An adaptive time stepping method with efficient error control for second-order evolution problems

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Abstract This work is concerned with time stepping finite element methods for abstract second order evolution problems. We will derive optimal order a posteriori error estimates and a posteriori nodal superconvergence error estimates using the energy approach and the duality argument. With the help of the a posteriori error estimator developed in this work, we will further propose an adaptive time stepping strategy. A number of numerical experiments are performed to illustrate the reliability and efficiency of the a posteriori error estimates and to assess the effectiveness of the proposed adaptive time stepping method.

Keywords A posteriori error analysis, adaptive algorithm, reconstruction, evolution problems

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1 Introduction

Adaptive time stepping methods are very important in developing efficient algorithms for solving evolution problems arising from fluid dynamics, epitaxial growth and many other applied sciences (cf. [11, 13, 18, 20]). Such methods enable us to adopt feasible time steps to carry out time discretization, so that we are able to take much less computational cost to get numerical solutions with desired accuracy. The strategy for choosing time steps adaptively is very technical and problem oriented, and one typical approach is based on the a posteriori error estimator corresponding to the underlying problem (cf. [5, 7]). Hence, a posteriori error analysis in time plays an important role in constructing adaptive time stepping methods.

As far as we know, there have existed a very sophisticated investigation on a posteriori error analysis for abstract first order evolution problems (cf. [1–4, 10]). Precisely speaking, with the help of higher order appropriate reconstructions of the approximate solutions, the optimal order a posteriori error estimates of some time discretization methods were established in [1–3, 10]. Furthermore, a posteriori superconvergence estimates for the error at the nodes for Galerkin and Runge-Kutta methods were derived in [4]. However, there are few results about a posteriori error analysis for abstract second order evolution problems, which frequently occur in structural analysis (cf. [6, 8, 9]).

In honor of Prof. Zhongci Shi's 80th birthday.

In this paper, we are interested in developing a posteriori error analysis for abstract second-order evolution problems. More precisely, for any real number $T > 0$, seek $u : [0, T] \to D(A)$ satisfying

$$\begin{cases} u''(t) + Au(t) = f(t), \quad 0 < t < T, \\ u(0) = u_0, \\ u'(0) = v_0, \end{cases} \tag{1.1}$$

where $(\cdot)'$ and $(\cdot)''$ denote respectively the first and second order derivatives in time, A is a positive definite, self-adjoint, linear operator on a Hilbert space $(H, \langle\cdot,\, \cdot\rangle)$ with domain $D(A)$ dense in H, and f is a function from $[0, T]$ into H. Throughout this paper, we assume that

$$u_0,\, v_0 \in D(A), \quad f \in L^2(0, T;\, H). \tag{1.2}$$

To discretize Problem (1.1), we use a standard finite element approach for handling the second-order evolution problems, see, e.g., [8,9]. To this end, we use a non-uniform subdivision for the time interval $I := (0, T)$:

$$0 = t_0 < t_1 < \cdots < t_N = T,$$

and introduce the notations

$$J_n = (t_{n-1},\, t_n], \quad k_n = t_n - t_{n-1}, \quad 1 \leqslant n \leqslant N.$$

Define

$$\begin{aligned} \mathcal{V}_2 &= \left\{ v : \bar{I} \to D(A); v \in C(\bar{I}),\ v|_{J_n}(t) = \sum_{j=0}^{2} t^j w_j,\ w_j \in D(A),\ 1 \leqslant n \leqslant N \right\}, \\ \mathcal{W}_3 &= \left\{ v : \bar{I} \to D(A); v \in C^1(\bar{I}),\ v|_{J_n}(t) = \sum_{j=0}^{3} t^j w_j,\ w_j \in D(A),\ 1 \leqslant n \leqslant N \right\}, \\ \mathcal{H}_q &= \left\{ v : \bar{I} \to H; v|_{J_n}(t) = \sum_{j=0}^{q} t^j w_j,\ w_j \in H,\ 1 \leqslant n \leqslant N \right\}, \quad q = 1,\, 2,\, 4. \end{aligned}$$

Let $\mathcal{V}_2(J_n)$ and $\mathcal{W}_3(J_n)$ consist of the restrictions to J_n of the elements of $\mathcal{V}_2$ and $\mathcal{W}_3$, respectively. Similarly, denote by $\mathcal{H}_q(J_n)$ the restriction of $\mathcal{H}_q$ to J_n. Then our C^0-continuous time stepping finite element method for (1.1) is to find $U \in \mathcal{V}_2$ such that

$$\begin{cases} \displaystyle\int_{J_n} \big(\langle U'',\, w'\rangle + \langle F(t,\, U),\, w'\rangle\big)\, \mathrm{d}t + \langle \dot{U}_+^{n-1} - \dot{U}_-^{n-1},\, \dot{w}_+^{n-1}\rangle = 0 \\ \qquad\qquad\qquad\qquad \forall\, w \in \mathcal{V}_2(J_n), \quad 1 \leqslant n \leqslant N, \\ U^0 = u_0, \quad \dot{U}_-^0 = v_0, \end{cases} \tag{1.3}$$

where

$$\begin{aligned} &\dot{w}_\pm^{n-1} := \lim_{s\to 0^+} w'(t_n \pm s), \quad w^{n-1} := w(t_{n-1}), \\ &F(t,\, U) := AU - f(t). \end{aligned}$$

For the method (1.3), in order to develop a posteriori error analysis with desired accuracy, we require as in [1–4, 10] to technically devise a higher order reconstruction $\tilde{U}$ or $\widehat{U}$ from U in advance. Then, in light of this reconstruction and using the energy method, we are able to obtain suboptimal/optimal a posteriori error estimates for $u - U$ and $(u - U)'$. Moreover, applying the duality method in [8, 9], we also derive a posteriori superconvergence error estimator at the time nodes. All the estimates (estimators) given before are computable quantities depending only on the discrete solution U and the prescribed data of the continuous problem, with the constants explicitly given. Based on the available a posteriori error estimates, using the error equidistribution strategy (cf. [5, 12]), and following some ideas implied in the Runge-Kutta-Felberg method (cf. [17]), we then design an adaptive time stepping method related to (1.3). Finally, we perform a series of numerical examples to show the reliability and efficiency of our a posteriori error estimates (estimators) as well as the effectiveness of our adaptive time stepping method.

The remainder of this paper is organized as follows. The higher order reconstruction $\tilde{U}$ or $\widehat{U}$ from U and the corresponding suboptimal/optimal a posteriori error analysis are given in Sections 2 and 3, respectively. The a posteriori superconvergence error estimator at the time nodes is provided in Section 4. The adaptive time stepping method is devised and discussed in Section 5. In Section 6, a series of numerical experiments are performed to illustrate the reliability and efficiency of our a posteriori error estimates (estimators) and to assess the effectiveness of our adaptive time stepping method. Some concluding remarks are given in the final section.

2 Suboptimal a posteriori error analysis

The usual way for bounding the error $e := u - U$ of (1.3) is based on the corresponding error equation $e''(t) + Ae(t) = -R(t)$, where the residual $R(t)$ is defined by

$$R(t) = U''(t) + AU(t) - f(t), \quad t \in J_n, \tag{2.1}$$

or equivalently,

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

in view of (1.1). However, by the error analysis for finite elements, the magnitude of the quantity $R(t)$ is $O(k_n)$, and hence we can not derive sharp estimate for the error $e(t)$ through the previous error equation. For completeness, we show $R(t)$ is exactly $O(k_n)$ by an example. Consider an ordinary differential equation $u''(t) = f(t) = ct + d$ with $c \neq 0$ and d two real constants. First of all, we recall from [9] that in any J_n,

$$\begin{aligned} U(t) = \Big(& U^{n-1}(t - t_n)^2 + U^n\big(- (t - t_{n-1})^2 + 2k_n(t - t_{n-1})\big) \\ & + \dot{U}^n_-\big(k_n(t - t_{n-1})^2 - k_n^2(t - t_{n-1})\big)\Big) \Big/ k_n^2, \end{aligned} \tag{2.3}$$

which together with (2.1) implies

$$R(t) = (2U^{n-1} - 2U^n + 2k_n\dot{U}^n_-)/k_n^2 - f(t), \quad t \in J_n. \tag{2.4}$$

On the other hand, we find after a direct manipulation that

$$U^n = u^n, \quad \dot{U}^n_- = u'(t_n), \quad 1 \leqslant n \leqslant N. \tag{2.5}$$

The combination of (2.4) and (2.5) then gives

$$\begin{aligned}
R(t) &= \big(2u^{n-1} - 2u^n + 2k_n u'(t_n)\big)/k_n^2 - f(t) \\
&= \frac{2}{k_n^2}\int_{t^{n-1}}^{t^n} (s - t_{n-1}) u''(s)\,\mathrm{d}s - f(t) \\
&= \frac{2}{k_n^2}\int_{t^{n-1}}^{t^n} (s - t_{n-1}) f(s)\,\mathrm{d}s - f(t) \\
&= \frac{2}{k_n^2}\int_{t^{n-1}}^{t^n} (s - t_{n-1})(cs + d)\,\mathrm{d}s - (ct + d) \\
&= c(t_{n-1} - t) + 2ck_n/3, \quad t \in J_n,
\end{aligned}$$

which implies that $R(t)$ is indeed of the size $O(k_n)$ in this case.

Therefore, as in [1–4,10], we require a higher order reconstruction $\widetilde{U}$ or $\widehat{U}$ from U, which are devised in an appropriate way, in order to establish our a posteriori error analysis with desired accuracy.

2.1 Reconstruction

We first introduce an invertible linear operator $\widetilde{I}_3$: $\mathcal{V}_2 \to \mathcal{W}_3$ as follows. With every $w \in \mathcal{V}_2$ we associate an element $\widetilde{w} := \widetilde{I}_3 w \in \mathcal{W}_3$ defined by locally interpolating in each subinterval $J_n (1 \leqslant n \leqslant N)$, i.e. $\widetilde{w}|_{J_n} \in \mathcal{W}_3(J_n)$ is uniquely determined by

$$\begin{cases}
\widetilde{w}(t_n) = w(t_n), \\
\widetilde{w}(t_{n-1}) = w(t_{n-1}), \\
\widetilde{w}'(t_n) = \dot{w}_-^n, \\
\widetilde{w}'(t_{n-1}) = \begin{cases} v_0, & n = 1, \\ \dot{w}_-^{n-1}, & 2 \leqslant n \leqslant N. \end{cases}
\end{cases} \tag{2.6}$$

We call $\widetilde{w}$ a time reconstruction of w. Conversely, if $\widetilde{w} \in \mathcal{W}_3$ is given and $I_2 : \mathcal{W}_3 \to \mathcal{V}_2$ is the interpolation operator defined by

$$\begin{cases}
(\dot{I_2 \varphi})_-^n = \varphi'(t_n), \\
I_2\varphi(t_n) = \varphi(t_n), \\
I_2\varphi(t_{n-1}) = \varphi(t_{n-1}),
\end{cases}$$

$1 \leqslant n \leqslant N$, we can recover w locally via interpolation, i.e. $w = I_2\widetilde{w}$. Thus, $I_2 = \widetilde{I}_3^{-1}$.

Using the reconstruction $\widetilde{U} \in \mathcal{W}_3$ of $U \in \mathcal{V}_2$ which is the solution of (1.3), we can deduce from (2.6) that

$$\int_{J_n} \langle \widetilde{U}' - U', w'' \rangle \,\mathrm{d}t = 0 \quad \forall\, w \in \mathcal{V}_2(J_n). \tag{2.7}$$

Hence, for every $w \in \mathcal{V}_2(J_n)$, $1 \leqslant n \leqslant N$ using integration by parts, (2.7) and (2.6) gives

$$
\begin{aligned}
& \int_{J_n} \langle \widetilde{U}'', w' \rangle \,\mathrm{d}t = \langle \widetilde{U}'(t_n), \dot{w}_-^n \rangle - \langle \widetilde{U}'(t_{n-1}), \dot{w}_+^{n-1} \rangle - \int_{J_n} \langle \widetilde{U}', w'' \rangle \,\mathrm{d}t \\
= \quad & \langle \widetilde{U}'(t_n), \dot{w}_-^n \rangle - \langle \widetilde{U}'(t_{n-1}), \dot{w}_+^{n-1} \rangle - \int_{J_n} \langle U', w'' \rangle \,\mathrm{d}t \\
= \quad & \langle \widetilde{U}'(t_n), \dot{w}_-^n \rangle - \langle \widetilde{U}'(t_{n-1}), \dot{w}_+^{n-1} \rangle - \Big(\langle \dot{U}_-^n, \dot{w}_-^n \rangle - \langle \dot{U}_+^{n-1}, \dot{w}_+^{n-1} \rangle - \int_{J_n} \langle U'', w' \rangle \,\mathrm{d}t \Big) \\
= \quad & \langle \dot{U}_+^{n-1} - \dot{U}_-^{n-1}, \dot{w}_+^{n-1} \rangle + \int_{J_n} \langle U'', w' \rangle \,\mathrm{d}t. \qquad (2.8)
\end{aligned}
$$

Plugging (2.8) into (1.3), we immediately obtain

$$
\int_{J_n} \big(\langle \widetilde{U}'', w' \rangle + \langle F(t, U), w' \rangle \big) \,\mathrm{d}t = 0 \quad \forall\, w \in \mathcal{V}_2(J_n), \quad 1 \leqslant n \leqslant N,
$$

which is equivalent to

$$
\int_{J_n} \big(\langle \widetilde{U}'', w' \rangle + \langle F(t, I_2\widetilde{U}), w' \rangle \big) \,\mathrm{d}t = 0 \quad \forall\, w \in \mathcal{V}_2(J_n), \quad 1 \leqslant n \leqslant N,
$$

i.e.

$$
\widetilde{U}'' + P_1 F(t, I_2\widetilde{U}) = 0 \quad \forall\, t \in J_n, \tag{2.9}
$$

where P_q $(q = 1, 2)$ is the (local) L^2 orthogonal projection operator onto $\mathcal{H}_q(J_n)$ (cf. [4]). Consequently, for each n,

$$
\int_{J_n} \langle P_q v - v, w \rangle \,\mathrm{d}t = 0 \quad \forall\, w \in \mathcal{H}_q(J_n).
$$

2.2 Energy estimates

Let $V := D(A^{1/2})$ and denote the norms in H and in V by $|\cdot|$ and $\|\cdot\|$, with $\|v\| := |A^{1/2}v| = \langle Av, v \rangle^{1/2}$, respectively. We also use the following norm notations:

$$
\|v\|_{L^\infty(G)} := \operatorname*{ess\,sup}_{t \in G} \|v(t)\|, \quad |v|_{L^\infty(G)} := \operatorname*{ess\,sup}_{t \in G} |v(t)|.
$$

Under the assumption (1.2), we know from [15] that there exists a unique weak solution $u \in C([0, T]; V) \bigcap C^1([0, T]; H)$ to the evolution problem (1.1).

Let $\widetilde{R}$ be the residual of $\widetilde{U}$ given by

$$
\widetilde{R}(t) := \widetilde{U}''(t) + A\widetilde{U} - f(t), \quad t \in J_n,\ 1 \leqslant n \leqslant N. \tag{2.10}
$$

Subtracting (2.10) from the differential equation in (1.1), we readily have

$$
\widetilde{e}''(t) + A\widetilde{e} = -\widetilde{R}(t), \tag{2.11}
$$

where $\widetilde{e} := u - \widetilde{U}$. Testing (2.11) by $\widetilde{e}'$ and integrating over $t \in [0, \tau]$ gives

$$
\int_0^\tau \big(\langle \widetilde{e}''(s), \widetilde{e}'(s) \rangle + \langle A\widetilde{e}(s), \widetilde{e}'(s) \rangle \big) \,\mathrm{d}s = \int_0^\tau \langle -\widetilde{R}(s), \widetilde{e}'(s) \rangle \,\mathrm{d}s, \tag{2.12}
$$

Using the fact that $\widetilde{e}(0) = \widetilde{e}'(0) = 0$ and integration by parts gives

$$\frac{1}{2}\left|\widetilde{e}'(\tau)\right|^2 + \frac{1}{2}\left\|\widetilde{e}(\tau)\right\|^2 = \int_0^\tau \langle -\widetilde{R}(s),\, \widetilde{e}'(s)\rangle\,\mathrm{d}s, \quad \tau \in [0, t], \tag{2.13}$$

which yields

$$\begin{aligned} &\frac{1}{2}\big(\max_{0\leqslant\tau\leqslant t} |\widetilde{e}'(\tau)|\big)^2 \\ \leqslant\ & \max_{0\leqslant\tau\leqslant t}\int_0^\tau |\langle \widetilde{R}(s),\, \widetilde{e}'(s)\rangle|\,\mathrm{d}s \\ \leqslant\ & \int_0^t |\langle \widetilde{R}(s),\, \widetilde{e}'(s)\rangle|\,\mathrm{d}s \leqslant \max_{0\leqslant\tau\leqslant t} |\widetilde{e}'(\tau)| \int_0^t |\widetilde{R}(s)|\,\mathrm{d}s. \end{aligned}$$

Consequently, we have

$$\max_{0\leqslant\tau\leqslant t} |\widetilde{e}'(\tau)| \leqslant 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s. \tag{2.14}$$

It then follows from (2.13)-(2.14) that

$$\begin{aligned} &\frac{1}{2}\big(\max_{0\leqslant\tau\leqslant t} \|\widetilde{e}(\tau)\|\big)^2 \leqslant \int_0^t |\langle \widetilde{R}(s),\, \widetilde{e}'(s)\rangle|\,\mathrm{d}s \\ \leqslant\ & \max_{0\leqslant\tau\leqslant t} |\widetilde{e}'(\tau)| \int_0^t |\widetilde{R}(s)|\,\mathrm{d}s \leqslant 2\big(\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s\big)^2, \end{aligned}$$

which leads to

$$\max_{0\leqslant\tau\leqslant t} \|\widetilde{e}(\tau)\| \leqslant 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s.$$

Obviously, using the triangle inequality we have

$$|(U-\widetilde{U})'|_{L^\infty((0,\,t))} \leqslant |(u-U)'|_{L^\infty((0,\,t))} + \max_{0\leqslant\tau\leqslant t} |(u-\widetilde{U})'(\tau)|. \tag{2.15}$$

Summarizing the above results, we can get a posteriori error estimates for the method (1.3) as described in the following theorem.

Theorem 2.1. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively and let $\widetilde{U}$ be the reconstruction of U by* (2.6)*. Then, for $t \in [0, T]$, there hold the following a posteriori error estimates:*

$$\max_{0\leqslant\tau\leqslant t} \left|(u-\widetilde{U})'(\tau)\right| \leqslant 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s, \tag{2.16}$$

$$\max_{0\leqslant\tau\leqslant t} \left\|(u-\widetilde{U})(\tau)\right\| \leqslant 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s, \tag{2.17}$$

where the a posteriori quantity $\widetilde{R}$ is given by (2.10)*. Moreover, we have the following lower estimate:*

$$|(U-\widetilde{U})'|_{L^\infty((0,\,t))} \leqslant |(u-U)'|_{L^\infty((0,\,t))} + \max_{0\leqslant\tau\leqslant t} |(u-\widetilde{U})'(\tau)|.$$

Let τ_1 and τ_2 be the zeroes of $l_2(t) := \sqrt{\frac{5}{8}}(3t^2 - 1)$, where $l_2(t)$ is exactly the third orthonormal Legendre polynomial in $[-1, 1]$. Write

$$t_{n,i} := \frac{t_{n-1} + t_n}{2} + \frac{k_n}{2}\tau_i, \quad i = 1, 2, \quad 1 \leqslant n \leqslant N.$$

Lemma 2.2. *For $s \in J_n$, $1 \leqslant n \leqslant N$,*

$$U(s) - \widetilde{U}(s) = -\frac{1}{6}k_n^3 \widetilde{U}^{(3)}\big(\frac{s - t_{n-1}}{k_n}\big)\big(\frac{s - t_n}{k_n}\big)^2, \tag{2.18}$$

$$U(s) - P_1U(s) = \frac{1}{8}k_n^2 U'' \prod_{i=1}^{2}\big(\frac{2s - t_{n-1} - t_n}{k_n} - \tau_i\big). \tag{2.19}$$

Moreover, for $t \in J_n$, $1 \leqslant n \leqslant N$, there holds

$$\begin{aligned} &2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s \qquad (2.20)\\ \leqslant &\sum_{m=1}^{n}\left(\frac{1}{36}k_m^4 |A\widetilde{U}^{(3)}|_{L^\infty(J_m)} + \frac{\sqrt{3}}{27}k_m^3 |AU''|_{L^\infty(J_m)} + 2\int_{J_m} |f(s) - P_1 f(s)|\,\mathrm{d}s\right). \end{aligned}$$

Proof. It follows from (2.6) that

$$(U - \widetilde{U})(t_{n-1}) = (U - \widetilde{U})(t_n) = \dot{U}_-^n - \widetilde{U}'(t_n) = 0,$$

which yields

$$U(s) - \widetilde{U}(s) = -\frac{1}{6}k_n^3 \widetilde{U}^{(3)}\left(\frac{s - t_{n-1}}{k_n}\right)\left(\frac{s - t_n}{k_n}\right)^2.$$

Let p_2 be the third Legendre polynomial shifted to J_n and normalized, i.e.

$$p_2(t) = \sqrt{\frac{2}{k_n}}\, l_2\left(\frac{2t - t_{n-1} - t_n}{k_n}\right), \quad t \in J_n.$$

Noting that

$$U(s) - P_1U(s) = P_2U(s) - P_1U(s) = \int_{J_n} U(t)p_2(t)\,\mathrm{d}t \cdot p_2(s),$$

we have

$$(U - P_1U)(t_{n,i}) = 0, \quad i = 1, 2,$$

from which it follows that

$$U(s) - P_1U(s) = \frac{1}{8}k_n^2 U'' \prod_{i=1}^{2}\left(\frac{2s - t_{n-1} - t_n}{k_n} - \tau_i\right), \quad s \in J_n.$$

From (2.9) and (2.10), $\widetilde{R}(s)$ can be expressed as

$$\widetilde{R}(s) = A(\widetilde{U} - U)(s) + A(U - P_1U)(s) - (f - P_1 f)(s). \tag{2.21}$$

Using (2.18)-(2.19) and (2.21), we can obtain (2.20) by some direct computation. □

We then differentiate (2.18) with respect to s to get

$$(U - \widetilde{U})'(s) = -\frac{1}{6}k_n^2 \widetilde{U}^{(3)}\Big(\big(\frac{s - t_n}{k_n}\big)^2 + 2\big(\frac{s - t_{n-1}}{k_n}\big)\big(\frac{s - t_n}{k_n}\big)\Big),$$

leading to

$$|(U - \widetilde{U})'|_{L^\infty(J_n)} = \frac{1}{6}k_n^2 |\widetilde{U}^{(3)}|_{L^\infty(J_n)}, \quad 1 \leqslant n \leqslant N. \tag{2.22}$$

Applying (2.16), (2.22) and noting that

$$|(u - U)'|_{L^\infty((0,t))} \leqslant \max_{0 \leqslant \tau \leqslant t} \big|(u - \widetilde{U})'(\tau)\big| + |(U - \widetilde{U})'|_{L^\infty((0,t))},$$

we obtain the following result.

Theorem 2.3. *Let u and U be the solutions of* (1.1) *and* (1.3), *respectively and let $\widetilde{U}$ be the reconstruction of U by* (2.6). *Then, for $t \in J_n$, $1 \leqslant n \leqslant N$, there holds*

$$|(u-U)'|_{L^\infty((0,\,t))} \leqslant \frac{1}{6} \max_{1\leqslant m\leqslant n} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)} + 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s.$$

The following result is a direct consequence of Theorems 2.1, 2.3 and (2.22).

Corollary 2.1. *Let u and U be the solutions of* (1.1) *and* (1.3), *respectively and let $\widetilde{U}$ be the reconstruction of U by* (2.6). *Then, for $t \in J_n$, $1 \leqslant n \leqslant N$, there hold the following lower and upper bounds:*

$$\begin{aligned}
&\frac{1}{6} \max_{1\leqslant m\leqslant n} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)} \\
&\leqslant |(u-U)'|_{L^\infty((0,\,t))} + \max_{0\leqslant \tau\leqslant t} \left|(u-\widetilde{U})'(\tau)\right| \\
&\leqslant \frac{1}{6} \max_{1\leqslant m\leqslant n} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)} + 4\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s,
\end{aligned}$$

where the a posteriori quantity $\widetilde{R}$ is given by (2.10).

Recall that $\widetilde{U}$ is C^1-continuous on $\bar{I}$ and its restriction to any J_n is a third order polynomial in the variable t, so $\widetilde{U}|_{J_n}$ is uniquely determined by U^{n-1}, U^n, $\dot{U}_-^{n-1}$ and $\dot{U}_-^n$. After some direct computation we have, for $t \in J_n$, $1 \leqslant n \leqslant N$,

$$\begin{aligned}
\widetilde{U}(t) \quad = \quad & U^{n-1}\lambda_0\left(\frac{t-t_{n-1}}{k_n}\right) + k_n\dot{U}_-^{n-1}\phi_0\left(\frac{t-t_{n-1}}{k_n}\right) \\
& + U^n\lambda_1\left(\frac{t-t_{n-1}}{k_n}\right) + k_n\dot{U}_-^{n}\phi_1\left(\frac{t-t_{n-1}}{k_n}\right),
\end{aligned}$$

where

$$\begin{aligned}
\lambda_0(\xi) &= (1-\xi)^2(2\xi+1), \quad & \phi_0(\xi) &= \xi(1-\xi)^2, \\
\lambda_1(\xi) &= \xi^2(3-2\xi), & \phi_1(\xi) &= -\xi^2(1-\xi),
\end{aligned}$$

which are the Hermite cubic interpolation basis functions on the reference interval [0, 1] (cf. [14,16]). Thus, it is easy to get

$$\widetilde{U}^{(3)}(t) = \frac{6}{k_n^3}\left(2U^{n-1} - 2U^n + k_n\dot{U}_-^{n-1} + k_n\dot{U}_-^n\right), \quad t \in J_n.$$

On the other hand, we note that

$$\begin{aligned}
U(t) \quad = \quad & U^{n-1}\lambda_0\left(\frac{t-t_{n-1}}{k_n}\right) + k_n\dot{U}_+^{n-1}\phi_0\left(\frac{t-t_{n-1}}{k_n}\right) \\
& + U^n\lambda_1\left(\frac{t-t_{n-1}}{k_n}\right) + k_n\dot{U}_-^{n}\phi_1\left(\frac{t-t_{n-1}}{k_n}\right),
\end{aligned}$$

which leads to

$$U - \widetilde{U} = k_n(\dot{U}_+^{n-1} - \dot{U}_-^{n-1})\phi_0\left(\frac{t-t_{n-1}}{k_n}\right), \quad t \in J_n.$$

Consequently, we obtain

$$\widetilde{U}^{(3)}(t) = -\frac{6}{k_n^2}(\dot{U}_+^{n-1} - \dot{U}_-^{n-1}), \quad t \in J_n. \tag{2.23}$$

That means, the a posteriori error estimate given in Theorem 2.3 can be expressed as

$$|(u-U)'|_{L^\infty((0,\,t))} \leqslant \max_{1\leqslant m\leqslant n} |\dot{U}_+^{n-1} - \dot{U}_-^{n-1}| + 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s, \tag{2.24}$$

which is quite similar to the a posteriori error estimate corresponding to the finite element method in space (cf. [19]).

Remark 1. If f admits two time derivatives and the discrete solution U admits the optimal a priori error estimates, then we can check from (2.20) that the magnitude of the quantity $\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s$ is of order 2 with respect to the time step k_m. Hence, noting that U is a piecewise polynomial of degree 2, we get the optimal order (2 order) a posteriori error estimates for the time derivative of the error $u-U$ (cf. Theorem 2.3 and Corollary 2.1). However, (2.17) only yields an a posteriori error estimate of order 2 for the error $u-U$, which is suboptimal (the best order is 3). To recover the optimal order a posteriori error estimate on $u-U$, we require to introduce a new reconstruction $\widehat{U}$ of the approximate solution U, as shown in the next section.

3 Optimal a posteriori error analysis

3.1 Optimal reconstruction

Denote $\widehat{U}(t) \in \mathcal{H}_4$ by

$$\widehat{U}(t) = \widetilde{U}(t) + \int_{t_{n-1}}^t \Big(\int_{t_{n-1}}^\sigma (P_2 - P_1)\big(-AU(s) + f(s)\big)\,\mathrm{d}s\Big)\,\mathrm{d}\sigma, \quad t \in J_n,\ 1 \leqslant n \leqslant N. \tag{3.1}$$

We call $\widehat{U}$ an optimal reconstruction of U. It is easy to check that $\widehat{U}(t_n) = \widetilde{U}(t_n) = U(t_n)$ by changing the order of integration in (3.1) and conclude $\widehat{U}$ is continuous in $[0,\,T]$. On the other hand, for $t \in J_n$,

$$\widehat{U}'(t) = \widetilde{U}'(t) + \int_{t_{n-1}}^t (P_2 - P_1)\big(-AU(s) + f(s)\big)\,\mathrm{d}s,$$

which implies

$$\widehat{U}'(t_n) = \widetilde{U}'(t_n) = \dot{U}_-^n \tag{3.2}$$

and $\widehat{U}'(t)$ is continuous in $[0,\,T]$. It is also easy to show that

$$\widehat{U}''(t) = \widetilde{U}''(t) + (P_2 - P_1)\big(-AU(t) + f(t)\big), \quad t \in J_n, \tag{3.3}$$

which combined with (2.9) gives

$$\widehat{U}''(t) = P_2\big(f(t) - AU(t)\big), \quad t \in J_n, \tag{3.4}$$

i.e. $\widehat{U}$ satisfies

$$\widehat{U}'' + P_2 F(t,\, I_2\widetilde{U}) = 0, \quad t \in J_n.$$

Let $\widehat{R}$ be the residual of $\widehat{U}$,

$$\widehat{R}(t) := \widehat{U}''(t) + A\widehat{U} - f(t), \quad t \in J_n,\, 1 \leqslant n \leqslant N. \tag{3.5}$$

Subtracting (3.5) from the differential equation in (1.1), we can get the error equation

$$\widehat{e}''(t) + A\widehat{e} = -\widehat{R}(t), \tag{3.6}$$

where $\widehat{e} := u - \widehat{U}$.

3.2 Error estimates

We first note that

$$\widehat{e}(0) = \widehat{e}'(0) = 0. \tag{3.7}$$

Then applying the similar argument for deriving Theorem 2.1 (see (2.12)-(2.15)), we can readily obtain the a posteriori error estimates for $u - \widehat{U}$ and its time derivative, as described in the following theorem.

Theorem 3.1. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively and let $\widehat{U}$ be the optimal reconstruction of U by* (3.1)*. Then, for $t \in [0, T]$, there hold*

$$\max_{0\leqslant\tau\leqslant t} \left|(u - \widehat{U})'(\tau)\right| \leqslant 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s, \tag{3.8}$$

$$\max_{0\leqslant\tau\leqslant t} \left\|(u - \widehat{U})(\tau)\right\| \leqslant 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s, \tag{3.9}$$

where the a posteriori quantity $\widehat{R}$ is given by (3.5)*. Moreover, we have the lower estimate*

$$\max_{0\leqslant\tau\leqslant t} \|(U - \widehat{U})(\tau)\| \leqslant \max_{0\leqslant\tau\leqslant t} \|(u - U)(\tau)\| + \max_{0\leqslant\tau\leqslant t} \|(u - \widehat{U})(\tau)\|.$$

Lemma 3.2. *For $s \in J_n$, $1 \leqslant n \leqslant N$,*

$$\widehat{U}(s) - \widetilde{U}(s) = \frac{1}{32}k_n^4\widehat{U}^{(4)}\psi\Big(\frac{2s - t_{n-1} - t_n}{k_n}\Big), \tag{3.10}$$

where $\psi(x) = \frac{1}{12}(x^2-1)^2$. Thus, for $1 \leqslant m \leqslant N$, we have

$$\|\widehat{U} - \widetilde{U}\|_{L^\infty(J_m)} = \frac{1}{384}k_m^4\|\widehat{U}^{(4)}\|_{L^\infty(J_m)}, \tag{3.11}$$

$$|(\widehat{U} - \widetilde{U})'|_{L^\infty(J_m)} = \frac{\sqrt{3}}{216}k_m^3|\widehat{U}^{(4)}|_{L^\infty(J_m)}. \tag{3.12}$$

Moreover, for $t \in J_n$, $1 \leqslant n \leqslant N$, there hold the following explicit upper estimates:

$$\max_{0\leqslant\tau\leqslant t} \|(U - \widehat{U})(\tau)\| \leqslant \frac{1}{384}\max_{1\leqslant m\leqslant n} k_m^4\|\widehat{U}^{(4)}\|_{L^\infty(J_m)} + \frac{1}{81}\max_{1\leqslant m\leqslant n} k_m^3\|\widetilde{U}^{(3)}\|_{L^\infty(J_m)}, \tag{3.13}$$

$$2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s \leqslant \sum_{m=1}^{n}\Big(\frac{1}{360}k_m^5|A\widehat{U}^{(4)}|_{L^\infty(J_m)} + \frac{1}{36}k_m^4|A\widetilde{U}^{(3)}|_{L^\infty(J_m)} + 2\int_{J_m}|f(s) - P_2 f(s)|\,\mathrm{d}s\Big). \tag{3.14}$$

Proof. It follows from (3.3) and the fact that $(\widehat{U}-\widetilde{U})''$ is a multiple of the Legendre polynomial of second order that

$$(\widehat{U}-\widetilde{U})''(t_{n,i}) = 0, \quad i = 1, 2, \tag{3.15}$$

$$(\widehat{U}-\widetilde{U})''(s) = \frac{1}{2}\widehat{U}^{(4)}(s-t_{n,1})(s-t_{n,2}). \tag{3.16}$$

Integrating (3.16) twice with respect to s gives (3.10), and a direct consequence of (3.10) yields (3.11) and (3.12). Moreover, the estimate (3.13) follows immediately from (3.11), (2.18) and the triangle inequality.

Owing to (3.4) and (3.5), $\widehat{R}(s)$ can be expressed as

$$\begin{aligned}\widehat{R}(s) &= A(\widehat{U}-U)(s) - (f-P_2 f)(s),\\ &= A(\widehat{U}-\widetilde{U})(s) + A(\widetilde{U}-U)(s) - (f-P_2 f)(s).\end{aligned}$$

Thus, using (2.18) and (3.10) we can get (3.14) by some direct computation. □

Remark 2. It follows from (3.4) that

$$\widehat{U}^{(4)} = \big(P_2(f-AU)\big)'' = -AU'' + (P_2 f)'',$$

so the constant $\widehat{U}^{(4)}$ can be computed easily.

Since $u-U = (u-\widehat{U})+(\widehat{U}-U)$, we can readily obtain the following result by using Theorem 3.1 and the triangle inequality.

Theorem 3.3. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively and let $\widehat{U}$ be the optimal reconstruction of U by* (3.1)*. Then, for $t \in J_n$, $1 \leqslant n \leqslant N$, there holds the following optimal order a posteriori error estimate:*

$$\max_{0\leqslant\tau\leqslant t} \big\|(u-U)(\tau)\big\| \leqslant 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s + \max_{0\leqslant\tau\leqslant t} \|(U-\widehat{U})(\tau)\|,$$

where the a posteriori quantity $\widehat{R}$ is given by (3.5)*.*

Applying Theorem 3.1 and Theorem 3.3 we can easily have

Corollary 3.1. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively. Let $\widehat{U}$ be the optimal reconstruction of U by* (3.1)*. Then, for $t \in J_n$, $1 \leqslant n \leqslant N$, there hold the following lower and upper bounds:*

$$\begin{aligned}&\max_{0\leqslant\tau\leqslant t} \|(U-\widehat{U})(\tau)\|\\ &\leqslant \max_{0\leqslant\tau\leqslant t} \|(u-U)(\tau)\| + \max_{0\leqslant\tau\leqslant t} \big\|(u-\widehat{U})(\tau)\big\|\\ &\leqslant \max_{0\leqslant\tau\leqslant t} \|(U-\widehat{U})(\tau)\| + 4\int_0^t |\widehat{R}(s)|\,\mathrm{d}s,\end{aligned}$$

where the a posteriori quantity $\widehat{R}$ is given by (3.5)*.*

Remark 3. If f admits three time derivatives and the discrete solution U admits the optimal a priori error estimates, then we have from (3.14) that the order of the quantity $\int_0^t |\widehat{R}(s)|\,\mathrm{d}s$ is 3. Hence, from (3.13) we find the optimal order (3 order) a posteriori error estimates are obtained in Theorem 3.3 and Corollary 3.1.

The following result is a direct consequence of Theorem 3.1, (3.11)-(3.12).

Corollary 3.2. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively. Let $\widetilde{U}$ be the reconstruction of U by* (2.6) *and $\widehat{U}$ be the optimal reconstruction of U by* (3.1)*. Then, for $t \in [0, T]$,*

$$\max_{0\leqslant\tau\leqslant t} \left|(u-\widetilde{U})'(\tau)\right| \leqslant 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s + \frac{\sqrt{3}}{216}\max_{1\leqslant m\leqslant n} k_m^3 |\widehat{U}^{(4)}|_{L^\infty(J_m)}, \tag{3.17}$$

$$\max_{0\leqslant\tau\leqslant t} \|(u-\widetilde{U})(\tau)\| \leqslant 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s + \frac{1}{384}\max_{1\leqslant m\leqslant n} k_m^4 \|\widehat{U}^{(4)}\|_{L^\infty(J_m)}, \tag{3.18}$$

where the a posteriori quantity $\widehat{R}$ is given by (3.5).

Using Theorems 2.1 and 2.3, (2.22) and (3.17), we can get the following result.

Corollary 3.3. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively. Let $\widetilde{U}$ be the reconstruction of U by* (2.6) *and $\widehat{U}$ be the optimal reconstruction of U by* (3.1)*. Then, for $t \in J_n$, $1 \leqslant n \leqslant N$,*

$$\begin{aligned}
&\frac{1}{6}\max_{1\leqslant m\leqslant n} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)} \\
&\leqslant |(u-U)'|_{L^\infty((0,\,t))} + \max_{0\leqslant\tau\leqslant t}\left|(u-\widetilde{U})'(\tau)\right| \\
&\leqslant \frac{1}{6}\max_{1\leqslant m\leqslant n} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)} + 2\int_0^t |\widetilde{R}(s)|\,\mathrm{d}s + 2\int_0^t |\widehat{R}(s)|\,\mathrm{d}s \\
&\qquad + \qquad \frac{\sqrt{3}}{216}\max_{1\leqslant m\leqslant n} k_m^3 |\widehat{U}^{(4)}|_{L^\infty(J_m)},
\end{aligned} \tag{3.19}$$

where the a posteriori quantities $\widetilde{R}$ and $\widehat{R}$ are given by (2.10) *and* (3.5)*, respectively.*

Remark 4. If f admits three time derivatives and the discrete solution U admits the optimal a priori error estimates, then all the right terms in (3.17)-(3.18) are of three order while those in (2.16)-(2.17) are of two order. Therefore, Corollaries 3.2 and 3.3 improve the results in Theorem 2.1 and Corollary 2.1, respectively.

4 Nodal superconvergence

In this section, we shall apply the duality method used in [8, 9] to obtain a posteriori error estimates at the time nodes.

For $n \in \{1, \ldots, N\}$, let g be the solution of the following backward homogeneous problem

$$\begin{cases} g''(t) + Ag(t) = 0, \quad 0 < t < t_n, \\ g(t_n) = \mu, \\ g'(t_n) = \nu. \end{cases} \tag{4.1}$$

It is easy to see that

$$\int_t^{t_n} \langle g'' + Ag,\, g'\rangle\,\mathrm{d}t = 0,$$

from which and the integration by parts it follows that

$$\|g(t)\|^2 + |g'(t)|^2 = \|\mu\|^2 + |\nu|^2, \quad t \in [0, t_n]. \tag{4.2}$$

Hence, we take $\mu = 0$, $\nu = \widehat{e}'(t_n)$ in (4.1) to get

$$\begin{aligned}
|\dot{e}_-^n|^2 = |\widehat{e}'(t_n)|^2 &= \int_0^{t_n} \langle \widehat{e}', g' \rangle' \, \mathrm{d}t = \int_0^{t_n} \big(\langle \widehat{e}'', g' \rangle + \langle \widehat{e}', g'' \rangle \big) \, \mathrm{d}t \\
&= \int_0^{t_n} \big(\langle \widehat{e}'', g' \rangle - \langle \widehat{e}', Ag \rangle \big) \, \mathrm{d}t = \int_0^{t_n} \big(\langle \widehat{e}'', g' \rangle + \langle \widehat{e}, Ag' \rangle \big) \, \mathrm{d}t \\
&= \int_0^{t_n} \langle \widehat{e}'' + A\widehat{e}, g' \rangle \, \mathrm{d}t = -\int_0^{t_n} \langle \widehat{R}, g' \rangle \, \mathrm{d}t \\
&\leqslant \max_{t \in [0,\, t_n]} |g'(t)| \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t \leqslant |\widehat{e}'(t_n)| \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t,
\end{aligned} \tag{4.3}$$

where we have used (3.2), (3.6), (3.7) and (4.2). It follows from (4.3) that

$$|\dot{e}_-^n| \leqslant \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t.$$

Similarly, choosing $\mu = \widehat{e}(t_n)$, $\nu = 0$ in (4.1) yields

$$\begin{aligned}
\|e(t_n)\|^2 = \|\widehat{e}(t_n)\|^2 &= \int_0^{t_n} \langle A\widehat{e}, g \rangle' \, \mathrm{d}t = \int_0^{t_n} \big(\langle A\widehat{e}, g' \rangle + \langle A\widehat{e}', g \rangle \big) \, \mathrm{d}t \\
&= \int_0^{t_n} \big(\langle A\widehat{e}, g' \rangle + \langle \widehat{e}', Ag \rangle \big) \, \mathrm{d}t = \int_0^{t_n} \big(\langle A\widehat{e}, g' \rangle + \langle \widehat{e}', -g'' \rangle \big) \, \mathrm{d}t \\
&= \int_0^{t_n} \big(\langle A\widehat{e}, g' \rangle + \langle \widehat{e}'', g' \rangle \big) \, \mathrm{d}t = -\int_0^{t_n} \langle \widehat{R}, g' \rangle \, \mathrm{d}t \\
&\leqslant \max_{t \in [0,\, t_n]} |g'(t)| \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t \leqslant \|\widehat{e}(t_n)\| \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t,
\end{aligned}$$

which implies

$$\|e(t_n)\| \leqslant \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t.$$

Thus, we obtain the following result, which gives a posteriori error estimates at the nodes.

Theorem 4.1. *Let u and U be the solutions of* (1.1) *and* (1.3)*, respectively. Then, for $1 \leqslant n \leqslant N$, there hold*

$$|\dot{e}_-^n| \leqslant \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t, \tag{4.4}$$

$$\|e(t_n)\| \leqslant \int_0^{t_n} |\widehat{R}| \, \mathrm{d}t. \tag{4.5}$$

where the a posteriori quantity $\widehat{R}$ is given by (3.5)*.*

Remark 5. If f admits three time derivatives and the discrete solution U admits the optimal a priori error estimates, then we have from (3.14) that the order of $\int_0^{t_n} |\widehat{R}| \, \mathrm{d}t$ with respect to the time step is three. Hence (4.4) gives us a superconvergent result at the nodes.

5 An adaptive algorithm

Based on the a posteriori error estimates given in Corollary 3.3, we are able to construct an adaptive time stepping method related to the method (1.3). Let ϵ be the total error tolerance allowed for the a posteriori error estimate in (3.19), i.e.

$$\begin{aligned}\eta :=& \frac{1}{6}\max_{1\leqslant m\leqslant N} k_m^2|\widetilde{U}^{(3)}|_{L^\infty(J_m)} + 2\int_0^T |\widetilde{R}(s)|\,\mathrm{d}s + 2\int_0^T |\widehat{R}(s)|\,\mathrm{d}s \\ &+ \frac{\sqrt{3}}{216}\max_{1\leqslant m\leqslant N} k_m^3|\widehat{U}^{(4)}|_{L^\infty(J_m)} \\ \leqslant& \epsilon. \end{aligned} \tag{5.1}$$

To ensure (5.1) holds, a natural way is to adjust the time step size k_m such that the following conditions are satisfied:

$$\begin{aligned}&\frac{1}{6}k_m^2|\widetilde{U}^{(3)}|_{L^\infty(J_m)} \leqslant \frac{1}{3}\epsilon, \\ &\frac{\sqrt{3}}{216}k_m^3|\widehat{U}^{(4)}|_{L^\infty(J_m)} \leqslant \frac{1}{3}\epsilon, \\ &2\frac{T}{k_m}\int_{t_{m-1}}^{t_m}\big(|\widetilde{R}(s)| + |\widehat{R}(s)|\big)\,\mathrm{d}s \leqslant \frac{1}{3}\epsilon,\end{aligned}$$

which motivates us to use the following time-stepping strategy

$$\begin{aligned}\Theta :=& 3\max\left\{\frac{1}{6}k_m^2|\widetilde{U}^{(3)}|_{L^\infty(J_m)},\, \frac{\sqrt{3}}{216}k_m^3|\widehat{U}^{(4)}|_{L^\infty(J_m)},\, 2\frac{T}{k_m}\int_{t_{m-1}}^{t_m}\big(|\widetilde{R}(s)| + |\widehat{R}(s)|\big)\,\mathrm{d}s\right\} \\ \leqslant& \epsilon. \end{aligned} \tag{5.2}$$

It deserves to point out that in the derivation of the above time stepping rule, we have used the well known error equidistribution strategy (cf. [5, 12]). Consequently, using (5.2) and following some ideas implied in the Runge-Kutta-Felberg method (cf. [17]), we can get the following adaptive algorithm to control the time step size at each time step m.

Algorithm 5.1. *(Time step size control)*

1. Given an error tolerance ϵ and a parameter $\delta \in (0, 1)$ (usually we take $\delta = \frac{1}{4}$). Also assume that we have maximum and minimum for the time step size, denoted $k_{\max}$ and $k_{\min}$. These terms may be specified by the user, or they may be set to default values in a given software package.
2. At the node t_{m-1}, begin with an initial step size, k_m.
3. Compute U^m and $\dot{U}_-^m$ using (1.3) with the step size k_m. And then get U, U' and Θ at this time step.
4. If $\delta\epsilon \leqslant \Theta \leqslant \epsilon$, then $U'(t)$ is an acceptable approximation of $u'(t)$, $t \in (t_{m-1}, t_{m-1} + k_m]$. The step size k_m is acceptable, and it is used to advance to the next grid point, $k_{m+1} = k_m$.
5. If $\Theta < \delta\epsilon$, the step size is more than adequate, and we try to increase it. We double the step size as long as the larger step size is still smaller than $k_{\max}$. That is, we set $k_{m+1} = 2k_m$.

6. `If` $\Theta > \epsilon$`, then we decrease the step size. Replace` $k_m = \frac{1}{2}k_m$ `provided that the smaller step size satisfies` $k_m \geqslant k_{\min}$`. Return to Step 3, where new values of` U^m, $\dot{U}_-^m$ `and` U, U', Θ `are computed for this smaller step size.`

Remark 6. If the time step k_m ($m = 1, 2, \cdots$) determined by the above algorithm all lie in $(k_{\min}, k_{\max})$, then we easily have from (3.19), (5.2) and the definition of η (cf. (5.1)) that

$$|(u - U)'|_{L^\infty((0,T))} \le \eta \le \epsilon.$$

Table 1 Example 1: order of Etd and $\mathcal{E}_2 + \mathcal{E}_3$

N	Etd	Order	$\mathcal{E}_2 + \mathcal{E}_3$	Order	$\mathcal{E}_1$	Order
2	1.5444e–01		7.6389e–01		8.8555e–01	
4	2.2409e–02	2.7849	1.0161e–01	2.9102	1.7984e–01	2.2998
8	3.2049e–03	2.8057	1.3080e–02	2.9577	4.3014e–02	2.0639
16	4.2320e–04	2.9209	1.6594e–03	2.9786	1.0545e–02	2.0283
32	5.4140e–05	2.9666	2.0904e–04	2.9888	2.6153e–03	2.0115
64	6.8387e–06	2.9849	2.6232e–05	2.9944	6.5204e–04	2.0039
128	8.5908e–07	2.9929	3.2854e–06	2.9972	1.6282e–04	2.0017
256	1.0764e–07	2.9965	4.1109e–07	2.9986	4.0681e–05	2.0008
512	1.3470e–08	2.9984	5.1411e–08	2.9993	1.0168e–05	2.0004
1024	1.6840e–09	2.9998	6.4276e–09	2.9997	2.5416e–06	2.0002

Table 2 Example 1: order of Et and $\mathcal{E}_2 + \mathcal{E}_4$

N	Et	Order	$\mathcal{E}_2 + \mathcal{E}_4$	Order	$\mathcal{E}_1$	Order
2	2.6461e–01		7.4734e–01		8.8555e–01	
4	3.3352e–02	2.9880	9.7186e–02	2.9429	1.7984e–01	2.2998
8	4.1044e–03	3.0225	1.2132e–02	3.0019	4.3014e–02	2.0639
16	5.0659e–04	3.0183	1.5075e–03	3.0086	1.0545e–02	2.0283
32	6.2854e–05	3.0107	1.8762e–04	3.0062	2.6153e–03	2.0115
64	7.8257e–06	3.0057	2.3392e–05	3.0037	6.5204e–04	2.0039
128	9.7620e–07	3.0030	2.9200e–06	3.0020	1.6282e–04	2.0017
256	1.2190e–07	3.0015	3.6474e–07	3.0010	4.0681e–05	2.0008
512	1.5230e–08	3.0007	4.5575e–08	3.0005	1.0168e–05	2.0004
1024	1.9032e–09	3.0004	5.6959e–09	3.0003	2.5416e–06	2.0002

Table 3 Example 1: order of Ed and $\mathcal{E}_1 + \mathcal{E}_5$

N	Ed	Order	$\mathcal{E}_1 + \mathcal{E}_5$	Order
2	1.3500		2.3185	
4	3.5796e–01	1.9150	5.5465e–01	2.0635
8	9.7078e–02	1.8826	1.4232e–01	1.9624
16	2.4735e–02	1.9726	3.5564e–02	2.0007
32	6.2218e–03	1.9912	8.8735e–03	2.0028
64	1.5611e–03	1.9947	2.2177e–03	2.0004
128	3.9090e–04	1.9977	5.5429e–04	2.0004
256	9.7796e–05	1.9989	1.3855e–04	2.0002
512	2.4458e–05	1.9995	3.4635e–05	2.0001
1024	6.1157e–06	1.9997	8.6584e–06	2.0001

6 Numerical Experiments

6.1 Efficiency of the estimators

Example 1. In this subsection, we perform a simple numerical example to illustrate the effectiveness of the a posteriori error estimates developed in the previous sections. Consider an initial value problem

$$\begin{cases} u''(t) + 2u(t) = 2e^t(\cos t - \sin t), \quad 0 < t < 2, \\ u(0) = 1, \\ u'(0) = 1, \end{cases}$$

which has the exact solution $u(t) = e^t \cos t$ and $\|\cdot\| = \sqrt{2}|\cdot|$.

In our numerical computation, for a given natural number N, we adopt the uniform parti-

Table 4 Example 1: order of $\mathcal{E}_5$ and $\mathcal{E}_7$

N	$\mathcal{E}_5$	Example 1: order	Ed	Ed+Etd	$\mathcal{E}_7$	Order
2	1.4329		1.3500	1.5044	3.0824	
4	3.7481e–01	1.9347	3.5796e–01	3.8037e–01	6.5627e–01	2.2317
8	9.9308e–02	1.9162	9.7078e–02	1.0028e–01	1.5540e–01	2.0783
16	2.5019e–02	1.9889	2.4735e–02	2.5158e–02	3.7223e–02	2.0617
32	6.2581e–03	1.9992	6.2218e–03	6.2759e–03	9.0825e–03	2.0350
64	1.5657e–03	1.9989	1.5611e–03	1.5680e–03	2.2440e–03	2.0170
128	3.9147e–04	1.9998	3.9090e–04	3.9176e–04	5.5757e–04	2.0088
256	9.7868e–05	2.0000	9.7796e–05	9.7904e–05	1.3896e–04	2.0045
512	2.4467e–05	2.0000	2.4458e–05	2.4472e–05	3.4686e–05	2.0022
1024	6.1168e–06	2.0000	6.1157e–06	6.1174e–06	8.6649e–06	2.0011

Table 5 Example 1: order of Ehd and Eh

N	Ehd	Order	Eh	Order	$\mathcal{E}_2$	Order
2	1.6022e–01		2.6461e–01		7.3328e–01	
4	1.9640e–02	3.0282	3.3352e–02	2.9880	9.5865e–02	2.9353
8	2.4953e–03	2.9765	4.1044e–03	3.0225	1.2009e–02	2.9969
16	3.0409e–04	3.0367	5.0658e–04	3.0183	1.4982e–03	3.0028
32	3.7656e–05	3.0136	6.2855e–05	3.0107	1.8699e–04	3.0022
64	4.6720e–06	3.0107	7.8256e–06	3.0057	2.3351e–05	3.0014
128	5.8197e–07	3.0050	9.7621e–07	3.0029	2.9173e–06	3.0008
256	7.2607e–08	3.0028	1.2190e–07	3.0015	3.6457e–07	3.0004
512	9.0672e–09	3.0014	1.5230e–08	3.0007	4.5565e–08	3.0002
1024	1.1330e–09	3.0005	1.9032e–09	3.0004	5.6952e–09	3.0001

Table 6 Example 1: order of E and $\mathcal{E}_2 + \mathcal{E}_6$

N	E	Order	$\mathcal{E}_2 + \mathcal{E}_6$	Order
2	1.6139e–01		1.0270	
4	2.5746e–02	2.6482	1.3419e–01	2.9362
8	4.1044e–03	2.6491	1.7188e–02	2.9647
16	5.0658e–04	3.0183	2.1533e–03	2.9968
32	6.2855e–05	3.0107	2.6891e–04	3.0013
64	7.8254e–06	3.0058	3.3601e–05	3.0005
128	9.7616e–07	3.0030	4.1989e–06	3.0004
256	1.2184e–07	3.0021	5.2476e–07	3.0003
512	1.5213e–08	3.0017	6.5588e–08	3.0001
1024	1.8994e–09	3.0017	8.1979e–09	3.0001

tions with $k_m = 2/N$, $1 \leqslant m \leqslant N$. For ease of exposition, write

$$\mathcal{E}_1 := 2\int_0^2 |\widetilde{R}(s)|\,\mathrm{ds}, \qquad \mathcal{E}_2 := 2\int_0^2 |\widehat{R}(s)|\,\mathrm{ds}, \qquad \mathcal{E}_3 := \frac{\sqrt{3}}{216}\max_{1\leqslant m\leqslant N} k_m^3 |\widehat{U}^{(4)}|_{L^\infty(J_m)},$$

$$\mathcal{E}_4 := \frac{1}{384}\max_{1\leqslant m\leqslant N} k_m^4 \|\widehat{U}^{(4)}\|_{L^\infty(J_m)}, \quad \mathcal{E}_5 := \frac{1}{6}\max_{1\leqslant m\leqslant N} k_m^2 |\widetilde{U}^{(3)}|_{L^\infty(J_m)}, \quad \mathcal{E}_6 := \max_{0\leqslant\tau\leqslant 2} \|(U-\widehat{U})(\tau)\|,$$

$$\mathrm{E} := \max_{0\leqslant\tau\leqslant 2} \|(u-U)(\tau)\|, \qquad \mathrm{Ed} := \big|(u-U)'\big|_{L^\infty((0,\,2))}, \qquad \mathrm{Et} := \max_{0\leqslant\tau\leqslant 2} \|(u-\widetilde{U})(\tau)\|,$$

$$\mathrm{Etd} := \max_{0\leqslant\tau\leqslant 2} |(u-\widetilde{U})'(\tau)|, \qquad \mathrm{Eh} := \max_{0\leqslant\tau\leqslant 2} \|(u-\widehat{U})(\tau)\|, \qquad \mathrm{Ehd} := \max_{0\leqslant\tau\leqslant 2} |(u-\widehat{U})'(\tau)|,$$

$$\mathrm{Es} := \|u(2) - U(2)\|, \qquad \mathrm{Esd} := |u'(2) - \dot{U}_-^N|, \qquad \mathcal{E}_7 := \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 + \mathcal{E}_5.$$

In Tables 1 and 2 we give the values of a posteriori error estimators $\mathcal{E}_2 + \mathcal{E}_3$, $\mathcal{E}_2 + \mathcal{E}_4$ and $\mathcal{E}_1$ as well as their orders. These numerical results confirm the theoretical results of Corollary 3.2 and (2.16)-(2.17). Similarly, the numerical results in Tables 3-8 validate the theoretical results of Theorem 2.3, Corollary 3.3, Theorems 3.1, 3.3, Corollary 3.1 and Theorem 4.1, respectively.

Table 7 Example 1: order of $\mathcal{E}_6$ and $2\mathcal{E}_2 + \mathcal{E}_6$

N	$\mathcal{E}_6$	Order	E+Eh	$2\mathcal{E}_2 + \mathcal{E}_6$	Order
2	2.9374e–01		4.2600e–01	1.7603	
4	3.8320e–02	2.9384	5.9098e–02	2.3005e–01	2.9358
8	5.1796e–03	2.8872	8.2088e–03	2.9197e–02	2.9780
16	6.5505e–04	2.9832	1.0132e–03	3.6515e–03	2.9993
32	8.1919e–05	2.9993	1.2571e–04	4.5590e–04	3.0017
64	1.0250e–05	2.9985	1.5651e–05	5.6952e–05	3.0009
128	1.2815e–06	2.9997	1.9524e–06	7.1162e–06	3.0006
256	1.6019e–07	3.0000	2.4374e–07	8.8933e–07	3.0003
512	2.0023e–08	3.0000	3.0443e–08	1.1115e–07	3.0002
1024	2.5026e–09	3.0002	3.8026e–09	1.3893e–08	3.0001

Table 8 Example 1: order of Esd and Es

N	Esd	Order	Es	Order	$\mathcal{E}_2/2$	Order
2	6.9299e–02		2.6461e–01		3.6664e–01	
4	1.2580e–02	2.4617	3.3353e–02	2.9880	4.7933e–02	2.9353
8	1.7970e–03	2.8075	4.1045e–03	3.0225	6.0044e–03	2.9969
16	2.3743e–04	2.9200	5.0660e–04	3.0183	7.4911e–04	3.0028
32	3.0436e–05	2.9636	6.2857e–05	3.0107	9.3495e–05	3.0022
64	3.8505e–06	2.9827	7.8259e–06	3.0057	1.1675e–05	3.0014
128	4.8414e–07	2.9915	9.7624e–07	3.0030	1.4587e–06	3.0008
256	6.0692e–08	2.9958	1.2190e–07	3.0015	1.8228e–07	3.0004
512	7.5974e–09	2.9979	1.5230e–08	3.0008	2.2782e–08	3.0002
1024	9.5035e–10	2.9990	1.9033e–09	3.0004	2.8476e–09	3.0001

Next, we study the efficiency of the lower and upper estimators in Corollaries 3.1 and 3.3, using the indices as given in [1]. With respect to the reference error E+Eh the lower effectivity index Effl and the upper effectivity index Effu are defined as

$$\text{Effl} := \frac{\mathcal{E}_6}{\text{E+Eh}}, \quad \text{Effu} := \frac{2\mathcal{E}_2 + \mathcal{E}_6}{\text{E+Eh}},$$

respectively. Similarly, with respect to the reference error Ed+Etd, we denote the lower and upper effectivity indices

$$\text{Effld} := \frac{\mathcal{E}_5}{\text{Ed+Etd}}, \quad \text{Effud} := \frac{\mathcal{E}_7}{\text{Ed+Etd}}.$$

We compute these indices in Table 9 and graphically demonstrate them in log-log scale in Figure 1. It is observed that Effld≈ 1, Effud$\approx \sqrt{2}$, Effl$\approx 2/3$, and Effu$\approx 11/3$.

Table 9 Example 1: effectivity indices of lower and upper estimators

N	Effld	Effud	Effl	Effu
2	0.9525	2.0489	0.6895	4.1322
4	0.9854	1.7253	0.6484	3.8927
8	0.9903	1.5496	0.6310	3.5568
16	0.9945	1.4796	0.6465	3.6040
32	0.9972	1.4472	0.6517	3.6266
64	0.9986	1.4311	0.6549	3.6389
128	0.9993	1.4233	0.6564	3.6449
256	0.9996	1.4194	0.6572	3.6486
512	0.9998	1.4174	0.6577	3.6512
1024	0.9999	1.4164	0.6581	3.6535

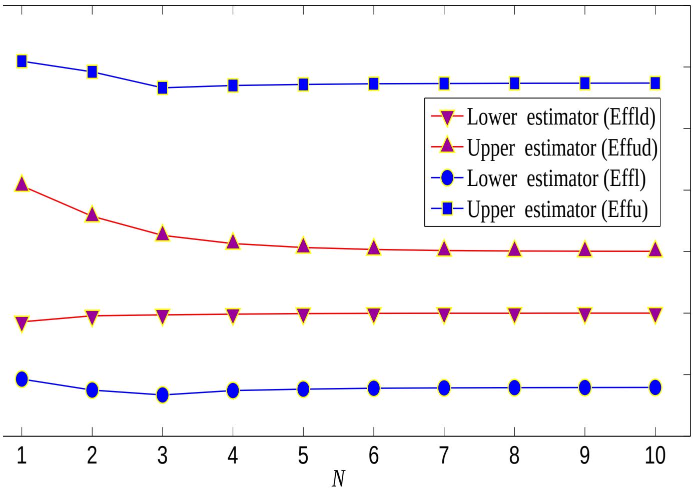


Figure 1 Log-log graphs of the effectivity indices of lower and upper estimators (the base of the logarithms is 2).

6.2 Efficiency of the adaptive algorithm

Example 2. In order to test the effectiveness of our adaptive Algorithm 5.1, we first consider the ODE case (cf. (1.1)) with $A = 2$, $T = 10$, and the right term f is taken such that the exact solution of (1.1) is

$$u(t) = \alpha(t) := e^{-800(\sin(\pi t/2)-1)^2}\sin(4\pi t). \tag{6.1}$$

We set $k_{\max} = 1$ in the computation. In Figure 2 we give the numerical solutions for u and u'. The error of $(u - U)'(t)$ is depicted in Figure 3(a) and the time stepsize trajectory is shown in Figure 3(b). In Table 10 we have reported the numerical results when running the adaptive algorithm for different values of ϵ and $k_{\min}$, where $(N_* - 1)$ is the total number of the time iterative step in the adaptive computation. Moreover, we adopt the uniform partitions to compute with the same iteration number $(N_* - 1)$, and the numerical results are shown in Table 11, from which we know the adaptive algorithm is very efficient.

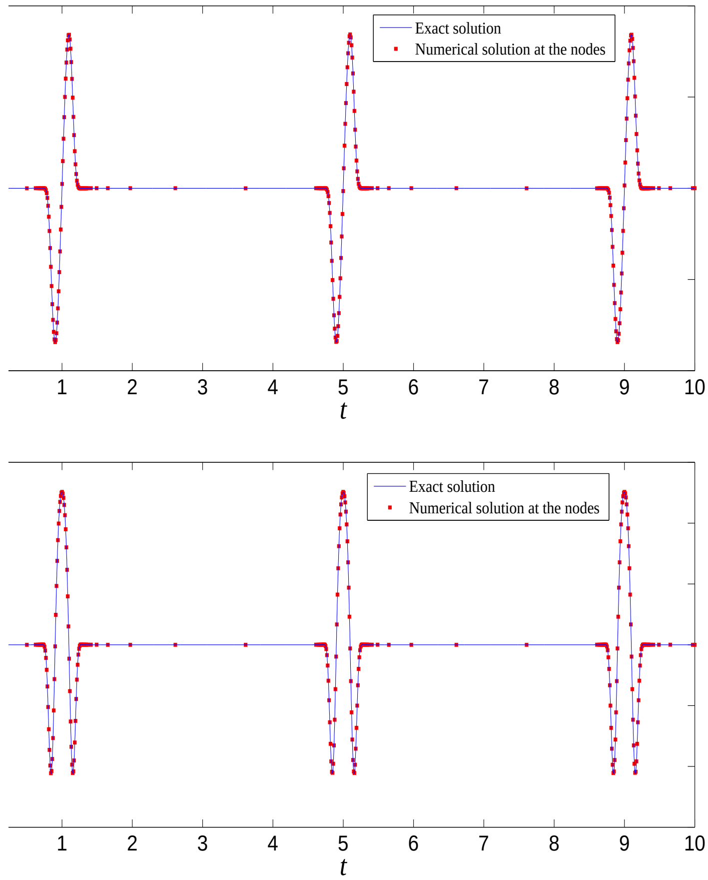


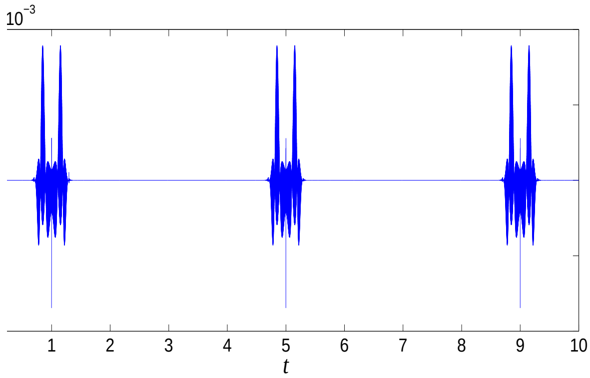
Figure 2 Example 2: solution curve (top) and derivative curve (bottom) with $\epsilon = 10^{-1}$, $k_{\min} = 10^{-2}$.

Table 10 Example 2: adaptive numerical results with different ϵ and $k_{\min}$

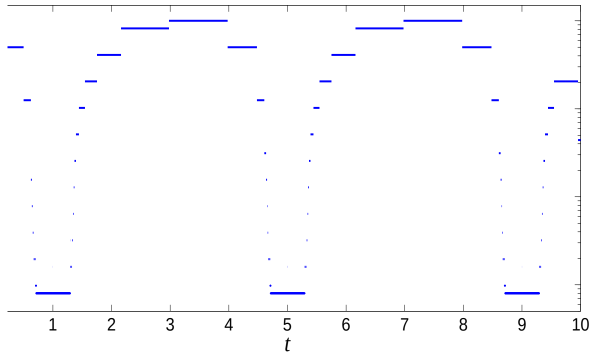
ϵ	$k_{\min}$	η	$\|(u-U)'\|_{L^\infty((0,T))}$	N	N_*
1e–1	1e–2	1.3458	1.3907e–1	237	265
1e–1	5e–3	3.2883e–1	3.4921e–2	432	465
1e–1	3e–3	1.1643e–1	1.2582e–2	670	713
1e–1	2e–3	5.1986e–2	5.5931e–3	960	1014
1e–1	1e–3	1.7596e–2	5.2996e–3	1748	1834
1e–2	8e–4	8.2489e–3	8.9507e–4	2373	2440

Table 11 Example 2: numerical results with uniform partitions

N_*	265	465	713	1014	1834	2440
η	2.0302e+1	6.4139	2.6775	1.3100	3.9251e–1	2.1752e–1
$\|(u-U)'\|_{L^\infty}$	1.8839	6.3710e–1	2.7348e–1	1.3554e–1	4.1577e–2	2.3495e–2



(a)



(b)

Figure 3 Example 2: (a) the error of $(u-U)'(t)$ and (b) the time stepsize trajectory with $\epsilon = 10^{-2}$, $k_{\min} = 8 * 10^{-4}$.

Example 3. Next, we turn to the results in the PDE case. The problem under consideration is

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - 2\dfrac{\partial^2 u}{\partial x^2} = f(x,\, t), & 0 < x < 1,\, 0 < t < T, \\ u(0,\, t) = u(1,\, t) = 0, & 0 \leqslant t \leqslant T, \\ u(x,\, 0) = u_0(x), \quad \dfrac{\partial u}{\partial t}(x,\, 0) = v_0(x), & 0 \leqslant x \leqslant 1, \end{cases} \tag{6.2}$$

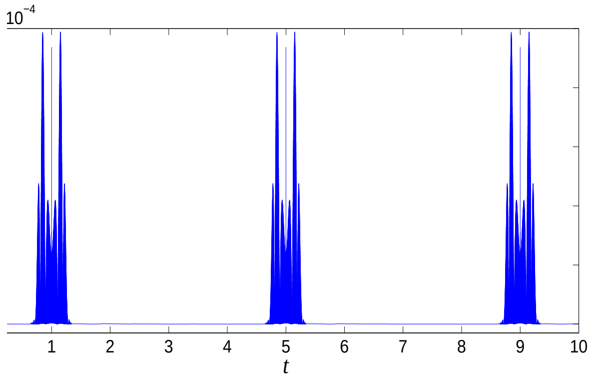
and define the solution of (6.2) by

$$\text{Case (a)} \qquad u(x,\, t) = \alpha(t) * \sin(\pi x), \quad T = 10, \tag{6.3}$$

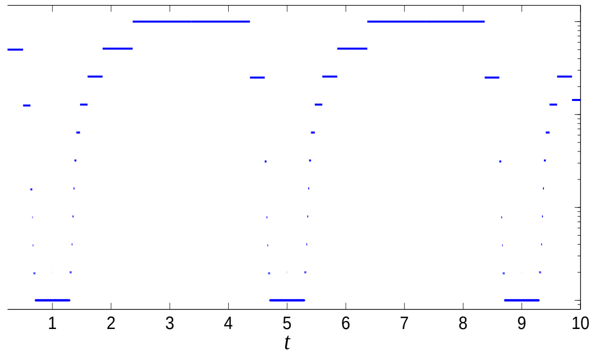
$$\text{Case (b)} \qquad u(x,\, t) = \beta(t) * \sin(\pi x), \quad T = 1, \tag{6.4}$$

where $\alpha(t)$ is given in (6.1) and $\beta(t) = 0.1 * (1 - e^{-10000*(t-1/2)^2})$, which is used in [5] for numerical experiments.

We apply the adaptive time stepping Algorithm 5.1 to solve these problems. In the space direction, we adopt linear finite element with uniform partitions, and the space step size is 1/1000. The error of $|(u-U)'(t)|$ and the time step size at each time step are displayed in Figures 4-5. The adaptive numerical results with different ϵ and $k_{\min}$ are shown in Tables 12-13.



(a)



(b)

Figure 4 Example 3: (a). the error of $|(u-U)'(t)|$ and (b) the time stepsize trajectory with $\epsilon = 10^{-2}$, $k_{\min} = 10^{-3}$, $k_{\max} = 1$, case (a).

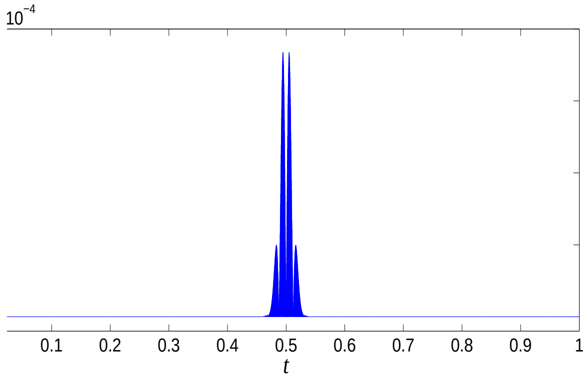
Table 12 Example 3: adaptive numerical results with different ϵ and $k_{\min}$, $k_{\max} = 1$, case (a)

ϵ	$k_{\min}$	η	$\|(u-U)'\|_{L^\infty((0,T))}$	N	N_*
1e–1	1e–2	9.3824e–1	9.8521e–2	232	256
1e–1	5e–3	2.2978e–1	2.4697e–2	428	463
1e–1	3e–3	8.1437e–2	8.8953e–3	665	716
1e–2	1e–3	9.0067e–3	9.8934e–4	1915	1965

Table 13 Example 3: adaptive numerical results with different ϵ and $k_{\min}$, $k_{\max} = 10^{-1}$, case (b)

ϵ	$k_{\min}$	η	$\|(u-U)'\|_{L^\infty((0,T))}$	N	N_*
1e–1	1e–3	1.3900e–1	4.5905e–2	88	96
1e–1	8e–4	8.8610e–2	2.9403e–2	103	111
1e–2	3e–4	1.2183e–2	4.1365e–3	257	271
1e–2	2e–4	5.4196e–3	1.8400e–3	361	375
1e–3	1e–4	1.3490e–3	4.6005e–4	736	749
1e–3	8e–5	8.6463e–4	2.9446e–4	893	909

(a)



(b)

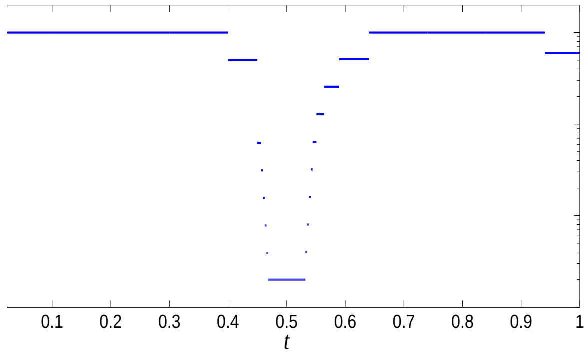


Figure 5 Same as Figure 4, except for case (b).

7 Concluding remarks

This work is concerned with developing adaptive time stepping methods for second-order evolution problems in terms of a posteriori error analysis. Based on the energy approach and the duality argument, optimal order a posteriori error estimates and a posteriori nodal superconvergence error estimates have been derived. Using these estimates, an adaptive time stepping strategy is developed. A number of numerical experiments are performed to assess the effectiveness of the proposed adaptive time stepping method.

We conclude this work by summarizing our main observations from the numerical results reported in the last section:

- The a posteriori error estimators developed in this paper are reliable and efficient. In particular, the estimator given in Corollary 3.3 performs better than the one given in Corollary 2.1.
- The adaptive time stepping Algorithm 5.1 is efficient for solving time evolution problems under consideration. This is seen by comparing the numerical errors obtained using the uniform partition and adaptive partition, i.e., Tables 11 and 10).
- For the adaptive time stepping Algorithm 5.1, the choice of $k_{\min}$ is critical for the efficiency of the algorithm. If it is taken too large, the total error may not be dominated by the prescribed error tolerance; and if too small, the algorithm may lead to over-refinement. Although $k_{\min}$ can be chosen quite easily by numerical experience, some theoretical justification is certainly needed.

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