, and, for $n \ge 3$, the restriction to J_n of the quadratic polynomial interpolating U^n, U^{n-1} and U^{n-2}.

As in [6, 2, 3], we consider the error functions e and $\hat e$,

$$e := u - U, \quad \hat e := u - \hat U. \tag{1.9}$$

Once an appropriate reconstruction $\hat U$ is in place, the derivation of a posteriori error estimates is elementary; cf. [2, 3]. Let $V := D(A^{1/2})$, $\|\cdot\|$ be the norm of V, $\|v\| := |A^{1/2}v|$, $V^\star$ be the (topological) dual of V and $\|\cdot\|_\star$ its norm, $\|v\|_\star := |A^{-1/2}v|$. As we will see in §2, the following upper and lower error bounds are valid, for $t \in [0, T]$,

$$\begin{aligned}\max_{0\le\tau\le t}\Big[|\hat e(\tau)|^2 + \int_0^\tau \Big(\|e(s)\|^2 + \frac{1}{2}\|\hat e(s)\|^2\Big)\,ds\Big]\\ \le \int_0^t \|\hat U(s) - U(s)\|^2\,ds + 2\int_0^t \|f(t) - \varphi(t)\|_\star^2\,ds,\end{aligned} \tag{1.10}$$

$$\frac{1}{3}\int_0^t \|\hat U(s) - U(s)\|^2\,ds \le \int_0^t \Big(\|e(s)\|^2 + \frac{1}{2}\|\hat e(s)\|^2\Big)\,ds. \tag{1.11}$$

In the sequel we will refer to the upper bound on the right-hand side of (1.10) as the *estimator* $\mathcal{E}$.

The above idea is related to earlier work on a posteriori analysis of time or space discrete approximations of evolution equations [6, 2, 3, 5]. It provides the means to establish optimal order error estimates with energy as well as with other stability techniques. In these references single step time stepping schemes were considered; the present work is devoted to a multistep scheme that is quite popular in the computations of parabolic equations.

The paper is organized as follows: In §2 we present two appropriate reconstructions and establish the upper and lower estimates (1.10) and (1.11). In §3 we show that the estimator $\mathcal{E}$ is of optimal order. In §4 we consider the scheme

$$\begin{cases}\frac{k}{2}\bar\partial^2 U^n + \bar\partial U^n + AU^n = f^n, \quad n = 2,\dots,N,\\ \bar\partial U^1 + AU^1 = f^1,\\ U^0 = u^0;\end{cases} \tag{1.12}$$

the only difference to (1.2) is that in this case U^1 is computed by the backward Euler scheme. This choice for U^1 is indeed more natural in the a priori error analysis. Since the backward Euler method is applied only once (in particular, a finite number of times, independent of the time step k), it is well known that the method (1.12) yields second order approximations U^m to u^m. Unfortunately, as illustrated in §4, our approach leads to a suboptimal a posteriori estimator for the scheme (1.12). Finally, in §5 we present numerical results that illustrate the theoretical results of §4 and demonstrate the effectivity of our upper and lower a posteriori error estimates.

2. A posteriori error estimates. In this section we present two appropriate BDF2 reconstructions and establish the estimates (1.10) and (1.11) for the errors e and $\hat{e}$.

First, we show that the residual $R(t) \in H$ of U is of first order. Indeed, from the differential equation in (1.1) and the definition (1.4) of the residual, we have

$$u' + Au = f, \quad U' + AU = f + R; \tag{2.1}$$

consequently,

$$R = -(u - U)' - A(u - U). \tag{2.2}$$

The second term on the right-hand side of (2.2) is of second order; however, the first term can be at most of first order, since u' is approximated by a piecewise constant function U' (and this is valid for any choice of piecewise linear function, not only for the specific approximation U); negative norms in time are excluded from this discussion.

A concrete example illustrating that $R(t)$ is of first order might be instructive here: In the case of the initial value problem for an o.d.e. $u'(t) = f(t)$, (1.4) yields

$$R(t) = \bar{\partial} U^n - f(t), \quad t \in J_n.$$

Let now f be an affine function, $f(t) = ct + d$, $c \neq 0$, and assume that $U^0 = u^0$. Since both the trapezoidal scheme and the BDF2 method integrate this o.d.e. exactly, we have $U^n = u^n$, $n = 1, \dots, N$, and thus

$$\begin{aligned} R(t) = \bar{\partial} u^n - f(t) &= \frac{1}{k} \int_{t^{n-1}}^{t^n} u'(s)\, ds - \frac{1}{k} \int_{t^{n-1}}^{t^n} f(t)\, ds \\ &= \frac{1}{k} \int_{t^{n-1}}^{t^n} \big[f(s) - f(t) \big]\, ds = \frac{1}{k} c \int_{t^{n-1}}^{t^n} (s - t)\, ds \\ &= c\big(t^{n-\frac{1}{2}} - t\big), \quad t \in J_n, \end{aligned}$$

whence the order of the residual is equal to one.

It is obvious from (2.2) that to obtain a second order residual by a piecewise polynomial function $\hat{U}$, we should allow $\hat{U}$ to be piecewise quadratic. We require two fundamental properties from the approximate solution $\hat{U}$: it should be continuous and its residual should be of second order.

Next, we introduce two appropriate reconstructions, $\hat{U}$ and $\tilde{U}$; they are associated to two piecewise linear functions $\hat{\varphi}$ and $\tilde{\varphi}$, given in (2.3) and in (2.19), (2.20) in the sequel, respectively.

First choice: Motivated by the discussion in the Introduction (see, in particular, (1.6) and (1.8)) and the fact that $\bar{\partial} f^n$ is a second order approximation to $f'(t^{n-\frac{1}{2}})$, our first choice is based on the piecewise linear approximation $\hat{\varphi}$ to f,

$$\hat{\varphi}(t) = (t - t^{n-\frac{1}{2}}) \bar{\partial} f^n + \bar{\partial} U^n + A U^{n-\frac{1}{2}}, \quad t \in J_n. \tag{2.3}$$

We then let $\hat{U}$ be given by (1.7), with φ replaced by $\hat{\varphi}$. Obviously,

$$\hat{U}(t) = U^{n-1} - A \int_{t^{n-1}}^{t} U(s)\, ds + \int_{t^{n-1}}^{t} \hat{\varphi}(s)\, ds, \quad t \in J_n. \tag{2.4}$$

Since both U and $\hat\varphi$ are affine in J_n, $\hat U$ is quadratic in J_n. In fact, it is easily seen that

$$\hat U(t) = U(t) + \frac{1}{2}(t-t^n)(t-t^{n-1})\bar\partial(f^n - AU^n) \quad \forall t\in J_n. \tag{2.5}$$

Obviously, $\hat U$ coincides with U at the nodes t^m; in particular, $\hat U$ is continuous. Also, relation (2.5) yields

$$\hat U(t) = U(t) + \frac{1}{2}(t-t^n)(t-t^{n-1})\hat U'' \quad \forall t\in J_n. \tag{2.6}$$

Let us also note, for later use, the relation between $\hat\varphi$ and f; we will denote by $I_1 f$ the piecewise linear interpolant of f at the nodes $t^0, t^1, \dots, t^N$. First, for $n=1$, we have

$$\hat\varphi(t) = (t-t^{\frac12})\bar\partial f^1 + \bar\partial U^1 + AU^{\frac12},$$

i.e., in view of (1.2),

$$\hat\varphi(t) = (t-t^{\frac12})\bar\partial f^1 + f^{\frac12} = (I_1 f)(t) \quad \forall t\in(t^0,t^1). \tag{2.7}$$

Furthermore, for $n\ge 2$ we have

$$\begin{aligned}\hat\varphi(t) &= \bar\partial U^n + AU^n - \frac{k}{2}\bar\partial AU^n + (t-t^n)\bar\partial f^n + \frac{k}{2}\bar\partial f^n\\ &= \bar\partial U^n + AU^n + \frac{k}{2}\bar\partial(f^n - AU^n) + (t-t^n)\bar\partial f^n,\end{aligned}$$

whence, in view of (1.2),

$$\hat\varphi(t) = f^n - \frac{k}{2}\bar\partial^2 U^n + \frac{k}{2}\bar\partial(f^n - AU^n) + (t-t^n)\bar\partial f^n,$$

i.e.,

$$\hat\varphi(t) = f^n + (t-t^n)\bar\partial f^n + \frac{k}{2}\bar\partial(f^n - AU^n - \bar\partial U^n);$$

thus

$$\hat\varphi(t) = (I_1 f)(t) + \frac{k}{2}\bar\partial(f^n - AU^n - \bar\partial U^n), \quad t\in(t^{n-1},t^n), \quad n\ge 2. \tag{2.8}$$

Therefore, using again (1.2), for $n\ge 3$,

$$\hat\varphi(t) = (I_1 f)(t) + \frac{k^2}{4}\bar\partial^3 U^n, \quad t\in(t^{n-1},t^n). \tag{2.9}$$

Remark 2.1 (Regularity of $\hat U$). A natural question is whether $\hat U(t)$ belongs to any space containing the approximations $U^0,\dots,U^N$. We will see that this is indeed the case, provided $u'(0)$ is contained in the same space; in particular, in the applications, $\hat U(t)$ satisfies the same boundary conditions as $U^0,\dots,U^N$.

First, let $n\ge 3$; then, (1.2) yields

$$\bar\partial(f^n - AU^n) = \bar\partial^2 U^n + \frac{k}{2}\bar\partial^3 U^n.$$

Therefore, from (2.5) we obtain

$$\hat U(t) = U(t) + \frac{1}{2}(t-t^n)(t-t^{n-1})\big(\bar\partial^2 U^n + \frac{k}{2}\bar\partial^3 U^n\big) \quad \forall t \in J_n, \quad n \geq 3, \tag{2.10}$$

and conclude that $\hat U(t)$ belongs, for $t \in [t^2, T]$, to any space containing the approximations $U^0, \dots, U^N$. (Note that, for $t \in [t^2, T]$, the assumption that $u'(0)$ is contained in the same space is not needed.)

Furthermore, since U^1 is computed by the trapezoidal method, the second relation in (1.2) yields

$$\frac{1}{2}(f^1 - AU^1) = \bar\partial U^1 - \frac{1}{2}(f^0 - AU^0),$$

i.e.,

$$f^1 - AU^1 = 2\bar\partial U^1 - u'(0). \tag{2.11}$$

Therefore,

$$\bar\partial(f^2 - AU^2) = \frac{1}{2}\bar\partial^2 U^2 + \frac{1}{k}\bar\partial U^2 - \frac{1}{k}\big[2\bar\partial U^1 - u'(0)\big]$$

and we easily conclude from (2.5) that $\hat U(t)$ belongs, for $t \in J_2$, to any space containing $u'(0)$ and the approximations U^0, U^1 and U^2.

Finally, combining (2.5) with (2.11), we see that $\hat U(t)$ belongs, for $t \in J_1$, to any space containing $u'(0)$ and the approximations U^0, U^1. □

Second choice: *The three-point reconstruction.*

In $J_1 \cup J_2$, we let the reconstruction $\tilde U$ be the quadratic interpolant of U^2, U^1 and U^0; for $n \geq 3$, we let $\tilde U$ in J_n be the restriction to J_n of the quadratic interpolant of U^n, U^{n-1} and U^{n-2}, i.e., $\tilde U(t^i) = U^i$, $i = n, n-1, n-2$. It is easily seen that

$$\tilde U(t) = U^n + (t-t^n)\bar\partial U^n + \frac{1}{2}(t-t^n)(t-t^{n-1})\bar\partial^2 U^n \quad \forall t \in J_n, \quad n \geq 2. \tag{2.12}$$

The three-point reconstruction was proposed in [4] for the trapezoidal scheme.

Let us note that, since $U(t) = U^n + (t-t^n)\bar\partial U^n$, $t \in J_n$, we have

$$\tilde U(t) = U(t) + \frac{1}{2}(t-t^n)(t-t^{n-1})\bar\partial^2 U^n \quad \forall t \in J_n. \tag{2.13}$$

Obviously,

$$\tilde U'(t) = \bar\partial U^n + (t - t^{n-\frac{1}{2}})\bar\partial^2 U^n, \quad t \in J_n,$$

i.e.,

$$\tilde U'(t) = \bar\partial U^n + (t-t^n)\bar\partial^2 U^n + \frac{k}{2}\bar\partial^2 U^n, \quad t \in J_n. \tag{2.14}$$

Therefore,

$$\tilde U'(t) + AU(t) = \bar\partial U^n + (t-t^n)\bar\partial^2 U^n + \frac{k}{2}\bar\partial^2 U^n + AU^n + (t-t^n)A\bar\partial U^n,$$

whence, in view of (1.2),

$$\tilde{U}'(t) + AU(t) = f^n + (t - t^n)\big(\bar{\partial}^2 U^n + A\bar{\partial}U^n\big), \quad t \in J_n, \tag{2.15}$$

$n \geq 2$. Furthermore, for $n \geq 3$, using again (1.2), we have

$$\begin{aligned}\tilde{U}'(t) + AU(t) &= f^n + (t - t^n)\bar{\partial}\big(\bar{\partial}U^n + AU^n\big) = f^n + (t - t^n)\bar{\partial}\big(f^n - \frac{k}{2}\bar{\partial}^2 U^n\big)\\ &= f^n + (t - t^n)\bar{\partial}f^n - \frac{k}{2}(t - t^n)\bar{\partial}^3 U^n,\end{aligned}$$

i.e.,

$$\tilde{U}'(t) + AU(t) = (I_1 f)(t) - \frac{k}{2}(t - t^n)\bar{\partial}^3 U^n, \quad t \in J_n, \quad n \geq 3. \tag{2.16}$$

Finally,

$$\tilde{U}(t) = U(t) + \frac{1}{2}t(t - t^1)\bar{\partial}^2 U^2 \quad \forall t \in J_1, \tag{2.17}$$

and we easily see that

$$\tilde{U}'(t) + AU(t) = (t - t^{\frac{1}{2}})\big(\bar{\partial}^2 U^2 + A\bar{\partial}U^1\big) + f^{\frac{1}{2}}, \quad t \in J_1. \tag{2.18}$$

Remark 2.2. Let

$$\tilde{\varphi}(t) := (t - t^{\frac{1}{2}})\big(\bar{\partial}^2 U^2 + A\bar{\partial}U^1\big) + f^{\frac{1}{2}}, \quad t \in J_1, \tag{2.19}$$

and

$$\tilde{\varphi}(t) := f^n + (t - t^n)\big(\bar{\partial}^2 U^n + A\bar{\partial}U^n\big), \quad t \in J_n, \quad n \geq 2; \tag{2.20}$$

see (2.15) and (2.18). Then, the three-point reconstruction $\tilde{U}$ could be alternatively defined by (1.7), with φ replaced by $\tilde{\varphi}$. □

Remark 2.3. From (2.16) and (2.9), we immediately obtain, for $n \geq 3$,

$$\tilde{\varphi}(t) = \hat{\varphi}(t) - \frac{k}{2}\big(t - t^{n-\frac{1}{2}}\big)\bar{\partial}^3 U^n, \quad t \in J_n. \tag{2.21}$$

In particular, in view of (2.3),

$$\tilde{\varphi}(t) = \big(t - t^{n-\frac{1}{2}}\big)\big(\bar{\partial}f^n - \frac{k}{2}\bar{\partial}^3 U^n\big) + \bar{\partial}U^n + AU^{n-\frac{1}{2}}, \quad t \in J_n. \tag{2.22}$$

Furthermore, for $n = 2$, it is easily seen from (2.20) that

$$\tilde{\varphi}(t) = \big(t - t^{\frac{3}{2}}\big)\big(\bar{\partial}^2 U^2 + A\bar{\partial}U^2\big) + \bar{\partial}U^2 + AU^{\frac{3}{2}}, \quad t \in J_2. \tag{2.23}$$

Finally, for $t \in J_1$, $\tilde{\varphi}$ is given in (2.19). □

Remark 2.4 (Regularity of $\tilde{U}$). Obviously, $\tilde{U}(t)$ belongs to any space containing the approximations $U^0, \dots, U^N$, for all $t \in [0, T]$. □

In the remaining part of this section, we let $\hat{U}$ be either one of the two reconstructions defined above and φ stand for either $\hat{\varphi}$ or $\tilde{\varphi}$, depending on the corresponding choice of $\hat U$. Once an appropriate reconstruction $\hat U$ is in place, the rest of the analysis is elementary as the following result illustrates; cf. [2, 3].

THEOREM 2.1 (Error estimates). *The upper and lower error bounds* (1.10) *and* (1.11) *are valid for the errors* $e = u - U$ *and* $\hat e = u - \hat U$, *for* $t \in [0, T]$.

Proof. Subtracting the differential equation in (1.7) from the one in (1.1), we obtain

$$\hat e'(t) + Ae(t) = f(t) - \varphi(t). \tag{2.24}$$

Taking in (2.24) the inner product with $\hat e(t)$ and using the identity $2\langle Ae(t), \hat e(t)\rangle = \|e(t)\|^2 + \|\hat e(t)\|^2 - \|\hat U(t) - U(t)\|^2$, we arrive at

$$\frac{d}{dt}|\hat e(t)|^2 + \|e(t)\|^2 + \|\hat e(t)\|^2 = \|\hat U(t) - U(t)\|^2 + 2\langle f(t) - \varphi(t), \hat e(t)\rangle. \tag{2.25}$$

Now,

$$2\langle f(t) - \varphi(t), \hat e(t)\rangle \le 2\|f(t) - \varphi(t)\|_\star^2 + \frac{1}{2}\|\hat e(t)\|^2,$$

and (2.25) yields

$$\frac{d}{dt}|\hat e(t)|^2 + \|e(t)\|^2 + \frac{1}{2}\|\hat e(t)\|^2 \le \|\hat U(t) - U(t)\|^2 + 2\|f(t) - \varphi(t)\|_\star^2,$$

whence, since $\hat e$ is continuous and $\hat e(0) = 0$,

$$\begin{aligned} |\hat e(t)|^2 &+ \int_0^t \Big(\|e(s)\|^2 + \frac{1}{2}\|\hat e(s)\|^2\Big)\, ds \\ &\le \int_0^t \|\hat U(s) - U(s)\|^2\, ds + 2\int_0^t \|f(s) - \varphi(s)\|_\star^2\, ds. \end{aligned} \tag{2.26}$$

This easily leads to the upper bound (1.10). Furthermore, obviously, $\|(\hat U - U)(s)\| \le \|e(s)\| + \|\hat e(s)\|$, and thus

$$\|(\hat U - U)(s)\|^2 \le 3\big[\|e(s)\|^2 + \frac{1}{2}\|\hat e(s)\|^2\big];$$

integrating in $[0, t]$, we obtain the lower bound (1.11). □

Combining (1.10) and (1.11), we immediately conclude

$$\begin{aligned} \frac{1}{3}\int_0^t \|\hat U(s) - U(s)\|^2\, ds &\le \int_0^t \Big(\|e(s)\|^2 + \frac{1}{2}\|\hat e(s)\|^2\Big)\, ds \\ &\le \int_0^t \|\hat U(s) - U(s)\|^2\, ds + 2\int_0^t \|f(s) - \varphi(s)\|_\star^2\, ds. \end{aligned} \tag{2.27}$$

3. Optimality of the estimator. In this section we show that the estimator $\mathcal{E}$ on the right-hand side of (1.10) is of optimal order, i.e., of order $O(k^4)$, for both reconstructions $\hat U$ and $\tilde U$ described in §2; see first and second choice in §2. We will present the details for the three-point estimator $\tilde U$. For the other estimator, $\hat U$, the proof goes along the same lines; we will briefly discuss this case in Remark 3.1.

Let

$$\mathcal{E}_1 := \int_0^T \|\tilde U(t) - U(t)\|^2\, dt \quad \text{and} \quad \mathcal{E}_2 := \int_0^T \|f(t) - \tilde\varphi(t)\|_\star^2\, dt \tag{3.1}$$

with $\tilde\varphi$ as described in detail in §2 and $\tilde U$ the corresponding, three-point reconstruction. In the sequel we show that both $\mathcal{E}_1$ and $\mathcal{E}_2$ are of order $O(k^4)$; thus, the estimator $\mathcal{E} = \mathcal{E}_1 + 2\mathcal{E}_2$ on the right-hand side of (1.10) is of optimal order for this reconstruction.

3.1. Optimality of $\mathcal{E}_1$. First, let $n \geq 2$. Then, using (2.13), we obtain

$$\int_{J_n} \|\tilde{U}(t) - U(t)\|^2\,dt = \frac{1}{4}\int_{J_n}(t^n - t)^2(t - t^{n-1})^2\,dt\,\|\bar{\partial}^2 U^n\|^2$$
$$= \frac{1}{4}k^5\int_0^1 (s-1)^2 s^2\,ds\,\|\bar{\partial}^2 U^n\|^2,$$

i.e.,

$$\int_{J_n} \|\tilde{U}(t) - U(t)\|^2\,dt = \frac{1}{120}k^5\|\bar{\partial}^2 U^n\|^2, \quad n \geq 2. \tag{3.2}$$

Similarly, in view of (2.17), we have

$$\int_{J_1} \|\tilde{U}(t) - U(t)\|^2\,dt = \frac{1}{120}k^5\|\bar{\partial}^2 U^2\|^2. \tag{3.3}$$

We readily conclude from (3.1), (3.2) and (3.3) that

$$\mathcal{E}_1 = \frac{k^4}{120}\,k\Big[2\|\bar{\partial}^2 U^2\|^2 + \sum_{n=3}^{N}\|\bar{\partial}^2 U^n\|^2\Big]. \tag{3.4}$$

We will estimate $\mathcal{E}_1$. We begin with some preparatory estimates for e^1 and e^2; actually, to estimate $\mathcal{E}_1$ we will only need an estimate for e^1, but since an estimate for e^2 will be needed in the next subsection to show that $\mathcal{E}_2$ is also of optimal order, we will provide here estimates for both e^1 and e^2.

Let E^1 denote the consistency error of the first step by the trapezoidal scheme,

$$E^1 := \bar{\partial}u^1 + Au^{1/2} - f^{1/2}, \tag{3.5}$$

and E^2 denote the consistency error of the BDF2 scheme in the second step,

$$E^2 := \frac{k}{2}\bar{\partial}^2 u^2 + \bar{\partial}u^2 + Au^2 - f^2. \tag{3.6}$$

It is well known and easily seen that, under obvious regularity assumptions,

$$\|E^1\|_\star + \|E^2\|_\star \leq Ck^2. \tag{3.7}$$

Now, we have

$$e^1 + \frac{k}{2}Ae^1 = kE^1;$$

taking here the inner product with e^1 and using elementary inequalities, we obtain

$$|e^1|^2 + \frac{k}{2}\|e^1\|^2 \leq k\|E^1\|_\star\,\|e^1\| \leq k\|E^1\|_\star^2 + \frac{k}{4}\|e^1\|^2,$$

whence

$$|e^1|^2 + \frac{k}{4}\|e^1\|^2 \leq k\|E^1\|_\star^2. \tag{3.8}$$

Combining (3.8) with (3.7), we arrive at the desired estimate for e^1,

$$|e^1|^2 + k\|e^1\|^2 \le Ck^5. \tag{3.9}$$

Similarly, we have

$$-2e^1 + \frac{3}{2}e^2 + kAe^2 = kE^2;$$

taking here the inner product with e^2, we obtain

$$\begin{aligned}\frac{3}{2}|e^2|^2 + k\|e^2\|^2 &= k\langle E^2, e^2\rangle + 2\langle e^1, e^2\rangle\\ &\le \frac{k}{2}\|E^2\|_\star^2 + \frac{k}{2}\|e^2\|^2 + |e^1|^2 + |e^2|^2,\end{aligned}$$

whence

$$|e^2|^2 + k\|e^2\|^2 \le k\|E^2\|_\star^2 + 2|e^1|^2. \tag{3.10}$$

Combining (3.10) with (3.7) and (3.9), we arrive at the desired estimate for e^2,

$$|e^2|^2 + k\|e^2\|^2 \le Ck^5. \tag{3.11}$$

We shall next use these preparatory estimates to estimate $\mathcal{E}_1$. It is well known from the a priori error analysis for the BDF2 method that, for sufficiently smooth u,

$$|e^n|^2 + k\sum_{\ell=2}^{n}\|e^\ell\|^2 \le C\big(|e^0|^2 + |e^1|^2 + k^4\big), \quad n = 2, \dots, N, \tag{3.12}$$

with $e^m := u^m - U^m$; cf. [7], [1]. In particular, in view of (3.9),

$$k\sum_{\ell=2}^{N}\|e^\ell\|^2 \le Ck^4. \tag{3.13}$$

Now,

$$\begin{aligned}k\sum_{n=2}^{N}\|\bar\partial^2 U^n\|^2 &\le 2k\sum_{n=2}^{N}\|\bar\partial^2 e^n\|^2 + 2k\sum_{n=2}^{N}\|\bar\partial^2 u^n\|^2\\ &\le C\frac{1}{k^3}\sum_{n=0}^{N}\|e^n\|^2 + 2k\sum_{n=2}^{N}\|\bar\partial^2 u^n\|^2,\end{aligned}$$

whence

$$k\sum_{n=2}^{N}\|\bar\partial^2 U^n\|^2 \le C\frac{1}{k^3}\|e^1\|^2 + C\frac{1}{k^3}\sum_{n=2}^{N}\|e^n\|^2 + C(u). \tag{3.14}$$

Using (3.13) in (3.14), we conclude

$$k\sum_{n=2}^{N}\|\bar\partial^2 U^n\|^2 \le C\frac{1}{k^3}\|e^1\|^2 + C. \tag{3.15}$$

Combining (3.15) with the estimate (3.9), we obtain

$$k\sum_{n=2}^{N}\|\bar\partial^2 U^n\|^2\le C, \tag{3.16}$$

and we arrive at the desired optimal order estimate for $\mathcal{E}_1$,

$$\mathcal{E}_1\le ck^4. \tag{3.17}$$

3.2. Optimality of $\mathcal{E}_2$. We split $\mathcal{E}_2$ in the form $\mathcal{E}_2=\mathcal{E}_{2,1}+\mathcal{E}_{2,2}$ with

$$\mathcal{E}_{2,1}:=\int_0^{2k}\|f(t)-\tilde\varphi(t)\|_\star^2\,dt,\quad \mathcal{E}_{2,2}:=\int_{2k}^{T}\|f(t)-\tilde\varphi(t)\|_\star^2\,dt. \tag{3.18}$$

First, for $t\in J_1$, using (2.19) and (1.2), we have

$$\begin{aligned}\tilde\varphi(t)&=\big(t-t^{\frac12}\big)(\bar\partial^2U^2+A\bar\partial U^1)+f^{\frac12}\\&=f^{\frac12}+\big(t-t^{\frac12}\big)\bar\partial f^1+\big(t-t^{\frac12}\big)(\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1),\end{aligned}$$

i.e.,

$$\tilde\varphi(t)=(I_1f)(t)+\big(t-t^{\frac12}\big)(\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1),\quad t\in J_1. \tag{3.19}$$

Thus, easily,

$$\|f(t)-\tilde\varphi(t)\|_\star\le Ck^2+\frac{k}{2}\|\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1\|_\star,\quad t\in J_1. \tag{3.20}$$

Now, using (1.2) and (1.1), we have

$$\begin{aligned}&\frac{k}{2}\big(\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1\big)=\frac{k}{2}\bar\partial^2U^2-\frac{k}{2}\bar\partial(f^1-AU^1)\\&=(f^2-\bar\partial U^2-AU^2)-\frac12(f^1-AU^1)+\frac12(f^0-Au^0)\\&=(f^2-AU^2)-\frac12(f^1-AU^1)+\frac12(f^0-Au^0)-\bar\partial U^2\\&=(f^2-Au^2)-\frac12(f^1-Au^1)+\frac12(f^0-Au^0)+Ae^2-\frac12Ae^1+\bar\partial e^2-\bar\partial u^2\\&=\big[u'(t^2)-\frac12u'(t^1)+\frac12u'(0)-\bar\partial u^2\big]+Ae^2-\frac12Ae^1+\bar\partial e^2,\end{aligned}$$

and we easily conclude that

$$\frac{k}{2}\|\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1\|_\star\le Ck^2+\|e^2\|+\frac12\|e^1\|+\|\bar\partial e^2\|_\star. \tag{3.21}$$

Using here the estimates (3.9) and (3.11), we obtain

$$\frac{k}{2}\|\bar\partial^2U^2+A\bar\partial U^1-\bar\partial f^1\|_\star\le Ck^{\frac32}. \tag{3.22}$$

Now (3.20) yields

$$\int_0^k\|f(t)-\tilde\varphi(t)\|_\star^2\,dt\le Ck^5+k^3\|\bar\partial^2U^2+AU^1-\bar\partial f^1\|_\star^2,$$

whence, in view of (3.22),

$$\int_0^k \|f(t)-\tilde\varphi(t)\|_\star^2\,dt \le Ck^4. \tag{3.23}$$

Furthermore, for $n=2$, in view of (2.20), we have

$$\begin{aligned} f(t)-\tilde\varphi(t) &= f(t)-\big[f^2+(t-t^2)\bar\partial f^2\big]-(t-t^2)\big(\bar\partial^2U^2+A\bar\partial U^2-\bar\partial f^2\big)\\ &= \big[f(t)-(I_1f)(t)\big]-(t-t^2)\big(\bar\partial^2U^2+A\bar\partial U^2-\bar\partial f^2\big),\quad t\in J_2, \end{aligned}$$

whence, easily,

$$\|f(t)-\tilde\varphi(t)\|_\star \le Ck^2+k\|\bar\partial^2U^2+A\bar\partial U^2-\bar\partial f^2\|_\star,\quad t\in J_2. \tag{3.24}$$

Now,

$$\begin{aligned} \frac{k}{2}\bar\partial(f^2-AU^2-\bar\partial U^2) &= \frac{k}{2}\bar\partial(f^2-AU^2)-\frac{k}{2}\bar\partial^2U^2\\ &= \frac{k}{2}\bar\partial(f^2-AU^2)+\bar\partial U^2+AU^2-f^2\\ &= \bar\partial U^2+AU^{\frac32}-f^{\frac32}\\ &= \bar\partial U^2+AU^{\frac32}-Au^{\frac32}-\frac12\big[u'(t^1)+u'(t^2)\big]\\ &= -\bar\partial e^2-Ae^{\frac32}+\Big[\bar\partial u^2-\frac12\big[u'(t^1)+u'(t^2)\big]\Big], \end{aligned}$$

whence

$$k\|\bar\partial(f^2-AU^2-\bar\partial U^2)\|_\star \le 2\|\bar\partial e^2\|_\star+2\|e^{\frac32}\|+Ck^2. \tag{3.25}$$

Estimating the first two terms on the right–hand side of (3.25) by (3.9) and (3.11), we get

$$k\|\bar\partial(f^2-AU^2-\bar\partial U^2)\|_\star \le Ck^{\frac32}. \tag{3.26}$$

Now (3.24) yields

$$\int_k^{2k} \|f(t)-\tilde\varphi(t)\|_\star^2\,dt \le Ck^5+2k^3\|\bar\partial(f^2-AU^2-\bar\partial U^2)\|_\star^2,$$

whence, in view of (3.26),

$$\int_k^{2k} \|f(t)-\tilde\varphi(t)\|_\star^2\,dt \le Ck^4. \tag{3.27}$$

From (3.23) and (3.27) we obtain the desired optimal order estimate for $\mathcal{E}_{2,1}$,

$$\mathcal{E}_{2,1} \le Ck^4. \tag{3.28}$$

To estimate $\mathcal{E}_{2,2}$, we first note that, in view of (2.16),

$$f(t)-\tilde\varphi(t) = \big[f(t)-(If)(t)\big]+\frac{k}{2}(t-t^n)\bar\partial^3U^n,\quad t\in J_n,$$

$n \geq 3$. Therefore,

$$\mathcal{E}_{2,2} \leq 2 \int_{2k}^{T} \|f(t) - (If)(t)\|_\star^2 \, dt + \frac{k^2}{2} \sum_{n=3}^{N} \int_{J_n} (t-t^n)^2 \, dt \, \|\bar\partial^3 U^n\|_\star^2,$$

whence

$$\mathcal{E}_{2,2} \leq Ck^4 + \frac{k^4}{6} k \sum_{n=3}^{N} \|\bar\partial^3 U^n\|_\star^2. \tag{3.29}$$

Therefore, it suffices to show

$$k \sum_{n=3}^{N} \|\bar\partial^3 U^n\|_\star^2 \leq C. \tag{3.30}$$

But (3.30) follows from the stability estimate

$$\begin{aligned} |A^{-1}\bar\partial^3 U^n|^2 + k \sum_{j=5}^{n} \|\bar\partial^3 U^j\|_\star^2 \leq C\Big[& |A^{-1}\bar\partial^3 U^3|^2 \\ & + |A^{-1}\bar\partial^3 U^4|^2 + k \sum_{j=5}^{n} \|A^{-1}\bar\partial^3 f^j\|_\star^2 \Big], \quad n = 5, \dots, N, \end{aligned} \tag{3.31}$$

cf. [7], [1], and the fact that $U^0, \dots, U^4$ are third order approximations to $u^0, \dots, u^4$, respectively, in the norm $|A^{-1} \cdot|$ and approximations of order $5/2$ in the norm $\|\cdot\|_\star$.

Remark 3.1. Here we briefly sketch the proof of the optimality of the estimator for the reconstruction $\hat U$ given by (2.4). With notation analogous to (3.1), with $\hat U$ and $\hat\varphi$ instead of $\tilde U$ and $\tilde\varphi$, respectively, it is easily seen that in this case

$$\mathcal{E}_1 = \mathcal{E}_{1,1} + \mathcal{E}_{1,2} \tag{3.32}$$

with

$$\begin{cases} \mathcal{E}_{1,1} := \dfrac{k^4}{120} k\big(\|\bar\partial(f^1 - AU^1)\|^2 + \|\bar\partial(f^2 - AU^2)\|^2\big) \\ \mathcal{E}_{1,2} := \dfrac{k^4}{120} k \displaystyle\sum_{n=3}^{N} \|\bar\partial^2 U^n + \frac{k}{2}\bar\partial^3 U^n\|^2. \end{cases} \tag{3.33}$$

We will now use (3.9) and (3.11) to estimate $\mathcal{E}_{1,1}$. First, in view of (2.11) and (1.1), we have

$$\bar\partial(f^1 - AU^1) = \frac{2}{k}\big[\bar\partial U^1 - u'(0)\big],$$

whence

$$\bar\partial(f^1 - AU^1) = -\frac{2}{k^2}e^1 + \frac{2}{k}\big[\bar\partial u^1 - u'(0)\big]. \tag{3.34}$$

Under obvious regularity requirements, the second term on the right-hand side of (3.34) can be easily estimated; we conclude

$$k\|\bar\partial(f^1 - AU^1)\|^2 \leq \frac{4}{k^3}\|e^1\|^2 + Ck.$$

Therefore, in view of (3.9),

$$k\|\bar\partial(f^1 - AU^1)\|^2 \le c. \tag{3.35}$$

Using (3.35) and the analogous estimate for $\bar\partial(f^2 - AU^2)$, we can easily see that $\mathcal{E}_{1,1} \le Ck^4$. Also, combining (3.16) with (3.30) we see that $\mathcal{E}_{1,2} \le Ck^4$. Therefore, $\mathcal{E}_1 \le Ck^4$.

Furthermore, in view of (3.28) and (2.9), we easily obtain

$$\mathcal{E}_2 := \int_0^T \|f(t) - \hat\varphi(t)\|_\star^2\,dt \le Ck^4 + \frac{k^4}{8} k \sum_{n=3}^N \|\bar\partial^3 U^n\|_\star^2;$$

using here (3.30), we conclude $\mathcal{E}_2 \le Ck^4$, i.e., the estimator $\mathcal{E}$ is of optimal order. □

4. Starting with the backward Euler scheme. Since we want to have a second order approximation U^1 to u^1, the first choice that comes to mind is to define U^1 by performing one step with the backward Euler method. Unfortunately, for this choice our estimator is of suboptimal order for both reconstructions. We illustrate this with two elementary examples.

Example 4.1. Let us first consider the initial value problem

$$\begin{cases} u'(t) = 2t, \quad 0 \le t \le 1,\\ u(0) = 0. \end{cases} \tag{4.1}$$

It is an easy task to derive a posteriori error estimates for (4.1) and we will not dwell upon this. Our purpose here is to study the order of our estimator $\mathcal{E}_2$ for this concrete example, cf. (3.1).

We first perform one step of the backward Euler method and get $U^1 = 2k^2$. Subsequently, we apply the BDF2 method to obtain the approximations $U^2, \dots, U^N$,

$$\begin{cases} \frac{1}{2}U^{n-2} - 2U^{n-1} + \frac{3}{2}U^n = 2k^2 n, \quad n = 2, \dots, N,\\ U^0 = 0,\ U^1 = 2k^2. \end{cases} \tag{4.2}$$

The solution U^n of (4.2) can be easily determined; since the order of the BDF2 method is two, and the exact solution u of (4.1) is a polynomial of degree two, $u^0, u^1, \dots, u^N$ is a particular solution of the inhomogeneous difference equation. Using also the general solution of the corresponding homogeneous equation and the given starting values U^0 and U^1, we obtain

$$U^n = \Big[\frac{3}{2}\big(1 - \frac{1}{3^n}\big) + n^2\Big]k^2, \quad n = 0, \dots, N. \tag{4.3}$$

Therefore, for the error $u^n - U^n$ we have

$$u^n - U^n = -\frac{3}{2}\big(1 - \frac{1}{3^n}\big)k^2, \quad n = 0, \dots, N; \tag{4.4}$$

in particular, U^n are second order approximations to u^n.

Furthermore, (4.3) yields

$$\frac{k}{2}\bar\partial^3 U^n = \frac{2}{3^{n-1}}, \quad n = 3, \dots, N. \tag{4.5}$$

Now, for $f(t) := 2t$, we obviously have $I_1 f = f$, and (2.16) yields, for $n \geq 3$,

$$f(t) - \tilde{\varphi}(t) = -\frac{k}{2}(t - t^n)\bar{\partial}^3 U^n, \quad t \in (t^{n-1}, t^n),$$

i.e.,

$$f(t) - \tilde{\varphi}(t) = -2(t - t^n)\frac{1}{3^{n-1}}, \quad t \in (t^{n-1}, t^n). \tag{4.6}$$

Thus, we have

$$\mathcal{E}_{2,2} = \int_{2k}^{1} |f(t) - \tilde{\varphi}(t)|^2 \, dt = \frac{4}{3} k^3 \sum_{n=3}^{N} \frac{1}{9^{n-1}},$$

and conclude that $\mathcal{E}_{2,2}$ is of suboptimal order $O(k^3)$.

Remark 4.1. Using the first reconstruction for the initial value problem (4.1) and the scheme (4.2), we get

$$\mathcal{E}_{2,2} = \int_{2k}^{1} |f(t) - \hat{\varphi}(t)|^2 \, dt = k^3 \sum_{n=3}^{N} \frac{1}{9^{n-1}},$$

and conclude that also in this case $\mathcal{E}_{2,2}$ is of suboptimal order $O(k^3)$. □

Remark 4.2. Let us discretize the initial value problem (4.1) by combining the BDF2 method with the trapezoidal scheme: We start with the exact initial value $U^0 = 0$, perform one step with the trapezoidal scheme to compute U^1 and subsequently apply the BDF2 method to obtain $U^2, \dots, U^N$. It is then easily seen that $U^n = u^n$, i.e.,

$$U^n = n^2 k^2, \quad n = 0, 1, \dots, N.$$

Therefore, we have $\bar{\partial}^3 U^n = 0, n = 3, \dots, N$, whence $\mathcal{E}_{2,2} = 0$. It is also easily seen that both $\hat{\varphi}$ and $\tilde{\varphi}$ coincide with f in the interval $[0, 2k]$; we conclude that $\mathcal{E}_2$ vanishes.

Furthermore, it is readily seen that both reconstructions $\hat{U}$ and $\tilde{U}$ of U considered in this paper coincide in this case with the exact solution u. Therefore, $\hat{e} = 0$ and the a posteriori estimate (2.26) holds as an equality for this problem,

$$\int_0^t |e(s)|^2 \, ds = \int_0^t |\hat{U}(s) - U(s)|^2 \, ds = \int_0^t |\tilde{U}(s) - U(s)|^2 \, ds, \quad t \in [0, 1]. \qquad \square$$

Example 4.2. Let us also consider the initial value problem

$$\begin{cases} u' + \dfrac{1}{2} u = 0, \quad 0 \leq t \leq 1, \\ u(0) = 1. \end{cases} \tag{4.7}$$

The BDF2 method for problem (4.7) is

$$\frac{3}{2} U^n - 2U^{n-1} + \frac{1}{2} U^{n-2} + \frac{1}{2} k U^n = 0,$$

i.e.,

$$(3 + k)U^n - 4U^{n-1} + U^{n-2} = 0. \tag{4.8}$$

We will first determine the approximations U^n, in terms of the starting approximation U^1; we will use the exact value $U^0 := 1$ and in the sequel will consider two cases, when U^1 is given by the backward Euler or the trapezoidal methods, respectively.

For the sake of brevity we will use the notation $\alpha := \sqrt{1-k}$. Since the roots of the characteristic polynomial ρ, $\rho(z) := (3+k)z^2 - 4z + 1$, of the difference equation (4.8) are

$$z_1 := \frac{2+\alpha}{3+k} \quad \text{and} \quad z_2 := \frac{2-\alpha}{3+k},$$

we have

$$U^n = c_1(z_1)^n + c_2(z_2)^n, \quad n \geq 0, \tag{4.9}$$

with constants c_1 and c_2 depending only on the starting approximations U^0 and U^1. From the relations $c_1 + c_2 = U^0 (= 1)$ and $c_1 z_1 + c_2 z_2 = U^1$, we obtain

$$c_1 = \frac{U^1 - z_2}{z_1 - z_2} \quad \text{and} \quad c_2 = -\frac{U^1 - z_1}{z_1 - z_2}, \tag{4.10}$$

and conclude that

$$U^n = \frac{U^1 - z_2}{z_1 - z_2} z_1^n - \frac{U^1 - z_1}{z_1 - z_2} z_2^n, \quad n \geq 0. \tag{4.11}$$

Now, according to (2.20), we have $\tilde{\varphi}(t) = (t - t^n)\big(\bar{\partial}^2 U^n + \frac{1}{2}\bar{\partial} U^n\big)$, $t \in J_n$, and conclude easily

$$\tilde{\varphi}(t) = \frac{t - t^n}{2k^2}\big[(2+k)U^n - (4+k)U^{n-1} + 2U^{n-2}\big], \quad t \in J_n, \quad n \geq 2,$$

whence, in view of (4.9),

$$\tilde{\varphi}(t) = \frac{t - t^n}{2k^2} \sum_{i=1}^{2} c_i \big[(2+k)z_i^2 - (4+k)z_i + 2\big] z_i^{n-2}, \quad t \in J_n, \quad n \geq 2. \tag{4.12}$$

Using the relation $(3+k)z_i^2 - 4z_i + 1 = 0$, we easily see that

$$(2+k)z_i^2 - (4+k)z_i + 2 = \big[4(1-z_i) - k(1+z_i)\big] z_i, \quad i = 1, 2;$$

thus, we rewrite (4.12) in the form

$$\tilde{\varphi}(t) = \frac{t - t^n}{2k^2} \sum_{i=1}^{2} c_i \big[4(1-z_i) - k(1+z_i)\big] z_i^{n-1}, \quad t \in J_n, \quad n \geq 2. \tag{4.13}$$

In the sequel we will distinguish two cases: In the first case U^1 is computed by the backward Euler method and in the second by the trapezoidal scheme.

First case: *Starting with the backward Euler method.* Performing one step with the backward Euler method for the initial value problem (4.7), we obtain $U^1 = 2/(2+k)$. Therefore, in view of (4.10), in this case we have

$$c_1 = \frac{2(1+\alpha) + \alpha k}{2\alpha(2+k)} \quad \text{and} \quad c_2 = -\frac{2(1-\alpha) - \alpha k}{2\alpha(2+k)}. \tag{4.14}$$

Now, it is easily seen that

$$(4.15)\qquad \begin{cases} c_1\big[4(1-z_1)-k(1+z_1)\big] = \dfrac{1-\alpha}{2\alpha(2+k)}\,k^2, \\ c_2\big[4(1-z_2)-k(1+z_2)\big] = -\dfrac{1+\alpha}{2\alpha(2+k)}\,k^2. \end{cases}$$

Using (4.15), from (4.13) we easily obtain

$$(4.16)\qquad \tilde\varphi(t) = \frac{t-t^n}{4\alpha(2+k)}\big[(1-\alpha)z_1^{n-1}-(1+\alpha)z_2^{n-1}\big], \quad t\in J_n, \quad n\ge 2.$$

Furthermore, using (2.19) we get

$$(4.17)\qquad \tilde\varphi(t) = \frac{1}{2(2+k)}\Big[\frac{1+k}{3+k}(t-t^{1/2})+\frac{k}{2}\Big], \quad t\in J_1.$$

From (3.1), (4.17) and (4.16), we easily obtain

$$\mathcal{E}_2 = \frac{k^3}{8(2+k)^2}\Big[1+\frac{1}{3}\big(\frac{1+k}{3+k}\big)^2+\frac{1}{3\alpha^2}\sum_{n=2}^{N}\big[(1-\alpha)z_1^{n-1}-(1+\alpha)z_2^{n-1}\big]^2\Big],$$

i.e.,

$$(4.18)\qquad \mathcal{E}_2 = \frac{k^3}{8(2+k)^2}\Big[1+\frac{1}{3}\big(\frac{1+k}{3+k}\big)^2+\frac{1}{3\alpha^2}\big[(1-\alpha)^2E_1-E_2+(1+\alpha)^2E_3\big]\Big]$$

with

$$(4.19)\qquad E_1 = z_1^2\frac{1-z_1^{2N-2}}{1-z_1^2}, \quad E_2 = 2kz_1z_2\frac{1-(z_1z_2)^{N-1}}{1-z_1z_2}, \quad E_3 = z_2^2\frac{1-z_2^{2N-2}}{1-z_2^2}.$$

Our next task is to determine the order of the terms E_1, E_2 and E_3. Let us start with E_2. In view of $k\le 1/2$, from $z_1z_2 = 1/(3+k)$ we obtain $2/7\le z_1z_2\le 1/3$ and conclude easily that

$$E_2 \ge 2k\frac{2}{7}\frac{1}{1-\frac{2}{7}}\big[1-(z_1z_2)^{N-1}\big] \ge \frac{4}{5}k(1-\frac{1}{3}) = \frac{8}{15}k$$

and

$$E_2 \le 2k\frac{1}{3}\frac{1}{1-\frac{1}{3}} = k;$$

summarizing, we have

$$(4.20)\qquad \frac{8}{15}k \le E_2 \le k.$$

Concerning E_3, from $z_2 = (2-\alpha)/(3+k)$ we obtain $1/3\le z_2\le 2/3$ and conclude

$$E_3 \le \frac{4}{9}\frac{1}{1-\frac{4}{9}} = \frac{4}{5}$$

and

$$E_3 \geq \frac{1}{9}\frac{1}{1-\frac{1}{9}}\big[1-\big(\frac{2}{3}\big)^{2N-2}\big] \geq \frac{1}{9}\frac{9}{8}\big(1-\frac{4}{9}\big) = \frac{5}{72};$$

thus

$$\frac{5}{72} \leq E_3 \leq \frac{4}{5}. \tag{4.21}$$

Furthermore, since $k \leq 1/2$, we have $2-(2-\sqrt{2})k \leq 1+\alpha \leq 2$ and thus

$$\frac{3}{2}+\sqrt{2} \leq (1+\alpha)^2 \leq 4. \tag{4.22}$$

From (4.21) and (4.22) we obtain

$$\frac{5}{72}\big(\frac{3}{2}+\sqrt{2}\big) \leq (1+\alpha)^2 E_3 \leq \frac{16}{5}. \tag{4.23}$$

Finally, as far as the order of E_1 is concerned, we first note that

$$1-\frac{1}{2}k \leq z_1 \leq 1-\frac{1}{3}k, \tag{4.24}$$

whence

$$\frac{2}{3}k-\frac{1}{9}k^2 \leq 1-z_1^2 \leq k;$$

consequently, since $k \leq 1/2$,

$$\frac{11}{18}k \leq 1-z_1^2 \leq k. \tag{4.25}$$

Therefore,

$$\frac{z_1^2}{1-z_1^2} \leq \frac{1}{\frac{11}{18}k} = \frac{18}{11}\frac{1}{k} \quad \text{and} \quad \frac{z_1^2}{1-z_1^2} \geq \frac{\frac{3}{4}}{k} = \frac{3}{4}\frac{1}{k},$$

i.e.,

$$\frac{3}{4}\frac{1}{k} \leq \frac{z_1^2}{1-z_1^2} \leq \frac{18}{11}\frac{1}{k}. \tag{4.26}$$

Using now (4.24) and the fact that

$$\lim_{N\to\infty}\big(1-\frac{1}{3}\frac{1}{N}\big)^N = \mathrm{e}^{-1/3} \quad \text{and} \quad \lim_{N\to\infty}\big(1-\frac{1}{2}\frac{1}{N}\big)^N = \mathrm{e}^{-1/2}$$

we easily conclude, in view of (4.26), that E_1 is of exactly order minus one with respect to k. Furthermore, we have

$$\frac{1}{2}k \leq 1-\alpha \leq k,$$

whence

$$\frac{1}{4}k^2 \leq (1-\alpha)^2 \leq k^2. \tag{4.27}$$

Now, (4.27) and the previous discussion leads to the conclusion that $(1-\alpha)^2 E_1$ is exactly of first order.

Summarizing, $\mathcal{E}_2$ is exactly of *third* order.

Next, we show that $\mathcal{E}_1$ is of *fourth* order. Indeed, first, in this case (3.4) takes the form

$$\mathcal{E}_1 = \frac{k^4}{240} k \big[2|\bar\partial^2 U^2|^2 + \sum_{n=3}^{N} |\bar\partial^2 U^n|^2 \big]. \tag{4.28}$$

Now, in view of (4.9),

$$\bar\partial^2 U^n = \frac{1}{k^2} \sum_{i=1}^{2} c_i (z_i^2 - 2z_i + 1) z_i^{n-2}. \tag{4.29}$$

Since $(3+k)z_i^2 - 4z_i + 1 = 0$, we have

$$z_i^2 - 2z_i + 1 = [2(1-z_i) - kz_i] z_i,$$

and, using (4.14), we easily see that

$$c_i (z_i^2 - 2z_i + 1) 2\alpha(2+k) = (-1)^{i+1} k^2 z_i, \quad i = 1, 2;$$

therefore, (4.29) takes the form

$$\bar\partial^2 U^n = \frac{1}{2\alpha(2+k)} \big(z_1^{n-1} - z_2^{n-1} \big). \tag{4.30}$$

Hence, (4.28) yields

$$\mathcal{E}_1 = \frac{k^4}{240(2\alpha)^2(2+k)^2} k \Big[(z_1 - z_2)^2 + \sum_{n=2}^{N} \big(z_1^{n-1} - z_2^{n-1} \big)^2 \Big],$$

i.e.,

$$\mathcal{E}_1 = \frac{k^4}{240(2\alpha)^2(2+k)^2} \Big[\frac{(2\alpha)^2}{(3+k)^2} k + (kE_1 - E_2 + kE_3) \Big] \tag{4.31}$$

with E_1, E_2 and E_3 as in (4.19). Thus, we easily conclude that $\mathcal{E}_1$ is of fourth order; see the discussion following (4.19).

Second case: *Starting with the trapezoidal method.* Here, we will consider the discretization of (4.7) by first performing one step with the trapezoidal method and subsequently applying the BDF2 method to compute $U^2, \dots, U^n$. It is easily seen that $U^1 = (4-k)/(4+k)$, whence, in view of (4.10),

$$c_1 = \frac{4(1+\alpha) - (1-\alpha)k - k^2}{2\alpha(4+k)} \quad \text{and} \quad c_2 = -\frac{4(1-\alpha) - (1+\alpha)k - k^2}{2\alpha(4+k)}. \tag{4.32}$$

Also, the analogous calculation to the one leading to (4.15) yields in this case

$$\begin{cases} c_1 \big[4(1-z_1) - k(1+z_1) \big] = \dfrac{1}{2\alpha(4+k)} k^3, \\ c_2 \big[4(1-z_2) - k(1+z_2) \big] = -\dfrac{1}{2\alpha(4+k)} k^3. \end{cases} \tag{4.33}$$

Using (4.33), from (4.13) we easily obtain

$$\tilde{\varphi}(t) = \frac{(t-t^n)k}{4\alpha(4+k)}\big(z_1^{n-1} - z_2^{n-1}\big), \quad t \in J_n, \quad n \geq 2. \tag{4.34}$$

Furthermore, using (2.19) we get

$$\tilde{\varphi}(t) = -\frac{k}{(4+k)(3+k)}(t - t^{1/2}), \quad t \in J_1. \tag{4.35}$$

From (3.1), (4.35) and (4.34), we easily obtain

$$\mathcal{E}_2 = \frac{k^5}{24\alpha^2(4+k)^2}\Big[\frac{4\alpha^2}{(3+k)^2} + \sum_{n=2}^{N}\big(z_1^{n-1} - z_2^{n-1}\big)^2\Big],$$

i.e.,

$$\mathcal{E}_2 = \frac{k^4}{24\alpha^2(4+k)^2}\Big[\frac{4\alpha^2 k}{(3+k)^2} + (kE_1 - E_2 + kE_3)\Big] \tag{4.36}$$

with E_1, E_2 and E_3 as in (4.19). In view of (4.20), (4.21) and the fact that kE_1 is of zeroth order, we conclude that $\mathcal{E}_2$ is of optimal order in this case, namely of order exactly four.

5. Numerical experiments. In this section we present numerical results for Example 4.2 for both methods (1.2) and (1.12). Our numerical calculations justify the theoretical results of §4 and illustrate the effectivity of our a posteriori error estimators in a simple case.

First, we use the three-point reconstruction $\tilde{U}$ of the approximation U; cf. (2.12). In Tables 5.1 and 5.2 we state the values of the parts $\mathcal{E}_1$ and $\mathcal{E}_2$ of (the square of) our a posteriori error estimator as well as their orders in the cases U^1 is computed by the trapezoidal method and the backward Euler scheme, respectively. It is clearly seen that while all other quantities are of optimal order four (since they estimate the square of the error), part $\mathcal{E}_2$ in the case of the backward Euler scheme is of reduced order three; this confirms the theoretical results in §4. For the computation of $\mathcal{E}_1$ and $\mathcal{E}_2$ we employed the Gauss–Legendre quadrature formula with three nodes in each subinterval J_n; notice that the integrand, as a polynomial of degree four, is integrated exactly by this formula. Furthermore, we employed the same quadrature formula to approximate the errors $\int_0^1 |e(s)|^2\,ds$ and $\int_0^1 |\hat{e}(s)|^2\,ds$ in the estimates (1.10) and (1.11). Also, we denote by Err_1 the square of the L^2 norm (in time) of the errors, $\mathrm{Err}_1 = \frac{1}{2}\int_0^1 \big(|e(s)|^2 + \frac{1}{2}|\hat{e}(s)|^2\big)ds$, and by Err_2 the sum of Err_1 and the discrete maximum norm (in time) of $\hat{e}$, $\mathrm{Err}_2 = \max|\hat{e}(t^n)|^2 + \mathrm{Err}_1$. The lower and upper estimators are $\mathcal{E}_1/3$ and $\mathcal{E}_1 + 2\mathcal{E}_2$, respectively; see (1.10) and (1.11). We present the results of this computation as well as their effectivity indices Eff_i,

$$\mathrm{Eff}_1 := \frac{\text{Lower estimator}}{\mathrm{Err}_1} \quad \text{and} \quad \mathrm{Eff}_2 := \frac{\text{Upper estimator}}{\mathrm{Err}_2}$$

in Tables 5.3 and 5.4, again for the trapezoidal and the backward Euler schemes, respectively. We graphically demonstrate the effectivity indices in log-log scale (with the base of the logarithms equal to two) in Figure 5.1.

Finally, we state the corresponding results for the reconstruction $\hat{U}$ given in (2.5) in Tables 5.5–5.8 and in Figure 5.2.

TABLE 5.1
Three-point reconstruction: Order of $\mathcal{E}_1$ and $\mathcal{E}_2$ when starting with the trapezoidal method

N	$\mathcal{E}_1$	Order	$\mathcal{E}_2$	Order
2	9.4482e−06		4.1992e−05	
4	6.6037e−07	3.8387	4.2416e−06	3.3075
8	4.1643e−08	3.9871	3.3528e−07	3.6611
16	2.5732e−09	4.0165	2.3088e−08	3.8601
32	1.5917e−10	4.0149	1.5072e−09	3.9372
64	9.8841e−12	4.0093	9.6171e−11	3.9701
128	6.1557e−13	4.0051	6.0717e−12	3.9854
256	3.8401e−14	4.0027	3.8138e−13	3.9928
512	2.3978e−15	4.0014	2.3895e−14	3.9964
1024	1.4979e−16	4.0007	1.4953e−15	3.9982

TABLE 5.2
Three-point reconstruction: Order of $\mathcal{E}_1$ and $\mathcal{E}_2$ when starting with the backward Euler scheme

N	$\mathcal{E}_1$	Order	$\mathcal{E}_2$	Order
2	3.4014e−06		4.2517e−04	
4	3.7834e−07	3.1684	7.0346e−05	2.5955
8	3.1585e−08	3.5824	1.0419e−05	2.7553
16	2.2394e−09	3.8181	1.4227e−06	2.8725
32	1.4841e−10	3.9154	1.8586e−07	2.9363
64	9.5427e−12	3.9591	2.3751e−08	2.9681
128	6.0481e−13	3.9798	3.0020e−09	2.9840
256	3.8064e−14	3.9900	3.7733e−10	2.9920
512	2.3872e−15	3.9950	4.7297e−11	2.9960
1024	1.4946e−16	3.9975	5.9203e−12	2.9980

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Table 5.3
Three-point reconstruction: Lower and upper estimators of the error and effectivity indices when starting with the trapezoidal method

N	$\frac{1}{3}\mathcal{E}_1$	Err_1	Err_2	$\mathcal{E}_1 + 2\mathcal{E}_2$	Eff_1	Eff_2
2	3.1494e−06	7.4620e−06	1.8725e−05	9.3432e−05	0.4221	4.9897
4	2.2012e−07	4.8769e−07	1.9597e−06	9.1435e−06	0.4514	4.6659
8	1.3881e−08	3.2741e−08	1.5766e−07	7.1221e−07	0.4240	4.5175
16	8.5772e−10	2.1323e−09	1.0937e−08	4.8750e−08	0.4022	4.4573
32	5.3056e−11	1.3568e−10	7.1581e−10	3.1736e−09	0.3910	4.4335
64	3.2947e−12	8.5464e−12	4.5716e−11	2.0223e−10	0.3855	4.4235
128	2.0519e−13	5.3603e−13	2.8873e−12	1.2759e−11	0.3828	4.4190
256	1.2800e−14	3.3557e−14	1.8139e−13	8.0116e−13	0.3814	4.4168
512	7.9926e−16	2.0990e−15	1.1366e−14	5.0189e−14	0.3808	4.4158
1024	4.9930e−17	1.3124e−16	7.1127e−16	3.1404e−15	0.3804	4.4153

Table 5.4
Three-point reconstruction: Lower and upper estimators of the error and effectivity indices when starting with the Euler method

N	$\frac{1}{3}\mathcal{E}_1$	Err_1	Err_2	$\mathcal{E}_1 + 2\mathcal{E}_2$	Eff_1	Eff_2
2	1.1338e−06	3.1789e−04	8.0369e−04	8.5374e−04	0.0036	1.0623
4	1.2611e−07	3.6681e−05	9.3291e−05	1.4107e−04	0.0034	1.5121
8	1.0528e−08	3.0576e−06	7.9768e−06	2.0869e−05	0.0034	2.6162
16	7.4647e−10	2.1793e−07	6.0875e−07	2.8476e−06	0.0034	4.6778
32	4.9470e−11	1.4509e−08	4.2307e−08	3.7186e−07	0.0034	8.7896
64	3.1809e−12	9.3540e−10	2.8199e−09	4.7512e−08	0.0034	16.8488
128	2.0160e−13	5.9372e−11	1.8274e−10	6.0045e−09	0.0034	32.8584
256	1.2688e−14	3.7394e−12	1.1651e−11	7.5470e−10	0.0034	64.7745
512	7.9574e−16	2.3461e−13	7.3687e−13	9.4597e−11	0.0034	128.3760
1024	4.9820e−17	1.4691e−14	4.6343e−14	1.1841e−11	0.0034	255.5046

Table 5.5
Reconstruction (2.5): *Order of $\mathcal{E}_1$ and $\mathcal{E}_2$ when starting with the trapezoidal method*

N	$\mathcal{E}_1$	Order	$\mathcal{E}_2$	Order
2	1.0400e−05		1.5747e−05	
4	6.4597e−07	4.0089	2.5413e−06	2.6314
8	4.0247e−08	4.0045	2.2851e−07	3.4753
16	2.5128e−09	4.0015	1.6546e−08	3.7877
32	1.5701e−10	4.0004	1.1055e−09	3.9038
64	9.8121e−12	4.0001	7.1334e−11	3.9539
128	6.1324e−13	4.0000	4.5287e−12	3.9774
256	3.8327e−14	4.0000	2.8525e−13	3.9888
512	2.3955e−15	4.0000	1.7897e−14	3.9944
1024	1.4972e−16	4.0000	1.1207e−15	3.9972

Table 5.6
Reconstruction (2.5): Order of $\mathcal{E}_1$ and $\mathcal{E}_2$ when starting with the Euler method

N	$\mathcal{E}_1$	Order	$\mathcal{E}_2$	Order
2	9.0349e−06		2.7041e−03	
4	6.1876e−07	3.8680	4.2429e−04	2.6720
8	3.9782e−08	3.9592	6.0128e−05	2.8190
16	2.5052e−09	3.9891	8.0251e−06	2.9054
32	1.5688e−10	3.9972	1.0372e−06	2.9518
64	9.8101e−12	3.9993	1.3185e−07	2.9757
128	6.1321e−13	3.9998	1.6622e−08	2.9878
256	3.8327e−14	4.0000	2.0866e−09	2.9939
512	2.3955e−15	4.0000	2.6138e−10	2.9969
1024	1.4972e−16	4.0000	3.2707e−11	2.9985

Table 5.7
Reconstruction (2.5): Lower and upper estimators of the error and effectivity index when starting with the trapezoidal method

N	$\frac{1}{3}\mathcal{E}_1$	Err_1	Err_2	$\mathcal{E}_1 + 2\mathcal{E}_2$	Eff_1	Eff_2
2	3.4665e−06	7.2836e−06	1.8547e−05	4.1894e−05	0.4759	2.2588
4	2.1532e−07	4.7253e−07	1.9445e−06	5.7286e−06	0.4557	2.9461
8	1.3416e−08	3.2062e−08	1.5698e−07	4.9726e−07	0.4184	3.1677
16	8.3761e−10	2.1079e−09	1.0913e−08	3.5605e−08	0.3974	3.2627
32	5.2335e−11	1.3487e−10	7.1500e−10	2.3679e−09	0.3880	3.3118
64	3.2707e−12	8.5204e−12	4.5690e−11	1.5248e−10	0.3839	3.3373
128	2.0441e−13	5.3521e−13	2.8865e−12	9.6707e−12	0.3819	3.3503
256	1.2776e−14	3.3532e−14	1.8136e−13	6.0883e−13	0.3810	3.3569
512	7.9849e−16	2.0982e−15	1.1365e−14	3.8189e−14	0.3806	3.3603
1024	4.9905e−17	1.3122e−16	7.1124e−16	2.3911e−15	0.3803	3.3619

Table 5.8
Reconstruction (2.5): Lower and upper estimators of the error and effectivity index when starting with the Euler method

N	$\frac{1}{3}\mathcal{E}_1$	Err_1	Err_2	$\mathcal{E}_1 + 2\mathcal{E}_2$	Eff_1	Eff_2
2	3.0116e−06	3.0580e−04	7.9159e−04	5.4172e−03	0.0098	6.8434
4	2.0625e−07	3.6095e−05	9.2706e−05	8.4921e−04	0.0057	9.1602
8	1.3261e−08	3.0366e−06	7.9559e−06	1.2030e−04	0.0044	15.1203
16	8.3507e−10	2.1724e−07	6.0805e−07	1.6053e−05	0.0038	26.4004
32	5.2295e−11	1.4486e−08	4.2285e−08	2.0746e−06	0.0036	49.0615
64	3.2700e−12	9.3469e−10	2.8192e−09	2.6372e−07	0.0035	93.5427
128	2.0440e−13	5.9349e−11	1.8272e−10	3.3244e−08	0.0034	181.9447
256	1.2776e−14	3.7387e−12	1.1650e−11	4.1732e−09	0.0034	358.2005
512	7.9848e−16	2.3459e−13	7.3685e−13	5.2276e−10	0.0034	709.4492
1024	4.9905e−17	1.4691e−14	4.6342e−14	6.5414e−11	0.0034	1411.5429

Fig. 5.1. *Three-point reconstruction*: Log-log *graphs of the effectivity indices, of upper and lower estimator, when starting with the Euler and the trapezoidal method, respectively*

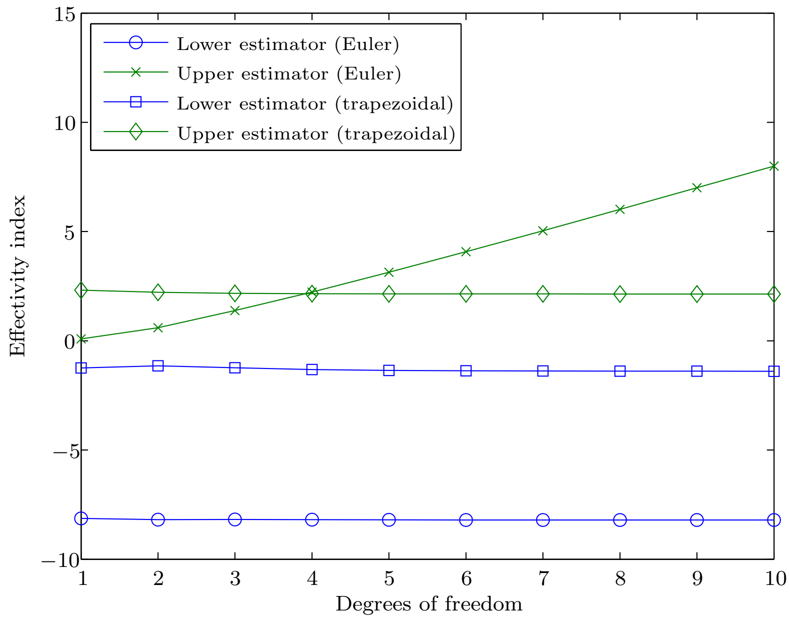

Fig. 5.2. *Reconstruction* (2.5): Log-log *graphs of the effectivity indices, of upper and lower estimator, when starting with the Euler and the trapezoidal method, respectively*