Backward Euler and Crank-Nicolson finite element variants with rational adaptivity and a-posteriori error estimates for a Volterra integrodifferential equation

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Abstract

Finite element methods are applied in time to a prototype problem involving an ODE with memory. These produce variants on the classical backward Euler (a piecewise constant approximation) and Crank-Nicolson (continuous piecewise linear approximation) methods. Using the Galerkin orthogonality of the error, and the strong stability of associated dual backward problems, a posteriori *error estimates are derived and then demonstrated numerically for some model problems. At this stage, as with many finite element schemes, the quadrature errors involved in the discrete inner product approximations are ignored, as is the quadrature error associated with the Volterra operator. The numerical results show that, at least when the quadrature errors can be made small relative to the Galerkin error, this can be an acceptable practice. In the penultimate section we then include a complete* a posteriori *error analysis of the quadrature replacements for the backward Euler variant. This work should be seen as a phase in the production of numerical schemes with* a posteriori *error analysis for space-time problems such as occur in viscoelasticity and hereditary heat conduction.*

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1. Introduction and summary. For some real number $T > 0$ we define the time intervals $\mathcal{J} := (0, T]$ and $\overline{\mathcal{J}} := [0, T]$ and by $W_p^m(\mathcal{J})$ we denote the usual Sobolev space of functions which, together with their first m derivatives, are of class $L_p(\mathcal{J})$.

In this note we consider, for some $p \in [1, \infty]$, finite element approximations to the prototype problem: find $u \in W_p^1(\mathcal{J})$ such that

$$f(t) = Au(t) := u'(t) + \sigma(t)u(t) - \Lambda u(t), \qquad u(0) = u_0 \text{ (given)}. \tag{1.1}$$

Here $\Lambda : L_p(\mathcal{J}) \mapsto L_p(\mathcal{J})$ is the Volterra operator defined through

$$\Lambda u(t) := \int_0^t \phi(t, s)u(s)\, ds,$$

and ϕ is the kernel of the operator. The following restrictions on the data are assumed to apply.

Assumptions 1.1. *Taking q conjugate to p, so that $p^{-1} + q^{-1} = 1$, we assume the following conditions hold.*

(i) $f \in L_p(\mathcal{J})$.

(ii) $\sigma \in L_\infty(\mathcal{J})$.

(iii) The kernel ϕ is such that

$$|||\phi||| := \left(\int_0^T \left(\int_0^t |\phi(t, s)|^q\, ds \right)^{p/q} dt \right)^{1/p} < \infty,$$

$$||||\phi|||| := \left(\int_0^T \left(\int_s^T |\phi(t, s)|^p\, dt \right)^{q/p} ds \right)^{1/q} < \infty,$$

with the obvious "ess sup" modification when p or $q = 1$.

(iv) A solution, u, to (1.1) exists uniquely in $W_p^1(\mathcal{J})$ for some $p \in [1, \infty]$.

(v) For every $\Upsilon \in (0, T]$ a unique solution, χ, to the dual problem (2.1) exists uniquely in $W_q^1(0, \Upsilon)$.

The dual problem referred to in (v) is used in proving the a posteriori *error estimates which follow. It is dealt with in detail in Section 2. Also, some more restrictive assumptions will be made later in Section 3 to facilitate the* a priori *error analysis for the backward Euler variant.* ■

Remark 1.1. *If Assumptions 1.1.iv and 1.1.v are satisfied in the slightly more restrictive case $p \in (1, \infty)$ then we also have $u \in C(\overline{\mathcal{J}})$ and $\chi \in C[0, \Upsilon]$. This follows from the Sobolev embedding theorem (see e.g. [1, Theorem 5.4, Part II, Case C′]) wherein $W_p^1(\mathcal{J}) \hookrightarrow C^{0,\alpha}(\overline{\mathcal{J}})$ and $C^{0,\alpha}(\overline{\mathcal{J}})$ is the space of functions that are Lipschitz continuous with order α. This embedding holds only for $1 < p < \infty$ and $0 < \alpha \leq 1 - 1/p$. This extra smoothness of the solutions to (1.1) and (2.1) is essential to the proof of Theorem 3.1 and is the reason why the extreme cases $p = 1$ or $p = \infty$ have been excluded in this result.* ■

Equation (1.1) serves as a prototype for studying the time discretization of the more general (linear) initial-history-boundary-value space-time problems that occur, for example, in theories of hereditary heat conduction, [12], and also in viscoelasticity theory, [18, Chap. 3], [14], where a hyperbolic integrodifferential equation can be converted to a system of type (1.1) by introducing an extra "unknown". For example, the generic hereditary heat conduction problem is simply the standard heat problem with memory:

$$u'(t) - \nabla^2 u(t) = f(t) - \int_0^t \nabla \cdot \phi(t, s)\nabla u(s)\, ds$$

(plus initial and boundary data), whilst the dynamic viscoelasticity problem can be expressed as

$$\begin{pmatrix} u'(t) \\ u''(t) \end{pmatrix} - \begin{pmatrix} 0 & I \\ \nabla^2 & 0 \end{pmatrix} \begin{pmatrix} u(t) \\ u'(t) \end{pmatrix} = \begin{pmatrix} 0 \\ f(t) \end{pmatrix} - \int_0^t \begin{pmatrix} 0 & 0 \\ \nabla \cdot \phi(t, s)\nabla & 0 \end{pmatrix} \begin{pmatrix} u(s) \\ u'(s) \end{pmatrix} ds$$

(here I is an identity). Also, if interpreted as a (large) system, (1.1) corresponds to the pure-time problems that result after these space-time problems have been semidiscretized in space.

Classical time discretization schemes for (1.1) have already been considered in, for example, [7], [3] (see also the book [11]) for the pure-time problem, and in [16], [17], [20], [4] for the space-time problem. However, as far as we are aware all of the error analyses for these schemes have been strictly *a priori*, and so adaptive time stepping is usually not considered and the algorithms provide little or no feedback to the user on the integrity of the calculated solution. On the other hand "parabolic" problems of type (1.1) can be converted to standard Volterra systems of the second kind by introducing an extra unknown function, see [11, Chap. 11§5], and numerical schemes for such problems are well established, again see [11] for some classical methods and [15] for the analogue of the approach taken below. Adaptive schemes for these standard Volterra second-kind problems do exist, see for example [2], [10] and [15].

Actually, quite apart from accuracy and reliability requirements, the need for efficient adaptive schemes for problems involving Volterra operators is much greater than for non-history-dependent problems. This is because of the tremendous demand placed on computer resources by the discretized Volterra term, $\Lambda^h u$ say. To illustrate the point suppose we have discretized (1.1) with the backward Euler method combined with a rectangle rule approximation to Λu. It is clear that at the discrete time t_i there will be $O(i)$ arithmetic operations required to evaluate the discrete history term. Thus, to march from time t_0 to time t_i will require a total number of operations proportional to $1 + 2 + \cdots + i = O(i^2)$. Not only this but, since all previous solutions have to be retained, the computer memory required at time level i is of order $O(i)$. Thus, to solve to the final time $T = t_N$ requires storage of order $O(N)$ and time of order $O(N^2)$, clearly it is highly desirable to minimise N without trading accuracy.

In [16] this problem was addressed by designing *sparse quadrature rules* which act in constant (or possibly piecewise constant) time stepping algorithms. The reduction in storage and execution time is dramatic but the discretization is classical, no *a posteriori* error analysis is attempted. Also, because the sparse rules require a substantially constant time step they do not obviate the basic motivation for adaptivity. Thus a solution which is only locally non-smooth still requires $O(N^{1+\epsilon})$ operations to solve to t_N (because the efficient history management attenuates the $O(N^2)$ term), and N could be "large". An adaptive scheme on the other hand has the potential to keep N "small" by allowing large time steps in smooth regions of the solution. In such a scheme the $O(N^2)$ estimate for the history calculation (which might not be attenuated by a special treatment) is not nearly so damaging.

Our purpose in this paper is to report on the applicability of the "Galerkin in time" discretization technique to the prototype form (1.1). Here we begin with a weighted residual formulation of (1.1) as: find $u \in W_p^1(\mathcal{J})$ such that

$$(Au, v) = (f, v) \qquad \forall v \in L_q(\mathcal{J}), \tag{1.2}$$

where $(\cdot,\cdot)$ denotes the usual $L_2(\mathcal{J})$ inner product. Introducing the finite dimensional trial and test spaces, U^h and V^h respectively, we then form a finite element scheme for (1.2) as: find $U \in U^h$ such that

$$(AU, v) = (f, v) \qquad \forall v \in V^h \subset L_q(\mathcal{J}).$$

Of course this methodology is well established for elliptic problems, but for general space, time or space-time dependent problems it has recently been developed and championed by Johnson and co-workers in, for example, [18, Chap. 6], [5], [6] and [9], and provides a framework for deriving rigorous *a posteriori* Galerkin-error estimates

for the finite element discretization. This technique has already been applied with a degree of success to the generic Volterra equation of the second kind in [15], and it is that success that has motivated the present study.

In the succeeding sections of this note we will develop, analyze and experiment with two finite element discretizations of (1.1) which are each capable of providing rigorous residual-based *a posteriori* Galerkin-error estimates, and therefore lend themselves naturally to solving in an adaptive mode with reliable error control. Discretizing the time interval into

$$\mathcal{J}^k := \{t_i \in \overline{\mathcal{J}} : 0 = t_0 < t_1 < \cdots < t_i < \cdots < t_N = T\},$$

for some integer $N > 0$, defining the "elements" $\mathcal{J}_i := (t_{i-1}, t_i)$ and time steps $k_i := t_i - t_{i-1}$, we first consider in Section 3 a finite element discretization of (1.1) based on piecewise constant trial and test functions. Here $U^h = V^h \not\subset W_p^1(\mathcal{J})$. The resulting algorithm is a variant of the classical backward Euler method and is a direct extension of the result in [9, Chap. 2§4], which deals with (1.1) in the case $\phi \equiv 0$. Also, in [5] a rigorous theory of adaptive error control based upon discontinuous Galerkin finite element approximation of nonlinear ODE systems is developed (see also [6]). In Theorem 3.1 we give the *a posteriori* Galerkin-error estimate:

$$\max_{1\le j\le i} |u(t_j) - U_j| \le C_1^s \max_{1\le j\le i} \left\{ k_j^{1/q} \|f - \sigma U + \Lambda U\|_{L_p(\mathcal{J}_j)} + |U_j - U_{j-1}| \right\},$$

where U_j is the (constant) finite element approximation to u in $\mathcal{J}_j$ and C_1^s is a strong data-stability constant associated with a certain continuous dual problem. In Section 4 we discuss the practical implementation of this algorithm, and also give the results of some numerical experiments performed on model problems for which the exact solution is known.

The finite element discretization introduced and analyzed in Section 5 is built on a trial space of continuous piecewise linears (this time $U^h \subset W_p^1(\mathcal{J})$) and a test space of piecewise constants. The resulting numerical scheme is a variant of the classical Crank-Nicolson method. In this case the *a posteriori* Galerkin-error estimate is given in Theorem 5.2 as:

$$|u(t_i) - U(t_i)| \le C_1^s \max_{1\le j\le i} \left\{ k_j^{1/q} \|f - U' - \sigma U + \Lambda U\|_{L_p(\mathcal{J}_j)} \right\}.$$

This time $U(t_i)$ is the nodal finite element approximation to $u(t_i)$. As with the Euler variant, Section 6 discusses the implementation and performance of the scheme.

Remark 1.2. *We are freely abusing convention here since "Galerkin" usually refers to the case where the trial and test spaces coincide. Here they do not but in the interests of brevity we shall retain the shorter: "Galerkin".* ■

The proofs of these error estimates each require some subsidiary results, and these are isolated and dealt with first in Section 2—the intention being to render Sections 3 thru 6 more sharply focused. In particular, in the finite element methodology of Johnson *et al.* the data-stability of associated dual problems plays a fundamental role in providing the link between the error, which in general is not computable, and the residual, which is. As a result the dual problem leaves its trace in the final bound in the form of the stability constant C_1^s, and it is therefore necessary to estimate this constant in order to use the error bound.

For problems of type (1.1) an upper bound on these constants can be established by appeal to various Gronwall lemmas; this proves the *form* of the data-stability. However, for many problems this results in a constant which is vastly larger in magnitude than is necessary, and then the stability bound is unduly pessimistic. In Section 2 we examine the dual problem and take this approach in proving that the stability estimates used in the error analyses are indeed of the correct form. However, we do not use these constants for the numerical results in Sections 4 and 6 but instead prefer to calculate them directly from numerical solutions. This, at first, may seem to be an unsatisfactory practice but we should observe that in general, only for certain special problems can these constants be sharply bounded. The need to solve the dual problem to calculate the constant, as well as solving the original problem is, it seems, the price of the *a posteriori* error estimates. Any quantitative error bound must contain some constant reflecting the stability of the operator and so the problem of estimating this constant cannot be avoided. The only exception to this seems to be when the underlying problem suggests a natural (or *energy*) norm for error control, and then the stability constant is unity.

An important point to note here at the outset is that the errors reported in the numerical experiments in Sections 4 and 6 are *not* those bounded by the *a posteriori* estimates given above. This is because the mechanism used here for deriving these estimates relies fundamentally on the *Galerkin orthogonality* of the error and, as with all finite element algorithms, this orthogonality is destroyed by introducing discrete inner products into the practical scheme. Moreover, unless $\phi(t,s)$ is of simple enough form, we also have to discretize the operator Λ by some quadrature rule. Thus the computed solutions are polluted by quadrature as well as Galerkin errors. Naturally it is desirable to be able to estimate and control both the Galerkin and various quadrature errors on an independent basis, and to this end we include a full analysis of the quadrature error for the backward Euler variant in Section 7. The resulting bound indicates that we are justified in discarding the quadrature errors in the results in Section 4 (i.e. the Galerkin error dominates) and, because it is computable in terms of the data, the bound could also be incorporated into the algorithm to provide guaranteed error control for the fully practical scheme.

2. Preparatory results. In this section we have isolated the results concerning the dual problem and the interpolation-error estimates that are common to the analysis of both the schemes to be given later. The section is designed to be referred *back* to from Section 3 onward, and so on a first reading one could omit Proposition 2.1 thru Lemma 2.2 (inclusive).

We begin with the dual problem which we consider in the following form. Let $\Upsilon \in (0,T]$ be given and set $\mathcal{I} := [0,\Upsilon) \subset \overline{\mathcal{J}}$. For $q \in [1,\infty]$ we assume (recall Assumption 1.1.v) that there is a unique $\chi \in W_q^1(\mathcal{I})$ such that:

$$\begin{aligned} &g(t) = A^*\chi(t) := -\chi'(t) + \sigma(t)\chi(t) - \Lambda^*\chi(t) \qquad \text{for } \Upsilon > t \geq 0, \\ &\chi(\Upsilon) = \chi_\Upsilon \ \text{(given)}, \end{aligned} \tag{2.1}$$

and $g \in L_q(\mathcal{I})$. Here Λ^* is the $L_2(\mathcal{I})$-adjoint to Λ given by

$$\Lambda^*\chi(t) := \int_t^\Upsilon \phi(s,t)\chi(s)\,ds, \tag{2.2}$$

so that if $\langle\cdot,\cdot\rangle$ is the $L_2(\mathcal{I})$ inner product we have $\langle\Lambda\cdot,\cdot\rangle = \langle\cdot,\Lambda^*\cdot\rangle$. Note also the duality between A and A^*:

$$\langle Av, w\rangle = \langle v, A^*w\rangle + v(\Upsilon)w(\Upsilon) - v(0)w(0), \tag{2.3}$$

for smooth enough v and w. It is the stability property of this problem that will play a key role in the *a posteriori* analyses given later and it is our goal here to prove that the strong stability estimates to be used later in the proofs of Theorems 3.1, 5.1 and 5.2 are indeed of the correct form. We first note that it is sufficient to study a standard forward problem rather than the non-standard backward problem given above.

Proposition 2.1. *The solution to (2.1) is given by* $\chi(t) = \gamma(\Upsilon - t)$, *where* γ *solves the forward problem,*

$$\begin{aligned} &\gamma'(\eta) + \overline{\sigma}(\eta)\gamma(\eta) - \int_0^\eta \overline{\phi}(\eta,\xi)\gamma(\xi)\,d\xi = \overline{g}(\eta), \qquad \text{for } 0 < \eta \leq \Upsilon, \\ &\gamma(0) = \chi_\Upsilon, \end{aligned} \tag{2.4}$$

and: $\overline{\phi}(\eta,\xi) := \phi(\Upsilon-\xi, \Upsilon-\eta)$, $\overline{\sigma}(\eta) := \sigma(\Upsilon-\eta)$, $\overline{g}(\eta) := g(\Upsilon-\eta)$.

Proof. Firstly, introduce the new independent variables $\xi := \Upsilon - s$ and $\eta := \Upsilon - t$ and substitute into (2.1), this gives

$$-\chi_t(\Upsilon-\eta) + \sigma(\Upsilon-\eta)\chi(\Upsilon-\eta) - \int_{s=t}^{s=\Upsilon} \overline{\phi}(\eta,\xi)\chi(\Upsilon-\xi)\,ds = g(\Upsilon-\eta).$$

Now, note that $-\chi_t(\Upsilon-\eta) = -\chi_\eta(\Upsilon-\eta)\eta'(t) = \gamma'(\eta)$; $ds = -d\xi$; $s = t \Rightarrow \xi = \eta$; and, $s = \Upsilon \Rightarrow \xi = 0$, then $\gamma(0) = \chi(\Upsilon)$ and the integrodifferential equation becomes

$$\gamma'(\eta) + \overline{\sigma}(\eta)\gamma(\eta) - \int_0^\eta \overline{\phi}(\eta,\xi)\gamma(\xi)\,d\xi = \overline{g}(\eta) \qquad \text{for } 0 < \eta \leq \Upsilon,$$

as claimed. ■

Remark 2.1. *In the case of a convolution kernel we have the replacement* $\phi(t,s) \leftarrow \phi(t-s)$ *and therefore* $\overline{\phi}(\eta,\xi) \leftarrow \phi(\eta-\xi)$. *It then follows that if* $\sigma(t)$ *and* $\overline{\sigma}(t)$ *evolve similarly through time (e.g.* σ *is periodic or a constant) then (1.1) and (2.4) will obey essentially the same stability bound.* ■

Before stating the stability estimates we need the following L_q generalization of Gronwall's lemma

Lemma 2.1. *For* $q \in [1,\infty)$ *let* α, β, $\psi \in L_q(\mathcal{J})$ *be non-negative a.e. in* $\mathcal{J}$. *Then:*

$$\alpha(t) \leq \beta(t) + \psi(t)\|\alpha\|_{L_q(0,t)} \qquad \Longrightarrow \qquad \|\alpha\|_{L_q(0,t)} \leq \frac{\|\beta\epsilon^{1/q}\|_{L_q(0,t)}}{1 - \big(1-\epsilon(t)\big)^{1/q}},$$

where $t \in \mathcal{J}$ *and* $0 < \epsilon(t) := \exp(-\|\psi\|^q_{L_q(0,t)}) \leq 1$.

Proof. See [19]. ■

Lemma 2.2. *For the standard forward problem, (2.4), under the assumptions stated in Section 1, there exist weak and strong data-stability constants, $C_q^w = C_q^w(\sigma,\phi,\Upsilon)$ and $C_q^s = C_q^s(\sigma,\phi,\Upsilon)$ respectively, such that*

$$\|\gamma\|_{L_q(0,t)} \le C_q^w(|\gamma(0)| + \|\overline{g}\|_{L_q(0,t)}) \quad \text{and} \quad \|\gamma'\|_{L_q(0,t)} \le C_q^s(|\gamma(0)| + \|\overline{g}\|_{L_q(0,t)}),$$

for all $t \in [0,\Upsilon]$ and $q \in [1,\infty]$ such that Assumptions 1.1 hold.

Proof. Choose an arbitrary $\tau \in [0,\Upsilon]$ and firstly note that, since $\Upsilon \le T$,

$$\int_0^\tau \left(\int_0^\eta |\overline{\phi}(\eta,\xi)|^p\,d\xi\right)^{q/p} d\eta = \int_{\eta=0}^{\eta=\tau} \left(\int_{\xi=0}^{\xi=\eta} |\phi(\Upsilon-\xi,\Upsilon-\eta)|^p\,d\xi\right)^{q/p} d\eta$$
$$= \int_{\Upsilon-\tau}^{\Upsilon} \left(\int_y^{\Upsilon} |\phi(x,y)|^p\,dx\right)^{q/p} dy \le |||\phi|||^q,$$

for conjugate p and q and $|||\phi|||$ as defined in Assumptions 1.1. (The obvious modification is intended if either p or $q=\infty$.) Now, define the operator $\overline{\Lambda}$ by

$$\overline{\Lambda}\gamma(\eta) := \int_0^\eta \overline{\phi}(\eta,\xi)\gamma(\xi)\,d\xi \qquad \text{for } \eta\in[0,\Upsilon],$$

and use Hölder's inequality with the result above to see that $\overline{\Lambda} : L_q(\mathcal{I}) \mapsto L_q(\mathcal{I})$ because

$$\|\overline{\Lambda}\gamma\|_{L_q(0,\tau)} = \left(\int_0^\tau \left|\int_0^\eta \overline{\phi}(\eta,\xi)\gamma(\xi)\,d\xi\right|^q d\eta\right)^{1/q} \le |||\phi|||\,\|\gamma\|_{L_q(0,\tau)} \quad \forall\tau\in\mathcal{I}. \tag{i}$$

Our first task is to prove the form of the weak stability estimate, the strong stability will then follow from this. To begin with we define the expedient:

$$J(\tau,t) := \exp\left(\int_t^\tau \overline{\sigma}(\xi)\,d\xi\right) \Longrightarrow \begin{cases} J(t,0) = \exp\left(\int_0^t \overline{\sigma}(\xi)\,d\xi\right), \\ J(0,t) = \exp\left(-\int_0^t \overline{\sigma}(\xi)\,d\xi\right), \end{cases}$$

which makes sense on finite time intervals due to our assumption on σ. Now we create an integrating factor, $I(t) := J(t,0)$, and note that $I'(t) = \overline{\sigma}(t)I(t)$ and then, with these definitions, we can write (2.4) as

$$\frac{d}{d\eta}\big(I(\eta)\gamma(\eta)\big) = I(\eta)\big(\overline{g}(\eta) + \overline{\Lambda}\gamma(\eta)\big).$$

Integrating this over $(0,\tau)$ yields

$$\gamma(\tau) = J(0,\tau)\gamma(0) + \int_0^\tau J(\eta,\tau)\big(\overline{g}(\eta) + \overline{\Lambda}\gamma(\eta)\big)\,d\eta$$

since: $I(0)=1$; $I(\tau)\ne 0$; $1/I(\tau) = J(0,\tau)$; and, $I(\eta)/I(\tau) = J(\eta,\tau)$. Now, setting

$$\beta(\tau) := J(0,\tau)|\gamma(0)| + \int_0^\tau J(\eta,\tau)|\overline{g}(\eta)|\,d\eta,$$

we get

$$|\gamma(\tau)| \le \beta(\tau) + \int_0^\tau J(\eta,\tau)\left|\overline{\Lambda}\gamma(\eta)\right|\,d\eta, \tag{ii}$$
$$\le \beta(\tau) + \|J(\cdot,\tau)\|_{L_p(0,\tau)}\left\|\overline{\Lambda}\gamma\right\|_{L_q(0,\tau)},$$
$$\le \beta(\tau) + \psi(\tau)\|\gamma\|_{L_q(0,\tau)},$$

using (i) and where $\psi(\tau) := \|J(\cdot,\tau)\|_{L_p(0,\tau)}|||\phi|||$. Therefore, for $q\in[1,\infty)$, from Lemma 2.1 we find

$$\|\gamma\|_{L_q(0,\tau)} \le \frac{\|\beta\|_{L_q(0,\tau)}}{1-\big(1-\epsilon(\tau)\big)^{1/q}},$$

where $0 < \epsilon(\tau) = \exp(-\|\psi\|^q_{L_q(0,\tau)}) \le 1$ for all $\tau\in[0,\Upsilon]$, and so there is a constant, C, such that $\|\gamma\|_{L_q(0,\tau)} \le C\|\beta\|_{L_q(0,\tau)}$. To estimate β we have

$$\|\beta\|_{L_q(0,\tau)} \le \|J(0,\cdot)\|_{L_q(0,\tau)}|\gamma(0)| + \left\|\int_0^t J(\eta,t)|\overline{g}(\eta)|\,d\eta\right\|_{L_q(0,\tau)},$$

and, from Hölder's inequality,

$$\left\|\int_0^t J(\eta,t)|\overline{g}(\eta)|\,d\eta\right\|_{L_q(0,\tau)} = \left(\int_0^\tau \left|\int_0^t \exp\left(\int_t^\eta \overline{\sigma}\,d\xi\right)|\overline{g}(\eta)|\,d\eta\right|^q dt\right)^{1/q},$$
$$\le \left(\int_0^\tau \left(\int_0^t \exp\left(p\int_t^\eta \overline{\sigma}\,d\xi\right)d\eta\right)^{q/p}\|\overline{g}\|^q_{L_q(0,t)}\,dt\right)^{1/q},$$
$$\le \left(\int_0^\tau \left(\int_0^t \exp\left(p\int_t^\eta \overline{\sigma}\,d\xi\right)d\eta\right)^{q/p} dt\right)^{1/q}\|\overline{g}\|_{L_q(0,\tau)}.$$

Thus we have obtained a bound for $\|\beta\|_{L_q(0,\tau)}$ which is a linear combination of $|\gamma(0)|$ and $\|\overline{g}\|_{L_q(0,\tau)}$ and this proves that the weak stability estimate is of the correct form for $q\in[1,\infty)$. When $q=\infty$ we return to (ii) to see that

$$|\gamma(\tau)| \le \beta(\tau) + \|J(\cdot,\tau)\|_{L_\infty(0,\tau)}\left\|\overline{\Lambda}\gamma\right\|_{L_1(0,\tau)},$$
$$\le \beta(\tau) + e^{t\|\sigma\|_{L_\infty(\mathcal{J})}}|||\phi|||\int_0^\tau|\gamma(\xi)|\,d\xi,$$
$$\Longrightarrow \|\gamma\|_{L_\infty(0,\tau)} \le C\|\beta\|_{L_\infty(0,\tau)},$$

from the standard Gronwall lemma. Reasoning as before we can again establish a bound on $\|\beta\|_{L_\infty(0,\tau)}$ as a linear combination of $|\gamma(0)|$ and $\|\overline{g}\|_{L_\infty(0,\tau)}$ and so we have verified the form of the weak stability estimate.

The strong stability estimate now follows immediately. Working from (2.4) we have, for all $q\in[1,\infty]$ such that Assumptions 1.1 are satisfied, and for all $\tau\in[0,\Upsilon]$:

$$\|\gamma'\|_{L_q(0,\tau)} = \left\|\overline{g} + \overline{\Lambda}\gamma - \overline{\sigma}\gamma\right\|_{L_q(0,\tau)},$$
$$\le \|\overline{g}\|_{L_q(0,\tau)} + (|||\phi||| + \|\overline{\sigma}\|_{L_\infty(0,\tau)})\|\gamma\|_{L_q(0,\tau)},$$
$$\le \|\overline{g}\|_{L_q(0,\tau)} + C_q^w(|\gamma(0)| + \|\overline{g}\|_{L_q(0,\tau)})(|||\phi||| + \|\overline{\sigma}\|_{L_\infty(0,\tau)}),$$

which clearly defines C_q^s implicitly. Hence it follows that the strong stability estimate is also of the correct form. ■

Returning now to the backward problem the following result is immediate.

Theorem 2.1. *Let Lemma 2.2 hold, then for the dual backward problem (2.1) there exist weak and strong stability constants, C_q^w and C_q^s, which depend only upon σ, ϕ and Υ and are such that*

$$\|\chi\|_{L_q(\Upsilon-t,\Upsilon)} \le C_q^w(|\chi(\Upsilon)| + \|g\|_{L_q(\Upsilon-t,\Upsilon)}),$$
$$\|\chi'\|_{L_q(\Upsilon-t,\Upsilon)} \le C_q^s(|\chi(\Upsilon)| + \|g\|_{L_q(\Upsilon-t,\Upsilon)}),$$

for all $t \in \mathcal{I}$ and for all $q \in [1,\infty]$ such that Assumptions 1.1 are satisfied.

Proof. Use a simple change of variable to show that $\|\chi\|_{L_q(\Upsilon-t,\Upsilon)} = \|\gamma\|_{L_q(0,t)}$ and $\|g\|_{L_q(\Upsilon-t,\Upsilon)} = \|\overline{g}\|_{L_q(0,t)}$, then use these, with $\gamma(0) = \chi(\Upsilon)$, in Lemma 2.2. ■

Remark 2.2. *Theorem 2.1 shows that the strong stability estimates to be used in the a posteriori error analyses in Sections 3 and 5 are of the correct form, but gives no a priori way of determining sharp values for the constants C_q^s. This is because these constants, as given in the proof above, derive from a Gronwall lemma and may therefore be hopelessly pessimistic for many actual problems. At the moment it seems that the only realistic way of obtaining accurate values is to solve the dual backward problem numerically (with suitable data) and then estimate the required constants from the computed solution. This is the approach taken for the numerical experiments in Sections 4 and 6 where, in view of Remark 2.1, we expect the dual stability to be closely related to the stability of the problem being solved, (1.1).* ■

There is however an exception to this remark and this is when $\overline{\phi}$ in (2.4) exhibits a certain kind of fading memory. The result we have in mind is due to Thomée and Wahlbin and is given in [17, Prop. 2.1]. Assume in (2.4) that: $\overline{\sigma} = \sigma =$ constant > 0; $\overline{\phi}(\eta,\xi)$ is a convolution kernel; and, for some B, $\alpha > 0$,

$$|\phi(\eta)| \le Be^{-\alpha\eta} \text{ such that } \int_0^\infty |\phi(s)|\,ds < \sigma.$$

Under these conditions Thomée and Wahlbin show that there is an $\epsilon > 0$ such that $|\gamma(\eta)| \le e^{-\epsilon\eta}|\gamma(0)|$. From this it follows that $\|\gamma\|_{L_q(0,\eta)} \le C_q(\eta)|\gamma(0)|$, where $C_q(\eta) := (1-e^{-q\epsilon\eta})/q\epsilon$ for $q \in [1,\infty)$, and $C_\infty = 1$. Using this weak stability estimate in the last part of the proof of Lemma 2.2 then gives $\|\gamma'\|_{L_q(0,\eta)} \le C_q(\eta)(|||\phi||| + \sigma)|\gamma(0)|$. This is clearly a much sharper result that the general one derived above.

With the dual stability estimates established we now move on to give some relevant interpolation-error estimates.

Lemma 2.3. *For the piecewise constant interpolate defined later in (3.7) the following interpolation-error estimate applies:*

$$\|w - \pi w\|_{L_q(\mathcal{J}_i)} \le \begin{cases} k_i^{1/q}\|w'\|_{L_1(\mathcal{J}_i)}, & \text{for } q \in [1,\infty), \\ \|w'\|_{L_1(\mathcal{J}_i)}, & \text{for } q = \infty, \end{cases}$$

for all $w \in W_1^1(\mathcal{J}_i)$.

Proof. For t, $s \in [t_{i-1}, t_i]$ we know that $w(s) = w(t) + \int_t^s w'(\xi)\,d\xi$ and therefore, using the definition of πw in (3.7), we get, after substituting for $w(s)$ in the integrand,

$$w(t) - \pi w(t) = \frac{-1}{k_i}\int_{t_{i-1}}^{t_i}\int_t^s w'(\xi)\,d\xi ds. \qquad \text{(i)}$$

Now, for $1 < p, q < \infty$ and p such that $p^{-1} + q^{-1} = 1$, we find by applying Hölder's inequality to this that:

$$\int_{t_{i-1}}^{t_i} |w(t) - \pi w(t)|^q\,dt \le k_i^{-q}\int_{t_{i-1}}^{t_i}\left(\int_{t_{i-1}}^{t_i}\left|\int_t^s w'(\xi)\,d\xi\right| ds\right)^q dt,$$
$$\le k_i^{-q+q/p}\int_{t_{i-1}}^{t_i}\int_{t_{i-1}}^{t_i}\left|\int_t^s w'(\xi)\,d\xi\right|^q dsdt.$$

Majorizing the inner integral gives

$$\|w - \pi w\|_{L_q(\mathcal{J}_i)}^q \le k_i^{2-q+q/p}\|w'\|_{L_1(\mathcal{J}_i)}^q,$$

which gives the required result since $2 - q + q/p = 1$. For $q = \infty$ we note that (i) implies $|w - \pi w|(t) \le \|w'\|_{L_1(\mathcal{J}_i)}$, but since $t \in \overline{\mathcal{J}}_i$ is arbitrary, and does not appear on the right hand side, we may replace $|w - \pi w|$ by $\|w - \pi w\|_{L_\infty(\mathcal{J}_i)}$. ■

Lemma 2.4. *For the piecewise constant interpolate defined later by (3.7) the following error estimate applies for all $t \in \mathcal{J}^k$,*

$$\|\kappa^{-1}(w - \pi w)\|_{L_q(0,t)} \le \|w'\|_{L_q(0,t)},$$

when $w \in W_q^1(0,t)$, for $q \in [1,\infty]$, and κ is the piecewise constant function such that $\kappa|_{\mathcal{J}_i} = k_i$ for $i = 1,\dots,N$.

Proof. For p conjugate to q apply Hölder's inequality to the right hand side of the result in Lemma 2.3, this gives: $\|w - \pi w\|_{L_q(\mathcal{J}_i)} \le k_i\|w'\|_{L_q(\mathcal{J}_i)}$. Now: divide through by k_i; raise each side to the power q; sum each side to the required $t \in \mathcal{J}^k$; and, finally, take q^{th} roots. ■

3. Analysis of the backward Euler variant. Our aim in this section is to produce a discontinuous piecewise polynomial approximation to the solution $u(t)$ of (1.1) and to analyze the Galerkin error, some numerical experiments will then be given in the next section to illustrate the error bounds derived below. Our main concern is with a piecewise constant approximation which produces a variant on the classical backward Euler method, but for the sake of generality some of the results below allow for polynomial degree $r \ge 0$.

Let $(\cdot,\cdot)$ be the usual $L_2(\mathcal{J})$ inner product, then a Galerkin formulation of (1.1) is: find $u \in W_p^1(\mathcal{J})$ such that

$$(Au, v) := (u' + \sigma u - \Lambda u, v) = (f, v) \qquad \forall v \in L_q(\mathcal{J}), \qquad (3.1)$$

with $u(0) = u_0$ and where q is conjugate to p so that $p^{-1} + q^{-1} = 1$. In the finite element formulation of (3.1) we will seek an approximating solution $U \in V_r^h$ where

$$V_r^h := \{v \in L_\infty(\mathcal{J}) : v \in \mathbb{P}_r(\mathcal{J}_i) \text{ for each } i = 1, \dots, N.\}, \tag{3.2}$$

and $\mathbb{P}_r(\mathcal{J}_i)$ denotes the set of all polynomials of degree r defined on $\mathcal{J}_i$. When $r = 0$ we will write $V^h := V_0^h$ for brevity. For such functions $w \in V_r^h$ we adopt the following convenient notation:

$$w_i^+ := \lim_{s\downarrow 0} w(t_i + s), \qquad w_i^- := \lim_{s\uparrow 0} w(t_i + s)$$

and $w_0^- := w(0)$ denote the limiting values either side of a possible discontinuity; $w_i := w(t)|_{\mathcal{J}_i}$ denotes the function that results from restricting w to a single $\mathcal{J}_i$; and, by $[\![w_i]\!]$ we mean the "jump" in w at a time $t_i \in \mathcal{J}^k$, that is,

$$[\![w_i]\!] := w_i^+ - w_i^-.$$

(So $[\![w_i]\!] = w_{i+1} - w_i$ when $r = 0$ since then: $w_{i-1}^+ = w_i^- = w_i$.) From time to time we will also use these notations for functions in spaces other than V_r^h.

With this approximating space we now encounter a technical difficulty, we cannot simply pose the finite element problem as: find $U \in V_r^h$ such that

$$(U' + \sigma U - \Lambda U, v) = (f, v) \qquad \forall v \in V_r^h, \tag{3.3}$$

since U is not smooth enough to permit the differentiation. However, U does have a distributional derivative which is symbolically given by

$$U'(t) + \sum_{i=0}^{N-1} [\![U_i]\!] \delta(t - t_i),$$

and motivated by this we *define* the finite element problem as: find $U \in V_r^h$ such that

$$(AU, v) := \sum_{j=1}^{N} \int_{t_{j-1}}^{t_j} U'v\,dt + (\sigma U - \Lambda U, v) + \sum_{i=0}^{N-1} v_i^+ [\![U_i]\!] = (f, v) \qquad \forall v \in V_r^h. \tag{3.4}$$

Note that if v were also smooth enough to be a test function for the space of distributions then this would follow directly from (3.3) by using the distributional derivative of U. That is: we would set $(U', v) := -(U, v')$ and integrate by parts in the latter term, see for example the summary account in [13, Chap. 2].

To obtain a time stepping algorithm for the piecewise constant case, $r = 0$, we now take $v = 1$ on $\mathcal{J}_i$ and $v = 0$ elsewhere, this yields the implicit method: for $i = 1, \dots, N$, find U_i such that

$$U_i - U_{i-1} + U_i \int_{t_{i-1}}^{t_i} \sigma(t)\,dt = \int_{t_{i-1}}^{t_i} f(t)\,dt + \int_{t_{i-1}}^{t_i} \Lambda U(t)\,dt, \tag{3.5}$$

with starting value $U_0 = U_0^- = u_0$. In the case when there is no history (i.e. $\phi \equiv 0$) this is a variant of the classical backward Euler scheme for (1.1) and is considered in [9, Chap. 2§4] and [5]. In order to arrive at a truly practical scheme we will have

to introduce some quadrature approximation to the inner products and history term, these are considered numerically in the next section and quantified later in Section 7. For the remainder of this section we will be concerned only with bounding the Galerkin error.

Below we shall derive *a posteriori* and *a priori* error estimates, the former will then be used in the next section to provide a basis for adaptive time stepping and error feedback. Prior to the analysis we need to outline some preliminary results, of which the first concerns the *Galerkin orthogonality* of the residual. Set $e = u - U$ and define the *partial residual*: $r(t) := f(t) - U'(t) - \sigma(t)U(t) + \Lambda U(t)$. Then, subtracting (3.4) from (3.1) we get

$$(Ae, v) = \sum_{i=0}^{N-1} \left(\int_{t_i}^{t_{i+1}} rv\,dt - v_i^+ [\![U_i]\!] \right) = 0 \qquad \forall v \in V_r^h.$$

In particular, it follows from this that for each $i \in \{1, \dots, N\}$

$$\int_{t_{i-1}}^{t_i} rv\,dt - v_{i-1}^+ [\![U_{i-1}]\!] = 0 \qquad \forall v \in \mathbb{P}_r(\mathcal{J}_i). \tag{3.6}$$

Secondly, if $w \in L_1(\mathcal{J})$ we can define a piecewise constant elementwise mean interpolate, $\pi w \in V_r^h$, to w as:

$$\pi w(t) := \frac{1}{k_i} \int_{t_{i-1}}^{t_i} w(\xi)\,d\xi \quad \text{ for } t \in \mathcal{J}_i \text{ and } i = 1, \dots, N. \tag{3.7}$$

With these in mind the first theorem of this section gives the *a posteriori* error estimate.

Theorem 3.1. *Let Assumptions 1.1 hold for some $p \in (1, \infty)$ and let Theorem 2.1 hold for q conjugate to p. Then, the Galerkin error in the backward Euler variant (3.4) satisfies the computable bound:*

$$\left.\begin{array}{ll} \text{(a)} & \max_{1\le j\le i} |u(t_j) - U_j^-| \\[1ex] \text{(b)} & \|u - U\|_{L_\infty(0,t_i)} \end{array}\right\} \le \widehat{E}_{\mathrm{BE}}(j, p) := C_1^s \max_{1\le j\le i} \left\{ k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)} + |U_j - U_{j-1}| \right\},$$

for every $i \in \{1, \dots, N\}$ and where C_1^s is a strong dual stability constant guaranteed by Theorem 2.1. In this bound $p \in [1, \infty]$ and $q = p/(p - 1)$.

Proof. We begin with the nodal error bound in Case (a). Pick an arbitrary $i \in \{1, \dots, N\}$ and set $e_i^- := u(t_i) - U_i^-$. Also, note from Remark 1.1 that with $p \in (1, \infty) \Rightarrow q \in (1, \infty)$ both u and χ are continuous on $[0, t_i]$. Consider first the dual backward problem (2.1) with the data: $\Upsilon = t_i$; $g = 0$; and, $\chi(\Upsilon) = e_i^-$, and observe that Theorem 2.1 gives a strong stability constant, C_1^s, such that $\|\chi'\|_{L_1(0,t_i)} \le C_1^s |e_i^-|$. Now, using this dual problem to add on zero we get

$$|e_i^-|^2 = |e_i^-|^2 + \sum_{j=1}^{i} \int_{t_{j-1}}^{t_j} (\sigma\chi - \chi' - \Lambda^*\chi) e\,dt.$$

Integrating this by parts to shift the time derivative onto e, and using Remark 1.1 and the definition of Λ^* in (2.2) as the $L_2(0,t_i)$-adjoint to Λ, we obtain the error representation

$$|e_i^-|^2 = \sum_{j=1}^{i} \int_{t_{j-1}}^{t_j} r\chi\,dt + e_0^+\chi_0^+ + \sum_{j=1}^{i-1} \chi_j^+(e_j^+ - e_j^-),$$

where $r = f - U' - \sigma U + \Lambda U$ is the partial residual defined earlier for (3.6). Expanding the notation we can see that $e_0^+ = -[\![U_0]\!]$ and $e_j^+ - e_j^- = -[\![U_j]\!]$, and so, with this and the Galerkin orthogonality (3.6):

$$\begin{aligned} |e_i^-|^2 &= \sum_{j=1}^{i} \left(\int_{t_{j-1}}^{t_j} \chi r\,dt - \chi_{j-1}^+[\![U_{j-1}]\!] \right), \qquad \text{(i)} \\ &= \sum_{j=1}^{i} \left(\int_{t_{j-1}}^{t_j} (\chi - \pi\chi) r\,dt - (\chi - \pi\chi)_{j-1}^+[\![U_{j-1}]\!] \right), \end{aligned}$$

where $\pi\chi \in V^h$ is the piecewise constant interpolate to χ as given by (3.7). Now using, in turn, the interpolation-error estimate for $q = \infty$ given in Lemma 2.3 and the strong stability estimate given in Theorem 2.1 we find:

$$\begin{aligned} |e_i^-|^2 &\le \sum_{j=1}^{i} \left(\|r\|_{L_1(\mathcal{J}_j)} + |U_j - U_{j-1}| \right) \|\chi - \pi\chi\|_{L_\infty(\mathcal{J}_j)}, \\ &\le \sum_{j=1}^{i} \left(\|r\|_{L_1(\mathcal{J}_j)} + |U_j - U_{j-1}| \right) \int_{t_{j-1}}^{t_j} |\chi'|\,dt, \\ &\le \int_0^{t_i} |\chi'|\,dt \quad \max_{1\le j\le i} \left\{ \|r\|_{L_1(\mathcal{J}_j)} + |U_j - U_{j-1}| \right\}, \\ \Longrightarrow |e_i^-| &\le C_1^s \max_{1\le j\le i} \left\{ k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)} + |U_j - U_{j-1}| \right\}. \end{aligned}$$

Since the right hand side of this inequality is a non-decreasing function of i it is possible to replace the left hand side with $\max\{|e_1^-|, \dots, |e_i^-|\}$, thus giving the desired result.

The proof of Case (b) proceeds in a similar manner but here, to keep the argument simple, we consider only the case $r = 0$. Set $e(t) = u(t) - U(t)$; pick an arbitrary $t_i \in \mathcal{J}^k$ and in (2.1) set $\Upsilon := t_i^-$ and $\chi(\Upsilon) = 0$. Use the strong stability for $q = 1$ from Theorem 2.1, let $\langle\cdot,\cdot\rangle$ denote the $L_2(0, t_i^-)$ inner product and use the dual problem to write $\langle e, g\rangle = \langle e, A^*\chi\rangle$. Now we need to verify that (2.3) holds for this non-smooth function e. Firstly note that $\langle e, \sigma\chi\rangle = \langle \sigma e, \chi\rangle$ and $\langle e, -\Lambda^*\chi\rangle = \langle -\Lambda e, \chi\rangle$ and so we are left to consider $\langle e, -\chi'\rangle$. For this we have:

$$-\int_0^{t_i} \chi' e\,dt = \sum_{j=1}^{i} \left(\chi e\Big|_{t_j^-}^{t_{j-1}^+} + \int_{t_{j-1}}^{t_j} e'\chi\,dt \right).$$

Now, using Remark 1.1 and $\chi(t_i^-) = 0$ we find:

$$\begin{aligned} \sum_{j=1}^{i} \chi e\Big|_{t_j^-}^{t_{j-1}^+} &= \sum_{j=1}^{i} \left(\chi(t_{j-1}^+) e(t_{j-1}^+) - \chi(t_j^-) e(t_j^-) \right) \\ &= \chi(t_0^+) e(t_0^+) + \sum_{j=1}^{i-1} \chi(t_j^+) \big(e(t_j^+) - e(t_j^-) \big) = -\sum_{j=0}^{i-1} \chi_j^+ [\![U_j]\!], \end{aligned}$$

similarly to before. Observing now that $e' = u'$ on each (t_{j-1}, t_j) we obtain:

$$\langle e, g\rangle = \langle u' + \sigma e - \Lambda e, \chi\rangle - \sum_{j=0}^{i-1} \chi_j^+ [\![U_j]\!] = \langle r, \chi\rangle - \sum_{j=1}^{i} \chi_{j-1}^+ [\![U_{j-1}]\!],$$

and we see that the right hand side here is identical to that in (i). Writing

$$\|e\|_{L_\infty(0,t_i^-)} = \sup\left\{ |\langle e, g\rangle| : \|g\|_{L_1(0,t_i^-)} = 1 \right\},$$

the required bound on $|\langle e, g\rangle|$ is now obtained exactly as before from (i). ■

The *a posteriori* error estimates just given depend upon the strong initial-data-stability of the continuous dual backward problem (2.1). This problem is, of course, discretization independent and has been dealt with already in Section 2. For the remainder of this section we will be concerned with deriving *a priori* Galerkin-error estimates for (3.4) in the case $r = 0$. For this we again adopt the methodology in [9], [18, Chap. 6] and [5] so that the *a priori* estimate will depend upon the strong initial-data-stability of a *discrete* dual backward problem. In what follows we firstly define an appropriate dual problem and then give a series of results which lead to the required strong stability estimate. With this we are then able to state the *a priori* Galerkin-error estimate in Theorem 3.2.

The main results in the remainder of this section are specialized to the case $r = 0$ in (3.2) and, in addition to Assumptions 1.1, are derived with respect to the following more restrictive assumptions.

Assumptions 3.1. *In addition to Assumptions 1.1 let the following also be satisfied:*

(i) $\exists K > 0$ *such that*

$$\int_a^b \sigma(t) - \int_t^b \phi(s,t)\,ds\,dt \ge 0 \quad \forall a, b \in \overline{\mathcal{J}} \text{ such that } b - a \in [0, K].$$

We can think of the largest such K as the maximum permitted time step.

(ii) Assumptions 1.1 are satisfied for $p = \infty$ and are also satisfied when $q \ge p$. This implies that the data are such that the dual problem (2.1) also makes sense for $q \ge 2$.

■

The appropriate discrete dual problem is arrived at by transposing (3.4). Note first that after a rearrangement (3.4) can be given in the conventional finite element way as: find $U \in V_r^h$ such that

$$\left.\begin{aligned} a(t_N;U,v) &= F(t_N;v) \qquad \forall v \in V_r^h, \\ &\text{where for } t_M \in \mathcal{J}^k \text{ we set} \\ a(t_M;U,v) &:= \sum_{i=1}^{M} \int_{t_{i-1}}^{t_i} (U' + \sigma U - \Lambda U)v\,dt \\ &\quad + \sum_{i=2}^{M} v_{i-1}^+ [\![U_{i-1}]\!] + v_0^+ U_0^+, \\ F(t_M;v) &:= \int_0^{t_M} fv\,dt + v_0^+ U_0^-, \\ U_0^- &:= u_0 \text{ (initial datum).} \end{aligned}\right\} \tag{3.8}$$

In the above we understand that backward summations are treated as zero so that $\sum_n^m \cdot := 0$ if $m < n$.

After noting (3.1) and recalling Remark 1.1 it is clear that with $u \in W_p^1(\mathcal{J})$ we have

$$a(t_M;u,v) = F(t_M;v) \qquad \forall v \in L_q(0,t_M) \text{ and } \forall t_M \in \mathcal{J}^k$$

since the jump terms vanish. Thus (3.6) can be written equivalently as

$$a(t_M;u-U,v) = 0 \qquad \forall v \in V^h \text{ and } \forall t_M \in \mathcal{J}^k. \tag{3.9}$$

In the remainder of this section we set $\Upsilon := t_M \in \mathcal{J}^k$ where $M \in \{1,\ldots,N\}$ is fixed but arbitrary. The discrete dual problem we require for the *a priori* error estimate now reads as: find $X \in W_r^h$ such that

$$\left.\begin{aligned} a^*(t_M;X,v) &= G(v) \qquad \forall v \in W_r^h, \\ &\text{where} \\ a^*(t_M;X,v) &:= \sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} (-X' + \sigma X - \Lambda^* X)v\,dt \\ &\quad - \sum_{j=1}^{M-1} v_j^- [\![X_j]\!] + v_M^- X_M^-, \\ G(v) &:= \int_0^{\Upsilon} gv\,dt + v_M^- X_M^+, \\ X_M^+ &:= \chi_\Upsilon \quad \text{(given),} \end{aligned}\right\} \tag{3.10}$$

and, analogously to (3.2),

$$W_r^h := \{v \in L_\infty(0,\Upsilon) : v \in \mathbb{P}_r(\mathcal{J}_i) \text{ for each } i = 1,\ldots,M\}. \tag{3.11}$$

In the above χ_Υ and g are exactly as in (2.1) and in fact X is a finite element approximation to χ in the same way as U is to u. That the superscripts $^+$ and $^-$ are reversed between (3.8) and (3.10) corresponds to time running in opposite directions in each.

This choice for the discrete dual problem results in the following relationships.

Lemma 3.1. *$a^*(t_M;v,w) = a(t_M;w,v)$ $\quad \forall v \in \cup_{i=1}^M W_q^1(\mathcal{J}_i)$ and $\forall w \in \cup_{i=1}^M W_p^1(\mathcal{J}_i)$ and therefore, that*

$$a^*(t_M;v,u-U) = a(t_M;u-U,v) = 0 \qquad \forall v \in W_r^h$$

follows immediately from (3.9).

Proof. This is simply a matter of integrating (3.8) by parts and rearranging terms to arrive at (3.10). Firstly, in (3.8) use the definition of Λ^* in (2.2) to see that

$$\int_0^{\Upsilon} (\sigma w - \Lambda w)v\,dt = \int_0^{\Upsilon} (\sigma v - \Lambda^* v)w\,dt. \tag{i}$$

Now, to switch the derivatives we partially integrate over each $\mathcal{J}_j$ and cancel and recollect the jump terms. From (3.8) we begin with

$$\sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} w'v\,dt = -\sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} v'w\,dt + \sum_{j=1}^{M} \left(v_j^- w_j^- - v_{j-1}^+ w_{j-1}^+\right),$$

from which it follows that

$$\begin{aligned} \sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} w'v\,dt &+ \sum_{j=1}^{M-1} v_j^+ [\![w_j]\!] + v_0^+ w_0^+ \\ &= \sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} -v'w\,dt + v_0^+ w_0^+ + v_M^- w_M^- - v_{M-1}^+ w_{M-1}^+ \\ &\quad + \sum_{j=1}^{M-1} \left(v_j^+ w_j^+ - v_{j-1}^+ w_{j-1}^+ - w_j^- [\![v_j]\!]\right) \\ &= \sum_{j=1}^{M} \int_{t_{j-1}}^{t_j} -v'w\,dt - \sum_{j=1}^{M-1} w_j^- [\![v_j]\!] + v_M^- w_M^-. \end{aligned} \tag{ii}$$

So, using (i) and (ii) with the definitions of the bilinear forms given in (3.8) and (3.10) shows that $a^*(t_M;v,w) = a(t_M;w,v)$, as required. ∎

Our route to the required strong stability estimate for (3.10) will be via a weak stability result. Henceforth we specialize our considerations to the case where $r = 0$ and set $W^h := W_0^h$ for brevity. Taking $v = 1$ on $\mathcal{J}_j$, for some $j \in \{1,\ldots,M\}$, and $v = 0$ elsewhere we have $v \in W^h$ and (3.10) gives

$$X_j = G_j(X_{j+1} + H_j(X) + g_j) \quad \text{ for } j = M, M-1, \ldots, 1 \tag{3.12}$$

with $X_M^+ = X_{M+1} = \chi_\Upsilon$. Here:

$$g_j := \int_{t_{j-1}}^{t_j} g\,dt; \qquad H_j(X) := \int_{t_{j-1}}^{t_j} \sum_{i=j}^{M-1} X_{i+1} \int_{t_i}^{t_{i+1}} \phi(s,t)\,ds\,dt$$

(with backward sums zero so that $H_M(X) = 0$); and $G_j := (1 + S_j - F_j)^{-1}$ with

$$S_j := \int_{t_{j-1}}^{t_j} \sigma\,dt \qquad \text{and} \qquad F_j := \int_{t_{j-1}}^{t_j} \int_t^{t_j} \phi(s,t)\,dsdt.$$

Also, due to Assumption 3.1.i we have $G_j \in (0,1]$ if $k_j \in (0,K]$. It is clear that without a restriction of this type we could have $G_j^{-1} = 0$ and then the numerical scheme would break down.

The following representation of the discrete dual solution will be useful.

Lemma 3.2. *Let Assumptions 1.1 and 3.1 hold and set*

$$P(j) := X_{M+1}\prod_{i=j}^{M} G_i + \sum_{i=j}^{M}\Big(H_i(X)+g_i\Big)\prod_{k=j}^{i} G_k,$$

then $X_j = P(j) \quad \forall j \in \{1,\dots,M\}$.

Proof. It is clear from (3.12) that $X_M = P(M)$ and so we assume that $X_{j+1} = P(j+1)$ for some $j \in \{1,\dots,M-1\}$. If this is the case then substituting it into (3.12) we find:

$$\begin{aligned} X_j &= G_j P(j+1) + G_j(H_j(X)+g_j) \\ &= X_{M+1}\prod_{i=j}^{M} G_i + \sum_{i=j+1}^{M}\Big(H_i(X)+g_i\Big)\prod_{k=j}^{i} G_k + G_j(H_j(X)+g_j) \\ &= P(j). \end{aligned}$$

Hence: $X_{j+1} = P(j+1) \Rightarrow X_j = P(j)$ and this completes the proof. ∎

With these preliminaries established we now give weak and strong stability estimates for (3.10).

Lemma 3.3. *Let Assumptions 1.1 and 3.1 hold. Then, if each $k_j \le K$, the solution to (3.12) obeys the data-stability bound:*

$$\|X\|_{L_q(t,\Upsilon)} \le C\big(|X_{M+1}| + \|g\|_{L_1(t,\Upsilon)}\big)$$

for all $t \in [0,\Upsilon]$.

Proof. Picking an arbitrary $j \in \{1,\dots,M\}$ we work directly from the expression $X_j = P(j)$ given in Lemma 3.2. Then, due to Assumption 3.1.i we have $|\Pi G_k| \le 1$ for all relevant limits on the product, and so

$$|X_j| \le |X_{M+1}| + \int_{t_{j-1}}^{\Upsilon} |g|\,dt + \sum_{i=j}^{M-1}\int_{t_{i-1}}^{t_i}\left|\sum_{n=i}^{M-1}\int_{t_n}^{t_{n+1}} X_{n+1}\phi(s,t)\,ds\right| dt. \qquad \text{(i)}$$

We now estimate the rightmost term in three stages. Firstly:

$$\left|\sum_{n=i}^{M-1}\int_{t_n}^{t_{n+1}} X_{n+1}\phi(s,t)\,ds\right| \le \|X\|_{L_q(t_i,\Upsilon)}\left(\int_{t_i}^{\Upsilon}|\phi(s,t)|^p\,ds\right)^{1/p},$$

Which follows by applying Hölder's inequality, first for the integral of a product and then for the resulting sum of a product. We have now bounded the integrand in (i) and so, secondly:

$$\int_{t_{i-1}}^{t_i} \|X\|_{L_q(t_i,\Upsilon)}\left(\int_{t_i}^{\Upsilon}|\phi|^p\,ds\right)^{1/p} dt \le k_i^{1/p}\|X\|_{L_q(t_i,\Upsilon)}\left(\int_{t_{i-1}}^{t_i}\left(\int_{t_i}^{\Upsilon}|\phi|^p\,ds\right)^{q/p} dt\right)^{1/q},$$

also from Hölder's inequality. Thirdly, we now sum this bound over $i = j,\dots,M-1$, this gives:

$$\begin{aligned} \sum_{i=j}^{M-1} k_i^{1/p}\|X\|_{L_q(t_i,\Upsilon)}&\left(\int_{t_{i-1}}^{t_i}\left(\int_{t_i}^{\Upsilon}|\phi|^p\,ds\right)^{q/p} dt\right)^{1/q} \\ &\le \|X\|_{L_q(t_j,\Upsilon)}\left(\sum_{i=j}^{M-1} k_i\right)^{1/p}\left(\int_{t_{j-1}}^{t_{M-1}}\left(\int_{t}^{\Upsilon}|\phi|^p\,ds\right)^{q/p} dt\right)^{1/q} \\ &\le \Upsilon^{1/p}|||\phi|||\,\|X\|_{L_q(t_j,\Upsilon)}, \end{aligned}$$

where we have used Hölder's inequality for sums together with

$$\sum_{i=j}^{M-1}\int_{t_{i-1}}^{t_i}\left(\int_{t_i}^{\Upsilon}|\phi|^p\,ds\right)^{q/p} dt \le \sum_{i=j}^{M-1}\int_{t_{i-1}}^{t_i}\left(\int_{t}^{\Upsilon}|\phi|^p\,ds\right)^{q/p} dt \le |||\phi|||^q.$$

Returning now to (i) we have found that

$$|X_j| \le \beta(t_j) + \psi\|X\|_{L_q(t_j,\Upsilon)}$$

where $\psi := \Upsilon^{1/p}|||\phi|||$ and $\beta(t) := |X_{M+1}| + \|g\|_{L_1(t,\Upsilon)}$. By adding non-negative quantities on to the right of this inequality we can then arrive at

$$|X| \le \beta(t) + \psi\|X\|_{L_q(t,\Upsilon)} \qquad \forall t \in [0,\Upsilon]$$

since $X|_{\mathcal{J}_j} = X_j$ and our choice of j is arbitrary. Before invoking Lemma 2.1 we need to turn this into a "forward" inequality. If the variable of integration in the above is s then we introduce the new variables and functions, ξ, τ, $\widehat{X}$ and $\widehat{\beta}$, given by:

$$\tau := \Upsilon - t, \quad \xi := \Upsilon - s, \quad \widehat{X}(\tau) := |X(\Upsilon-\tau)| \quad \text{and} \quad \widehat{\beta}(\tau) := \beta(\Upsilon-\tau).$$

Substituting these into the inequality and using Lemma 2.1 we then get:

$$\begin{aligned} &\widehat{X}(\tau) \le \widehat{\beta}(\tau) + \psi\|\widehat{X}\|_{L_q(0,\tau)} \\ \Longrightarrow\quad &C\big(|X_{M+1}| + \|g\|_{L_1(t,\Upsilon)}\big) \ge \|\widehat{X}\|_{L_q(0,\tau)} = \|X\|_{L_q(t,\Upsilon)} \end{aligned}$$

for all $t \in [0,\Upsilon]$. This completes the proof. ∎

Lemma 3.4. *Let Assumptions 1.1 and 3.1 hold. For the piecewise constant discrete dual backward problem (3.10): find $X \in W^h$ such that*

$$a^*(t_M; X, v) = v_M^- X_M^+ \qquad \forall v \in W^h \text{ and } M \in \{1,\dots,N\},$$

there exists a constant, C, such that

$$\sqrt{\iota\int_0^{\Upsilon}\sigma X^2\,dt} + \sum_{j=1}^{M}\big|[\![X_j]\!]\big| + |X_1| \le C|X_M^+|.$$

Here: $\iota := 2$ iff $\sigma \ge 0$ almost everywhere in $(0,\Upsilon)$ and then $C = C(K,\Upsilon,|||\phi|||)$, otherwise $\iota := 0$ and $C = C(K,\Upsilon,|||\phi|||,\|\sigma\|_{L_\infty(0,\Upsilon)})$.

Proof. Pick $v = 2X \in W^h$ in (3.10), for $X_{M+1} := X_M^+$ this gives

$$2\int_0^\Upsilon \sigma X^2\,dt + \sum_{j=1}^{M} [\![X_j]\!]^2 + X_1^2 = X_{M+1}^2 + 2\int_0^\Upsilon X\Lambda^* X\,dt \tag{i}$$

because: $2X_j^-[\![X_j]\!] = -[\![X_j]\!]^2 - (X_j^-)^2 + (X_j^+)^2$. We now use Lemma 3.3 to bound the Volterra term:

$$\begin{aligned}\left|2\int_0^\Upsilon X\Lambda^* X\,dt\right| &\le 2\|X\|_{L_q(0,\Upsilon)}\left\|\int_t^\Upsilon \phi(s,t)X(s)\,ds\right\|_{L_p(0,\Upsilon)}\\ &\le 2\|X\|_{L_q(0,\Upsilon)}\left\|\left(\int_t^\Upsilon |\phi|^p\,ds\right)^{1/p}\|X\|_{L_q(t,\Upsilon)}\right\|_{L_p(0,\Upsilon)}\\ &\le 2\Upsilon^{1/p-1/q}|\!|\!|\!|\phi|\!|\!|\!|\,\|X\|_{L_q(0,\Upsilon)}^2.\end{aligned}$$

This last step follows since $q \ge p$ by Assumption 3.1.ii and for $P, Q \in [1,\infty]$ such that $1/P + 1/Q = 1$ we find

$$\begin{aligned}\left(\int_0^\Upsilon\left(\int_t^\Upsilon |\phi|^p\,ds\right)dt\right)^{1/p} &\le \|1\|_{L_Q(0,\Upsilon)}^{1/p}\left(\int_0^\Upsilon\left(\int_t^\Upsilon |\phi|^p\,ds\right)^P dt\right)^{1/pP}\\ &\le \Upsilon^{1/p-1/q}|\!|\!|\!|\phi|\!|\!|\!|,\end{aligned}$$

by setting $P = q/p \ge 1$ so that $1/pP = 1/q$ and $1/pQ = 1/p - 1/q$. So, returning to (i) we get

$$2\int_0^\Upsilon \sigma X^2\,dt + \sum_{j=1}^{M}[\![X_j]\!]^2 + X_1^2 \le C|X_{M+1}|^2 \tag{ii}$$

after using Lemma 3.3 to bound $\|X\|_{L_q(0,\Upsilon)}^2$ (in this problem $g = 0$). Now, in (3.10) we pick $v = [\![X_i]\!]$ in $\mathcal{J}_i$ and $v = 0$ elsewhere, thus for any $i \in \{1,\dots,M\}$ we obtain

$$\begin{aligned}[\![X_i]\!]^2 = \int_{t_{i-1}}^{t_i}(\sigma X - \Lambda^* X)[\![X_i]\!]\,dt &\le \frac{k_i}{2}\int_{t_{i-1}}^{t_i}|\sigma X - \Lambda^* X|^2\,dt + \frac{1}{2}[\![X_i]\!]^2,\\ \implies \frac{1}{k_i}[\![X_i]\!]^2 &\le \int_{t_{i-1}}^{t_i}|\sigma X - \Lambda^* X|^2\,dt,\end{aligned}$$

where we used the inequality: $2ab \le \epsilon a^2 + b^2/\epsilon$. Using the result above we find:

$$\begin{aligned}\sum_{j=1}^M |[\![X_j]\!]| &\le \left(\sum_{j=1}^M k_j\right)^{1/2}\left(\sum_{j=1}^M \frac{1}{k_j}[\![X_i]\!]^2\right)^{1/2} \le \Upsilon^{1/2}\left(\int_0^\Upsilon |\sigma X - \Lambda^* X|^2\,dt\right)^{1/2},\\ &\le \sqrt{2\Upsilon\left(|\!|\!|\!|\phi|\!|\!|\!|^2 + \|\sigma\|_{L_\infty(0,\Upsilon)}^2\right)}\,\|X\|_{L_2(0,\Upsilon)},\end{aligned}$$

after using Assumption 3.1.ii to take $p = q = 2$ in Assumption 1.1.iii to see that

$$\begin{aligned}\int_0^\Upsilon |\Lambda^* X|^2\,dt = \int_0^\Upsilon\left[\int_t^\Upsilon \phi(s,t)X(s)\,ds\right]^2 dt &\le \int_0^\Upsilon\int_t^\Upsilon |\phi|^2\,ds\int_t^\Upsilon |X|^2 ds\,dt,\\ &\le |\!|\!|\!|\phi|\!|\!|\!|^2\|X\|_{L_2(0,\Upsilon)}^2,\end{aligned}$$

and also using

$$\int_0^\Upsilon |\sigma X|^2\,dt \le \|\sigma\|_{L_\infty(0,\Upsilon)}^2\|X\|_{L_2(0,\Upsilon)}^2.$$

From Lemma 3.3 we therefore have

$$\sum_{j=1}^M |[\![X_j]\!]| \le C(\Upsilon,\phi,\sigma)|X_{M+1}|$$

and using this with (ii) gives

$$2\int_0^\Upsilon \sigma X^2\,dt + \left(\sum_{j=1}^M |[\![X_j]\!]|\right)^2 + X_1^2 \le C|X_{M+1}|^2.$$

If $\sigma \ge 0$ almost everywhere in $(0,\Upsilon)$ we now take square roots to obtain the desired result with $\iota = 2$. Otherwise the term in σ can be brought to the right-hand side and estimated by Lemma 3.3 in the following manner:

$$2\left|\int_0^\Upsilon \sigma X^2\,dt\right| \le 2\|\sigma\|_{L_\infty(0,\Upsilon)}\|X\|_{L_2(0,\Upsilon)}^2 \le C|X_{M+1}|^2.$$

In this case the lemma holds with $\iota = 0$ and C depending on σ in the way just demonstrated. ■

Recalling now that the original choice of M was arbitrary the following *a priori* Galerkin-error estimate can now be proven.

Theorem 3.2. *Let Assumptions 1.1 and 3.1 hold. Then, if $u \in W_\infty^1(\mathcal{J})$, the nodal Galerkin-error in the piecewise constant approximation to (1.1) by (3.5) obeys*

$$|(u-U)_M^-| \le (C_s + 1)\|\kappa u'\|_{L_\infty(0,t_M)} \qquad \forall M \in \{1,\dots,N\},$$

where C_s is a strong discrete dual stability constant and $\kappa \in V^h$ is defined by $\kappa|_{\mathcal{J}_i} = k_i$ for $i = 1,\dots,N$ and is restricted such that $\|\kappa\|_{L_\infty(\mathcal{J})} \le K$.

Proof. Let $X \in W^h$ solve the discrete dual backward problem: $a^*(t_M; X, v) = v_M^- E_M^-$ $\forall v \in W^h$. Here $E := \pi u - U \in W^h$ where πu is given by (3.7). In this problem we take $v = E$ and use the orthogonality (3.9) with Lemma 3.1 to get

$$|E_M^-|^2 = a^*(t_M; X, E) = a^*(t_M; X, \pi u - u),$$

and so, recalling the definition of the bilinear form in (3.10):

$$\begin{aligned}|E_M^-|^2 &= \int_0^\Upsilon (\sigma X - \Lambda^* X)(\pi u - u)\,dt - \sum_{j=1}^{M-1}(\pi u - u)_j^-[\![X_j]\!] + (\pi u - u)_M^- X_M^-\\ &\le \left(\int_0^\Upsilon |\sigma X - \Lambda^* X|\,dt + \sum_{j=1}^{M-1}|[\![X_j]\!]| + |X_M^-|\right)\|\pi u - u\|_{L_\infty(0,\Upsilon)}.\end{aligned}$$

Now, firstly note that

$$\sum_{j=1}^{M-1} \big|[\![X_j]\!]\big| + |X_M^-| = \sum_{j=1}^{M-1} \big|[\![X_j]\!]\big| + |(X_M^- - X_M^+) + X_M^+|,$$
$$\leq \sum_{j=1}^{M} \big|[\![X_j]\!]\big| + |X_M^+| \leq C|X_M^+|$$

from Lemma 3.4. Also,

$$\int_0^\Upsilon |\sigma X|\,dt \leq \sqrt{\int_0^\Upsilon |\sigma|\,dt \int_0^\Upsilon |\sigma| X^2\,dt} \leq C|X_M^+|$$

from Lemma 3.3 or 3.4 depending upon the positive semi-definiteness of σ. For the Volterra term we get

$$\int_0^\Upsilon |\Lambda^* X|\,dt \leq \int_0^\Upsilon \left(\int_t^\Upsilon |\phi|^p\,ds\right)^{1/p} dt\,\|X\|_{L_q(0,\Upsilon)}$$
$$\leq \Upsilon^{1/p} |||\phi||| \,\|X\|_{L_q(0,\Upsilon)} \leq C|X_M^+|$$

from Lemma 3.3. Collecting these last few results together we then obtain

$$\int_0^\Upsilon |\sigma X - \Lambda^* X|\,dt + \sum_{j=1}^{M-1} \big|[\![X_j]\!]\big| + |X_M^-| \leq C_s|X_M^+|.$$

It is evident that in the dual problem we have chosen the initial datum as $X_M^+ = E_M^-$ and therefore the above implies that $|E_M^-| \leq C_s\|\pi u - u\|_{L_\infty(0,\Upsilon)}$. Using an interpolation-error estimate similar to that of Lemma 2.4 we therefore obtain:

$$\begin{aligned}\big|(u-U)_M^-\big| &\leq \big|(u-\pi u)_M^-\big| + \big|(\pi u - U)_M^-\big| \\ &\leq (C_s+1)\|u-\pi u\|_{L_\infty(0,\Upsilon)} \\ &\leq (C_s+1)\|\kappa u'\|_{L_\infty(0,\Upsilon)}.\end{aligned}$$

This completes the proof. ∎

4. Numerical implementation of the Euler variant. This section is devoted to a practical numerical implementation of the backward Euler variant (3.5). The computational algorithm given below is formed by replacing Λ and the inner products in (3.5) with quadrature rules which have a truncation error significantly smaller than the Galerkin error. We then give below the results of some numerical experiments performed on data for which the exact solutions are known. The adaptive algorithm is derived from the *a posteriori* Galerkin-error estimate, (a), in Theorem 3.1 and, once we establish some "defensive programming" rules, none of the numerical experiments below suggest that it is necessary to consider the quadrature errors. This view is supported by the quadrature-error analysis given below in Section 7, which demonstrates an *a posteriori* error estimate which could be incorporated into the algorithm to account for quadrature errors.

In (3.5) the terms involving σ and f are each calculated with the standard (3 point) Simpson rule, with truncation error of order $O(k_i^5)$. To deal with the history term we use the midpoint rule on the outer integral with Simpson's rule on the inner integral, that is:

$$\begin{aligned}\int_{t_{i-1}}^{t_i} \Lambda U(t)\,dt &\approx k_i U_i \int_{t_{i-1}}^{t_{i-1/2}} \phi(t_{i-1/2},s)\,ds + k_i \sum_{j=1}^{i-1} U_j \int_{t_{j-1}}^{t_j} \phi(t_{i-1/2},s)\,ds \\ &= k_i U_i \Phi(t_{i-1},t_{i-1/2},t_{i-1/2}) + k_i \sum_{j=1}^{i-1} U_j \Phi(t_{j-1},t_j,t_{i-1/2}).\end{aligned}$$

Here:

$$\Phi(a,b,c) := \int_a^b \phi(c,s)\,ds \tag{4.1}$$

and each of these are approximated with a single Simpson's rule. The truncation error here is nominally of order $O(k_i^3)$.

These discrete replacements turn (3.5) into a practical computational scheme, but to implement the adaptivity we need some more approximations. The norms, $\|\cdot\|_{L_p(\mathcal{J}_i)}$, are replaced with discrete approximations indicated by $\|\cdot\|_{L_p^h(\mathcal{J}_i)}$. For $p \in [1,\infty)$ a single Simpson's rule is employed over $\mathcal{J}_i$, and for $p=\infty$ the *value* of the normed quantity is sampled three times within each $\mathcal{J}_i$, at the midpoint and endpoints (taking care to allow for discontinuities), and the maximum $|value|$ taken. Finally, we want the freedom to evaluate the partial residual, $r(t) = f - \sigma U + \Lambda U$, for any $t \in \overline{\mathcal{J}}$. We choose to split Λ into the "far" and "near" history terms thus:

$$\Lambda U(t) = \int_0^{t_{i-1}} \phi(t,s)U(s)\,ds + \int_{t_{i-1}}^t \phi(t,s)U(s)\,ds,$$

for $t \in [t_{i-1},t_i]$ and $i \in \{1,\ldots,N\}$. The former term is approximated with a single Simpson's rule over each of the $\{\mathcal{J}_j\}_{j=1}^{i-1}$, and the latter with a single trapezoidal rule; the truncation error here is of order $O(k_i^3 + k_1^5 + \cdots + k_{i-1}^5)$. We will emphasize this particular "variational crime" by writing r^h for the approximate partial residual so obtained.

Now that we have a practical realization of (3.5), in which we expect the Galerkin error to dominate, our goal is to compute approximate solutions to (1.1) for which

$$e_{\mathrm{BE}}(t_i) := \max_{1\leq j\leq i} |u(t_j) - U_j^-| \leq \mathcal{E} \qquad \forall i \in \{1,\ldots,N\},$$

where $\mathcal{E}$ is a user-specified tolerance. From Theorem 3.1.(a) we see that this will be guaranteed, modulo quadrature errors, if we ensure that

$$E_{\mathrm{BE}}(i,p) \leq \mathcal{E} \qquad \forall i \in \{1,\ldots,N\} \tag{4.2}$$

where now

$$E_{\mathrm{BE}}(i,p) := C_1^s \left(k_i^{1/q}\|r^h\|_{L_p^h(\mathcal{J}_i)} + |U_i - U_{i-1}|\right),$$

since we will then have

$$e_{\mathrm{BE}}(t_i) \leq \widehat{E}_{\mathrm{BE}}(i,p) := \max_{1\leq j\leq i}\{E_{\mathrm{BE}}(j,p)\} \leq \mathcal{E} \tag{4.3}$$

datum	P1	P2	P3	P4	P5
σ	4	4	4	80	80
B	-1.9	-1.9	-1.9	$-3.9(+2)$	$-3.9(+2)$
A	0	$-4.7(+3)$	$-4.7(+3)$	0	$-4.7(+4)$
b	—	3	0.6	—	1.9
a	—	$>T$	0.8	—	2.5
I	—	1	7	0	3
u_0	—	$1.0(+3)$	$1.0(+3)$	—	$-1.5(+3)$
C_1^s	—	1.16	1.16	—	1.1
T	12				
k_{init}	1				

Table 4.1 Datum values for the test problems P1,..., P5, derived from (4.8).

providing $\|r^h\|_{L_p^h(\mathcal{J}_i)}$ is "close" to $\|r\|_{L_p(\mathcal{J}_i)}$. Thus, suppose we already have the solutions $\{U_j\}_{j=0}^{i-1}$, for some $i \in \{1,\ldots,N\}$, and we now want to compute U_i. Given a starting value for k_i it is natural to iterate: define k_i^{new} from

$$k_i^{\mathrm{new}} := \left(\frac{\mathcal{E}/C_1^s - |U_i - U_{i-1}|}{\|r^h\|_{L_p^h(\mathcal{J}_i)}}\right)^q \qquad \text{for } q \in [1,\infty); \tag{4.4}$$

set $k_i := k_i^{\mathrm{new}}$, and thus redefine $\mathcal{J}_i$; recompute U_i; and repeat until $k_i^{\mathrm{new}} \geq k_i$. In this case $E_{\mathrm{BE}}(i,p) \leq \mathcal{E}$, and if this process has also been applied to define each of the $\{\mathcal{J}_j\}_{j=1}^{i-1}$ we get

$$e_{\mathrm{BE}}(t_i) \leq \max_{1\leq j\leq i}\{E_{\mathrm{BE}}(j,p)\} \leq \mathcal{E},$$

as required. The starting value for k_1 must either be set to a fixed value in the algorithm or supplied by the user, whilst, for $i > 1$ it is natural to use the most recent k_{i-1}^{new} as the starting value for k_i. Once the condition $k_i^{\mathrm{new}} \geq k_i$ is met the algorithm then advances to the next time level.

In principle this scheme is workable for "small enough" time steps, and is implemented later for some model problems; in practice it is not *robust* without some additional defensive programming. There are three significant limitations to (4.4) which demand that we take extra care in choosing k_i^{new}, we take each in turn.

1 Theorem 3.1 does not specify an upper bound on the time steps and therefore it could certainly happen that $\mathcal{E}/C_1^s - |U_i - U_{i-1}| \leq 0$. Clearly this will cause (4.4) to fail and so we would require some other rule for selecting k_i^{new}. When this happens our approach is to suppose that $E_{\mathrm{BE}}(i,p) = O(k_i)$ and note that $\exists\alpha > 1$ such that $E_{\mathrm{BE}}(i,p) = \alpha\mathcal{E}$. We now attempt to choose k_i^{new} to bring α to unity and so we write:

$$\frac{1}{\alpha}O(k_i) = \frac{1}{\alpha}E_{\mathrm{BE}}(i,p) = \mathcal{E} = E_{\mathrm{BE}}^{\mathrm{new}}(i,p) = O(k_i^{\mathrm{new}}).$$

Thus we obtain a contingency rule:

$$\textit{if (4.4) fails: } k_i^{\mathrm{new}} := k_i/\alpha \text{ with } \alpha := \frac{E_{\mathrm{BE}}(i,p)}{\mathcal{E}}. \tag{4.5}$$

k	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N,\infty)$	$\widehat{E}_{\mathrm{BE}}(N,2)$	$N = T/k$
0.4	$2.164(+2)$	$1.710(+3)$	$1.655(+3)$	30
0.2	$1.265(+2)$	$1.201(+3)$	$1.177(+3)$	60
0.1	$7.371(+1)$	$7.729(+2)$	$7.689(+2)$	120
0.05	$4.001(+1)$	$4.517(+2)$	$4.511(+2)$	240
0.025	$2.085(+1)$	$2.466(+2)$	$2.465(+2)$	480
0.0125	$1.065(+1)$	$1.292(+2)$	$1.292(+2)$	960
0.00625	$5.383(+0)$	$6.620(+1)$	$6.620(+1)$	1920
0.003125	$2.707(+0)$	$3.351(+1)$	$3.351(+1)$	3840
0.0015625	$1.357(+0)$	$1.686(+1)$	$1.686(+1)$	7680

Table 4.2 Results of solving P2 with the backward Euler variant in the constant time step mode; $C_1^s := 1.16$.

$\mathcal{E}$	$p=\infty$			$p=2$		
	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N,\infty)$	work ratio	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N,2)$	work ratio
256	$4.577(+1)$	$2.486(+2)$	43/52	$5.293(+1)$	$2.364(+2)$	39/45
128	$2.529(+1)$	$1.278(+2)$	74/85	$2.813(+1)$	$1.279(+2)$	68/78
64	$1.357(+1)$	$6.380(+1)$	130/146	$1.428(+1)$	$6.377(+1)$	126/143
32	$7.047(+0)$	$3.198(+1)$	243/267	$7.232(+0)$	$3.200(+1)$	239/262
16	$3.608(+0)$	$1.600(+1)$	467/505	$3.657(+0)$	$1.600(+1)$	463/504
8	$1.826(+0)$	$8.000(+0)$	914/985	$1.839(+0)$	$7.999(+0)$	908/979
4	$9.175(-1)$	$4.000(+0)$	1797/1921	$9.312(-1)$	$4.000(+0)$	1797/1929
2	$4.606(-1)$	$2.000(+0)$	3571/3811	$4.720(-1)$	$2.000(+0)$	3567/3812
1	$2.348(-1)$	$1.000(+0)$	7111/7577	$2.379(-1)$	$1.000(+0)$	7114/7594

Table 4.3 Results of solving P2 with the backward Euler variant in the adaptive mode: $C_1^s := 1.16$, $k_{\mathrm{init}} = 1.0$.

Of course, if the need arises we iteratively apply (4.5) until (4.4) becomes a valid rule again.

2 The second weakness of (4.4) has already been touched upon above. The quadrature approximations to r by r^h, and to $\|\cdot\|_{L_p(\mathcal{J}_i)}$ by $\|\cdot\|_{L_p^h(\mathcal{J}_i)}$, can undershoot if the solution (or data) is "rough" in a neighbourhood of $\mathcal{J}_i$. This can cause (4.4) to give $k_i^{\mathrm{new}} \geq k_i$ which then triggers the advance of the algorithm to the next time level. In this way we can step over a singularity without capturing it. On the other hand the quadrature approximations can also overshoot and give much smaller values of k_i^{new} than are necessary, especially in a smooth phase of the solution occuring immediately prior to a singularity. This time the adaptivity does not fail but the algorithm can become grossly inefficient—taking small time steps in a smooth region of the solution. One way to deal with both of these possibilities would be to implement adaptive quadrature rules so as to derive a more accurate approximation $\|r^h\|_{L_p^h(\mathcal{J})}$ to $\|r\|_{L_p(\mathcal{J})}$, but for most problems this may be unnecessarily complex. The type of singularity that we have in mind is where a certain derivative of a numerically integrated function undergoes a step discontinuity. For the data $\{\sigma, f, \phi\}$ it should usually be safe to assume that the algorithm can be given, as input, a set, $D = \{t_i^d\}_{i=1}^{N_d}$ of times at which

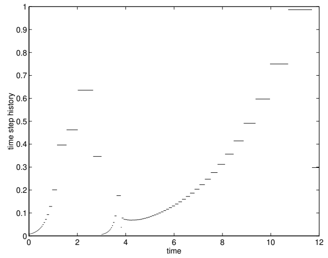

Figure 4.1 Evolution of the time steps when solving P2 in the adaptive mode for $\mathcal{E} = 64$ and $p = \infty$.

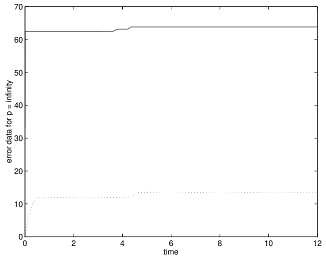

Figure 4.2 Evolution of the nodal error, e, and estimator, $E_{\mathrm{BE}}(i, \infty)$, when solving P2 for $\mathcal{E} = 64$, $k_{\mathrm{init}} = 1.0$.

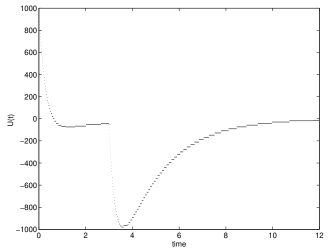

Figure 4.3 Evolution of the approximate solution to P2 for $\mathcal{E} = 64$ and $p = \infty$.

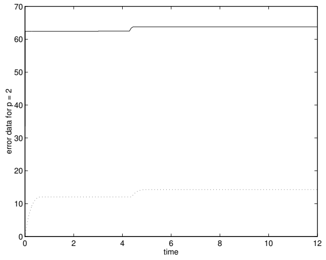

Figure 4.4 Evolution of the nodal error, e, and estimator, $E_{\mathrm{BE}}(i, 2)$, when solving P2 for $\mathcal{E} = 64$, $k_{\mathrm{init}} = 1.0$.

these type of singularities occur. The modification to the rule (4.4), while computing U_i, is then:

$$\text{while } \exists t \in D \cap (t_{i-1}, t_i) \text{ set } t_i := t. \tag{4.6}$$

When this loop terminates the data will be smooth in $\mathcal{J}_i$ and the singular behaviour will be at t_i, this will no longer affect the quadrature errors.

3 The third limitation of (4.4) is, unlike the previous two, related not to effectiveness but to efficiency. To illustrate our point we assume that $\|r^h\|_{L_p^h(\mathcal{J}_i)} = O(k_i^{1/p})$ and $|U_i - U_{i-1}| = O(k_i)$. Suppose, for some i, we obtain from (4.4), (4.5) and (4.6) a $k_i^{\mathrm{new}} > k_i$, then we would accept U_i, set $k_{i+1} := k_i^{\mathrm{new}}$ and advance to the next time level. The problem we have in mind occurs if the approximation on $\mathcal{J}_i$ is "very good", then it is reasonable to expect $k_i^{\mathrm{new}} \gg k_i$ and, upon partially inserting k_i^{new} into $E_{\mathrm{BE}}(i, p)$ we would find an $\alpha > 1$ given by:

$$\alpha = \frac{\widetilde{E}_{\mathrm{BE}}(i,p)}{\mathcal{E}} \quad \text{where} \quad \widetilde{E}_{\mathrm{BE}}(i,p) := C_1^s \left((k_i^{\mathrm{new}})^{1/q} \|r^h\|_{L_p^h(\mathcal{J}_i)} + |U_i - U_{i-1}| \right).$$

So, all other things remaining equal it can (and frequently did in the examples given below) happen that at the first "visit" to $\mathcal{J}_{i+1}$ (where $k_{i+1} = k_i^{\mathrm{new}}$) we would find $E_{\mathrm{BE}}(i+1, p) = \alpha\mathcal{E}$. Thus (4.2) is not satisfied and we are forced to iterate at least once to determine a k_{i+1}^{new}. For a solution that becomes less "flatter" through time this

k	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N, \infty)$	$\widehat{E}_{\mathrm{BE}}(N, 2)$	$N = T/k$
0.4	5.550(+2)	2.314(+3)	2.221(+3)	30
0.2	1.985(+2)	1.419(+3)	1.398(+3)	60
0.1	1.087(+2)	8.830(+2)	8.796(+2)	120
0.05	5.729(+1)	5.064(+2)	5.059(+2)	240
0.025	2.947(+1)	2.738(+2)	2.737(+2)	480
0.0125	1.495(+1)	1.427(+2)	1.427(+2)	960
0.00625	7.534(+0)	7.293(+1)	7.293(+1)	1920
0.003125	3.781(+0)	3.687(+1)	3.687(+1)	3840
0.0015625	1.894(+0)	1.854(+1)	1.854(+1)	7680

Table 4.4 Results of solving P3 with the backward Euler variant in the constant time step mode; $C_1^s := 1.16$.

$\mathcal{E}$	$p = \infty$			$p = 2$		
	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N, \infty)$	work ratio	$e_{\mathrm{BE}}(t_N)$	$\widehat{E}_{\mathrm{BE}}(N, 2)$	work ratio
256	4.372(+1)	2.368(+2)	118/155	4.551(+1)	2.347(+2)	117/154
128	2.446(+1)	1.277(+2)	213/247	2.487(+1)	1.235(+2)	214/246
64	1.317(+1)	6.379(+1)	398/432	1.429(+1)	6.319(+1)	400/432
32	6.842(+0)	3.185(+1)	771/807	7.303(+0)	3.166(+1)	771/805
16	3.509(+0)	1.599(+1)	1508/1549	3.721(+0)	1.600(+1)	1507/1549
8	1.833(+0)	7.995(+0)	2977/3023	1.893(+0)	7.997(+0)	2974/3022
4	9.404(−1)	3.999(+0)	5911/5971	9.565(−1)	4.000(+0)	5914/5976
2	4.768(−1)	2.000(+0)	11779/11863	4.809(−1)	2.000(+0)	11777/11862
1	2.401(−1)	1.000(+0)	23519/23654	2.412(−1)	1.000(+0)	23519/23657

Table 4.5 Results of solving P3 with the backward Euler variant in the adaptive mode: $C_1^s := 1.16$, $k_{\mathrm{init}} = 1.0$.

implies that we would often be forced to solve at least twice on *every* time level. The adaptivity, (4.2), does not fail here but produces an expensive algorithm. What is needed is a rule to prevent k_i^{new}/k_i becoming too large. From the assumptions above we expect that $E_{\mathrm{BE}}(i, p) = O(k_i)$ and thus infer

$$O(k_i^{\mathrm{new}}) = E_{\mathrm{BE}}(i+1, p) = \mathcal{E} \sim \widetilde{E}_{\mathrm{BE}}(i,p)/\alpha = O(k_i/\alpha).$$

And so we place an additional restriction on k_i^{new} as

$$k_i^{\mathrm{new}} \le k_i/\alpha \tag{4.7}$$

(note the similarity with (4.5)). Admittedly this is a rather loose argument, but when (4.7) was implemented for the model problems below it resulted in a dramatic reduction in the number of solutions of the discrete system required in order to satisfy (4.2).

To present a numerical demonstration of this practical version of (3.5) we need an exact solution to a problem of type (1.1). We consider the following example problem: find u such that

$$u'(t) + \sigma u(t) = f(t) + B \int_0^t u(s)\, ds \text{ with } t \in (0, 12] \tag{4.8}$$

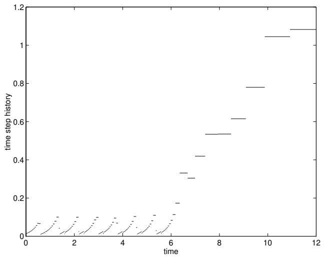

Figure 4.5 Evolution of the time steps when solving P3 in the adaptive mode for $\mathcal{E} = 128$ and $p = \infty$.

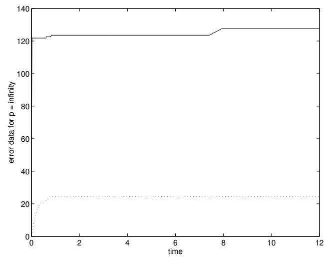

Figure 4.6 Evolution of the nodal error, e, and estimator, $E_{\rm BE}(i, \infty)$, when solving P3 for $\mathcal{E} = 128$, $k_{\rm init} = 1.0$.

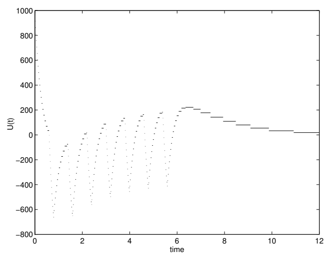

Figure 4.7 Evolution of the approximate solution to P3 for $\mathcal{E} = 128$ and $p = \infty$.

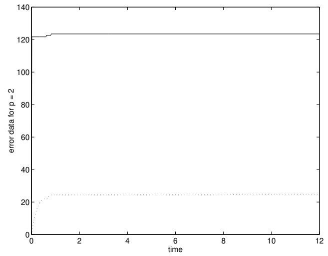

Figure 4.8 Evolution of the nodal error, e, and estimator, $E_{\rm BE}(i, 2)$, when solving P3 for $\mathcal{E} = 128$, $k_{\rm init} = 1.0$.

and $u(0) = u_0$. Here $\sigma = \text{constant} > 0$, $B = \text{constant} > \sigma^2/4$ and the loading is a step function given by $f(t) = 0$ for $t \in [0, b)$, $f(t) = A$ for $t \in [b, a)$, and $f(t + ia) = f(t)$ for $i = 0, 1, \ldots, I$. Here a, b and A are constants, with $0 \le b \le a$, and $I < \infty$ is a nonnegative integer.

The exact solution to this problem is continuous on $[0, T]$ but non-smooth in that u' suffers jump discontinuities at those points where f does. Moreover, by varying the parameters we can create a variety of test problems which exhibit varying degrees of "smoothness", and then use these to demonstrate the performance of the backward Euler variant.

We have remarked in the introduction that the only practical way of obtaining a sharp dual strong stability constant, C_1^s, seems to be to compute it from a numerical solution. This we do in Section 6 where we implement the Crank-Nicolson variant (to be developed in the next Section). For the moment we consider (4.8) in the specific instances of problems P1, P2, P3, P4 and P5, where the parameters for these problems are given in Table 4.1. Before discussing this table we need to emphasize a very important point regarding the constant C_1^s.

Remark 4.1. *On examining the proofs of Theorem 3.1.(a) and Theorem 5.2 (later) it is obvious that the stability constant C_1^s is related only to the strong initial-data stability of the dual problem. Thus when computing C_1^s from a discrete solution of*

k	$e_{\rm BE}(t_N)$	$\widehat{E}_{\rm BE}(N, \infty)$	$\widehat{E}_{\rm BE}(N, 2)$	$N = T/k$
0.4	3.938(+2)	1.811(+4)	8.132(+3)	30
0.2	1.410(+2)	6.075(+3)	3.298(+3)	60
0.1	2.028(+2)	3.292(+3)	3.008(+3)	120
0.05	3.216(+2)	2.845(+3)	2.701(+3)	240
0.025	3.306(+2)	2.307(+3)	2.244(+3)	480
0.0125	2.110(+2)	1.700(+3)	1.675(+3)	960
0.00625	1.221(+2)	1.119(+3)	1.111(+3)	1920
0.003125	6.649(+1)	6.665(+2)	6.640(+2)	3840
0.0015625	3.494(+1)	3.686(+2)	3.679(+2)	7680

Table 4.6 Results of solving P5 with the backward Euler variant in the constant time step mode; $C_1^s := 1.1$.

$\mathcal{E}$	$p = \infty$			$p = 2$		
	$e_{\rm BE}(t_N)$	$\widehat{E}_{\rm BE}(N, \infty)$	work ratio	$e_{\rm BE}(t_N)$	$\widehat{E}_{\rm BE}(N, 2)$	work ratio
256	4.112(+1)	2.543(+2)	138/178	4.907(+1)	2.527(+2)	126/166
128	2.316(+1)	1.278(+2)	218/264	2.685(+1)	1.233(+2)	204/255
64	1.255(+1)	6.397(+1)	370/422	1.498(+1)	6.353(+1)	339/381
32	6.847(+0)	3.192(+1)	654/725	7.671(+0)	3.175(+1)	609/667
16	3.654(+0)	1.599(+1)	1196/1286	3.896(+0)	1.600(+1)	1151/1253
8	1.896(+0)	7.999(+0)	2279/2435	1.966(+0)	8.000(+0)	2226/2395
4	9.686(−1)	4.000(+0)	4402/4658	9.871(−1)	3.999(+0)	4342/4619
2	4.897(−1)	2.000(+0)	8660/9148	4.946(−1)	2.000(+0)	8565/9049
1	2.463(−1)	1.000(+0)	17114/18019	2.475(−1)	1.000(+0)	17034/17965

Table 4.7 Results of solving P5 with the backward Euler variant in the adaptive mode: $C_1^s := 1.1$, $k_{\rm init} = 1.0$.

the dual problem (2.1), it suffices to consider the simpler case where $g = 0$. ■

With regard to Remark 4.1 the constants C_1^s in Table 4.1 have indeed been computed from the simplified dual problem (this, actually, is (4.8) with $f = 0$, see Proposition 2.1), see Tables 6.1—3 later. However, the numerical scheme used in these instances was the Crank-Nicolson variant (since it is then easier to differentiate the discrete solution) which we have not yet discussed. We return to this matter in Section 6 and for now just note that by using the exact solution to (4.8) it is easy to show that

$$\|u'\|_{L_1(0,T)} = |u(0) - 2u(t^*)| + \epsilon, \tag{4.9}$$

for $T \gg 0$ and $T > t^*$ where t^* is the unique $t \in [0, T]$ where u' changes sign. Dropping the ϵ and setting $u(0) = 1$ it is clear that any constant C for which $C > |u(0) - 2u(t^*)|$ can be used as C_1^s. In the case of P1 and P4 we find from this the respective values $C_1^s = 1.159\ldots$ and $C_1^s = 1.094\ldots$. In fact the reason for including P1 and P4 is that they are the problems used later in Section 5 for computing the stability constants. That is: P1 is used to compute C_1^s for P2 and P3, and P4 is used to compute C_1^s for P5, hence the "$u(0)$" and "C_1^s" rows are blank in Table 4.1 for P1 and P4.

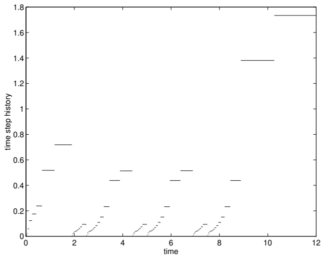

Figure 4.9 Evolution of the time steps when solving P5 in the adaptive mode for $\mathcal{E} = 256$ and $p = \infty$.

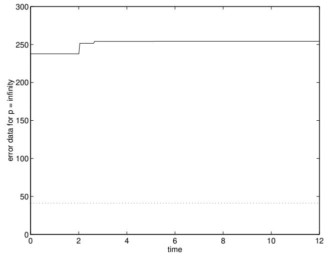

Figure 4.10 Evolution of the nodal error, e, and estimator, $E_{\mathrm{BE}}(i, \infty)$, when solving P5 for $\mathcal{E} = 256$, $k_{\mathrm{init}} = 1.0$.

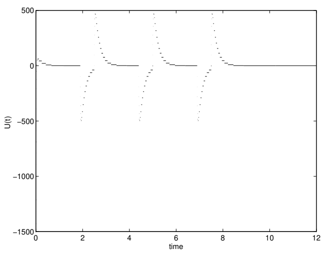

Figure 4.11 Evolution of the approximate solution to P5 for $\mathcal{E} = 256$ and $p = \infty$.

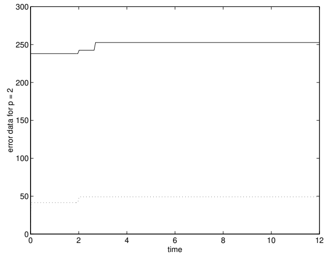

Figure 4.12 Evolution of the nodal error, e, and estimator, $E_{\mathrm{BE}}(i, 2)$, when solving P5 for $\mathcal{E} = 256$, $k_{\mathrm{init}} = 1.0$.

The accompanying numerical results for problems P2, P3 and P5 show the results of applying our practical version of (3.5) in various instances. Tables 4.2, 4.4 and 4.6 show the error

$$e_{\mathrm{BE}}(t_N) = \max_{1 \le i \le N} |u(t_i) - U_i^-|,$$

and the estimators $\widehat{E}_{\mathrm{BE}}(N, 2)$ and $\widehat{E}_{\mathrm{BE}}(N, \infty)$ resulting when constant time steps, k, are employed. Tables 4.3, 4.5 and 4.7 show these same quantities when solving in the adaptive mode, described earlier in this section, for various values of the tolerance $\mathcal{E}$. Also included in these results is the "work ratio". This is the ratio of two integers: ℓ/i, where $\ell = N + 1$ is the total number of time levels visited during the solution, and i is the total number of solutions required of the discrete equation. Necessarily we have $\ell \le i$ but it is possible to have $\ell < i$ since more than one solution may be required at a given time level. We see this work ratio as an indication of the efficiency of the adaptive criteria developed above. To get a feel for how the algorithm behaves Figures 4.1—4 (for P2), 4.5—8 (for P3) and 4.9—12 (for P5) show some graphical results for particular values of $\mathcal{E}$. For each of P2, P3 and P5 we show the evolution of: the solution, U; the time steps, k_i (as a piecewise constant); and, the error $e_{\mathrm{BE}}(t_i)$ (dotted lines) and estimators $E_{\mathrm{BE}}(i, \infty)$ and $E_{\mathrm{BE}}(i, 2)$ (solid lines).

5. Analysis of the Crank-Nicolson variant. The backward Euler variant is a robust scheme in the sense that it requires very little regularity of the exact solu-

tion. The price of this advantage is the relatively low accuracy of the scheme that results from the truncation error when interpolating with a piecewise constant function. When it is known that the exact solution possesses higher regularity then it is reasonable to seek a more accurate (i.e. smaller truncation error) approximate solution. The phrase "more accurate" seems rather glib since any scheme is as accurate as any other with appropriate choices of time steps, we mean of course accurate relative to computational work. In this section we retain the test space, $V^h = V_0^h$, as in (3.2), but now use a trial space, U^h, of continuous piecewise linears. The resulting finite element scheme is a variant of the classical Crank-Nicolson scheme as it would apply to (1.1) in the non-hereditary case $\phi \equiv 0$.

However, this scheme is *not* a Galerkin finite element method, nor is it "close" to one. It seems here that the discrete trial and test spaces are now too different for us to be able to construct a useful discrete dual backward problem, and thereby derive an *a priori* error estimate a similar manner to that in Section 3. Nonetheless, *a posteriori* estimates can be derived in essentially the same way as for the backward Euler variant and the numerical results presented in the next section suggest that the *a posteriori* error bound derived below is both reliable and useful. *A priori* error analyses for the classical finite difference Crank-Nicolson method for (1.1) can be found in [16] and, for more general space-time discretization, in [4] and [20]. Although we do not attempt to prove it, it seems that the Crank-Nicolson variant we describe below could be interpreted as a finite difference scheme and analyzed (although with perhaps considerably more effort) in a similar way. Also, see the analysis of the continuous Galerkin method for ODE's given by Estep and French in [6]. We do not wish to get involved with this, our purpose here is to demonstrate that, if the finite-element overhead can be tolerated, what is essentially the Crank-Nicolson method can be implemented for (1.1) along with a reliable *a posteriori* error estimator which can be used to construct an adaptive solver.

Let $(\cdot, \cdot)$ again be the usual $L_2(\mathcal{J})$ inner product. As before we begin with a "Galerkin" formulation of (1.1): find $u \in W_p^1(\mathcal{J})$ such that

$$(Au, v) := (u' + \sigma u - \Lambda u, v) = (f, v) \qquad \forall v \in L_q(\mathcal{J}), \tag{5.1}$$

with $u(0) = u_0$ and where q is conjugate to p. In the finite element method of this section the discrete test space, $V^h = V_0^h$, remains as before in (3.2), but now we will seek solutions in the discrete trial space given by

$$U^h := C(\overline{\mathcal{J}}) \bigcap \bigcup_{i=1}^{N} \mathbb{P}_1(\overline{\mathcal{J}}_i). \tag{5.2}$$

That is: U^h is the space of bounded continuous functions that are linear over each $\mathcal{J}_i$. Thus the finite element problem is: find $U \in U^h$ such that

$$(AU, v) := (U' + \sigma U - \Lambda U, v) = (f, v) \qquad \forall v \in V^h, \tag{5.3}$$

with $U(0) := u_0$. Due to the fact that U now varies over each $\mathcal{J}_i$ it is not so easy to write down here, as in (3.5), the resulting time stepping algorithm. For this reason we will defer further discussion of the numerical implementation of this scheme until the next section and, in the remainder of this section, we will be concerned only with the Galerkin-error analysis.

The first result we state is a flexible *a posteriori* L_p-error estimate for the scheme which could be used to provide reliable error feedback to the user, but firstly we should note the Galerkin-orthogonality of the error. Subtracting (5.3) from (5.1) and setting $e = u - U$ we obtain $(Ae, v) = 0$ for all $v \in V^h$. Defining the residual,

$$r(t) := Ae(t) = (f - U' - \sigma U + \Lambda U)(t),$$

this is equivalent to:

$$(r, v) = 0 \quad \forall v \in V^h. \tag{5.4}$$

Equipped with this observation the proof of the following *a posteriori* error estimate is now straightforward.

Theorem 5.1. *Let Assumptions 1.1 and Theorem 2.1 hold and also let $\kappa \in V^h$ be such that $\kappa|_{\mathcal{J}_i} = k_i$ for $i = 1, \dots, N$. Then the following a posteriori Galerkin-error estimate holds for the Crank-Nicolson variant (5.3):*

$$\|u - U\|_{L_p(0,t_i)} \le C_q^s \|\kappa r\|_{L_p(0,t_i)},$$

for q conjugate to $p \in [1, \infty]$, every $t_i \in \mathcal{J}^k$ and where C_q^s is a strong dual stability constant guaranteed by Theorem 2.1.

Proof. Define $e(t) = u(t) - U(t)$ and note that $e(0) = 0$. Now pick an arbitrary $t_i \in \mathcal{J}^k$ and consider the dual problem, (2.1), with the data: $\Upsilon = t_i$; $\chi(\Upsilon) = 0$; q conjugate to p; and, $g \in L_q(0, t_i)$ arbitrary. Then Theorem 2.1 gives the strong stability estimate: $\|\chi'\|_{L_q(0,t_i)} \le C_q^s \|g\|_{L_q(0,t_i)}$. Denote the $L_2(0, t_i)$ inner product by $\langle \cdot, \cdot \rangle$ and use: the dual property (2.3); the residual, $r = Ae$; and, the Galerkin orthogonality, (5.4), with the piecewise constant interpolate $\pi\chi \in V^h$, as defined in (3.7), to see that

$$\begin{aligned}\langle e, g\rangle &= \langle e, A^*\chi\rangle = \langle Ae, \chi\rangle = \langle r, \chi - \pi\chi\rangle \\ &= \langle \kappa r, \kappa^{-1}(\chi - \pi\chi)\rangle,\end{aligned}$$

since $e(0) = \chi(t_i) = 0$ and $\kappa\kappa^{-1} = 1$. Using now the interpolation-error estimate of Lemma 2.4 and invoking the strong stability the above implies:

$$\begin{aligned}|\langle e, g\rangle| = |\langle \kappa r, \kappa^{-1}(\chi - \pi\chi)\rangle| &\le \|\kappa r\|_{L_p(0,t_i)} \|\kappa^{-1}(\chi - \pi\chi)\|_{L_q(0,t_i)}, \\ &\le \|\kappa r\|_{L_p(0,t_i)} \|\chi'\|_{L_q(0,t_i)} \le C_q^s \|\kappa r\|_{L_p(0,t_i)} \|g\|_{L_q(0,t_i)}.\end{aligned}$$

Hence, for $p > 1$ we get

$$\|e\|_{L_p(0,t_i)} = \sup\left\{ |\langle e, g\rangle| : \|g\|_{L_q(0,t_i)} = 1 \right\} \le C_q^s \|\kappa r\|_{L_p(0,t_i)},$$

(see e.g. [8, Chap. 4§14]), and for $p = \infty$ we take $g = 1$ for $e \ge 0$ and $g = -1$ otherwise, then $|\langle e, g\rangle| = \|e\|_{L_1(0,t_i)}$ and $\|g\|_{L_\infty(0,t_i)} = 1$. Since the original choice of t_i was arbitrary this completes the proof. ∎

Theorem 5.1 provides a reliable and flexible *a posteriori* Galerkin-error bound which can be employed to check the integrity of the computed solution. However, the estimate refers to all previous times and so it is not useful for constructing a rational adaptive time stepping criterion. We now give a discrete pointwise Galerkin-error bound which is.

Theorem 5.2. *Let Assumptions 1.1 and Theorem 2.1 hold, then for any $t_i \in \mathcal{J}^k$ the nodal Galerkin error satisfies*

$$|u(t_i) - U(t_i)| \le C_1^s \max_{1 \le j \le i} k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)},$$

where q is conjugate to $p \in [1, \infty]$ and C_1^s is a strong dual stability constant guaranteed by Theorem 2.1.

Proof. Define $e(t) := u(t) - U(t)$ and $e_i := e(t_i)$, for an arbitrary $i \in \{1, \dots, N\}$, also, let $\langle \cdot, \cdot \rangle$ denote the $L_2(0, t_i)$ inner product and invoke the dual backward problem, (2.1), with the data: $\Upsilon = t_i$; $g = 0$; and, $\chi_\Upsilon = e_i$. Theorem 2.1 then gives a strong stability constant, C_1^s, such that $\|\chi'\|_{L_1(0,t_i)} \le C_1^s |e_i|$ and (2.3) gives: $e_i^2 + \langle e, A^*\chi\rangle = \langle Ae, \chi\rangle$, since $e(0) = 0$. Using, in turn, this duality and the fact that $A^*\chi = 0$ in $(0, t_i)$; the residual, $r = Ae$; the orthogonality (5.4) with the piecewise constant interpolate $\pi\chi \in V^h$ given by (3.7); the interpolation-error estimate of Lemma 2.3; and, the strong stability, we obtain

$$\begin{aligned} e_i^2 = \langle Ae, \chi\rangle = \langle r, \chi - \pi\chi\rangle &\le \sum_{j=1}^{i} \|r\|_{L_p(\mathcal{J}_j)} \|\chi - \pi\chi\|_{L_q(\mathcal{J}_j)}, \\ &\le \sum_{j=1}^{i} k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)} \|\chi'\|_{L_1(\mathcal{J}_j)} \le \|\chi'\|_{L_1(0,t_i)} \max_{1 \le j \le i} k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)}, \\ \Longrightarrow |e_i| \le C_1^s \max_{1 \le j \le i} k_j^{1/q} \|r\|_{L_p(\mathcal{J}_j)}, \end{aligned}$$

as required. ∎

The performance of this estimator is demonstrated for some model problems in the following section.

6. Numerical implementation of the Crank-Nicolson variant. Our task in this section, in direct analogy to Section 4, is to produce a practical computational implementation of the Crank-Nicolson variant, (5.3), and to give the results of some numerical experiments. For comparison purposes the test problems are the same as those used in Section 4. The practical algorithm is again derived by replacing the inner product and history terms with quadrature rules which have a small truncation error relative to the Galerkin error. We then construct an adaptive time step selection criteria based on the result in Theorem 5.2. As we have already remarked in Section 4, we prefer to use this scheme for calculating the stability constant, C_1^s (from Theorem 2.1), required in Theorem 5.2 because the finite element solution is differentiable. Accordingly our first numerical results are concerned with the computation of this constant for the problems P1 and P4. The section concludes with numerical experiments presented in the same format as those in Section 4.

As a first step in building an algorithm from (5.3) we pick an arbitrary $i \in \{1, \dots, N\}$ and take $v = 1$ on $\mathcal{J}_i$ and $v = 0$ elsewhere. Clearly $v \in V^h$ and so, from (5.3), we obtain

$$\int_{t_{i-1}}^{t_i} U' + \sigma U \, dt = \int_{t_{i-1}}^{t_i} f \, dt + H,$$

where the history is contained in H, given by:

$$H := \int_{t_{i-1}}^{t_i} \int_0^t \phi(t,s)U(s)\,dsdt.$$

If we write $U_i := U(t_i)$, for $i = 0, \dots, N$, then it is easy to see that $\int_{t_{i-1}}^{t_i} U'\,dt = U_i - U_{i-1}$. Also, the integrals involving σ and f are dealt with in the same way as in Section 4 by a Simpson's rule replacement (remembering that this time U is linear over $\mathcal{J}_i$). Since we expect the Galerkin error in this scheme to be of second order accuracy, and we want to ensure that it dominates the quadrature errors, we can no longer use the Simpson and midpoint rules for H as we did in Section 4. Simpson's rule is now used exclusively for H, but before we apply it we can make this term a little more manageable by exploiting the interchange relationship:

$$\int_{t_{i-1}}^{t_i} \int_0^t \cdot \,dsdt = \int_0^{t_{i-1}} \int_{t_{i-1}}^{t_i} \cdot \,dtds + \int_{t_{i-1}}^{t_i} \int_s^{t_i} \cdot \,dtds.$$

Therefore we write $H := H_1 + H_2$ where:

$$H_1 := \int_0^{t_{i-1}} U(s)\Phi_i(t_{i-1},s)\,ds \qquad \text{and} \qquad H_2 := \int_{t_{i-1}}^{t_i} U(s)\Phi_i(s,s)\,ds,$$

and in each

$$\Phi_i(a,b) := \int_a^{t_i} \phi(t,b)\,dt. \tag{6.1}$$

The history term, H, is now discretized by replacing Φ_i by a single Simpson's rule over each $\mathcal{J}_i$, and by replacing H_1 with the composite Simpson's rule derived from a single rule applied over each $\{\mathcal{J}_j\}_{j=1}^{i-1}$. The term H_2 is also replaced with a single Simpson rule. The residual, $r(t) = f - U' - \sigma U + \Lambda U$ $\big($see (5.4)$\big)$ for $t \in [t_{i-1}, t_i]$, is approximated as before with a single trapezoid rule over $[t_{i-1}, t)$ and Simpson's rule over each $\{\mathcal{J}_j\}_{j=1}^{i-1}$. Again we write $r^h(t)$ to emphasize the approximation. The discrete L_p^h norms remain as described earlier in Section 4.

We now use Theorem 5.2 to design a time step selection criteria which will control the nodal error such that

$$e_{\mathrm{CN}}(t_i) := \max_{1\le j\le i} |u(t_j) - U_j| \le \mathcal{E} \qquad \forall i \in \{1, \dots, N\},$$

where $\mathcal{E}$ is, again, a user-specified tolerance. From Theorem 5.2 this leads us to require that

$$E_{\mathrm{CN}}(i,p) \le \mathcal{E} \qquad \forall i \in \{1, \dots, N\},$$

where

$$E_{\mathrm{CN}}(i,p) := C_1^s k_i^{1/q} \|r^h\|_{L_p^h(\mathcal{J}_i)},$$

and we set

$$\widehat{E}_{\mathrm{CN}}(i,p) := \max_{1\le j\le i} E_{\mathrm{CN}}(j,p). \tag{6.2}$$

So, given a starting value for U_i we iteratively determine a new $\mathcal{J}_i$, and hence a new U_i, by choosing a new time step, k_i^{new}, such that

$$k_i^{\mathrm{new}} = \left(\frac{\mathcal{E}}{C_1^s \|r^h\|_{L_p^h(\mathcal{J}_i)}} \right)^q, \qquad q \ne \infty. \tag{6.3}$$

u_0	Constant time step, k						
	0.4	0.2	0.1	0.05	0.025	0.0125	0.00625
1	1.177	1.163	1.160	1.159	1.159	1.159	1.159
10	1.177	1.163	1.160	1.159	1.159	1.159	1.159
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
10^4	1.177	1.163	1.160	1.159	1.159	1.159	1.159

Table 6.1. Results of applying (5.3) in the constant time step mode for the problem P1 to determine the ratio $\|U'\|_{L_1^h(\mathcal{J})}/|U_0| \approx C_1^s$.

u_0	Constant time step, k					
	0.1	0.05	0.025	0.0125	0.00625	0.003125
1	5.926	2.187	1.112	1.096	1.094	1.094
10	5.926	2.187	1.112	1.096	1.094	1.094
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
10^4	5.926	2.187	1.112	1.096	1.094	1.094

Table 6.2 Results of applying (5.3) in the constant time step mode for the problem P4 to determine the ratio $\|U'\|_{L_1^h(\mathcal{J})}/|U_0| \approx C_1^s$.

u_0	Scaled tolerance: $\widehat{\mathcal{E}} = u_0\mathcal{E} \times 10^{-4}$					
	256	128	64	$\cdots$ $\cdots$ $\cdots$	2	1
1	1.255:108	1.181:115	1.137:129	$\cdots$	1.094:223	1.094:276
10	1.255:108	1.181:115	1.137:129	$\cdots$	1.094:223	1.094:276
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
10^4	1.255:108	1.181:115	1.137:129	$\cdots$	1.094:223	1.094:276

Table 6.3 Results of applying (5.3) in the adaptive mode to P4, with $C_1^s = 6$ and $k_{\mathrm{init}} = 1.0$. The table shows the calculated C_1^s and the number of solutions of the discrete problem required to obtain it.

As before, if $k_i^{\mathrm{new}} \ge k_i$ we accept U_i and march forward to the next time level, $t_{i+1} = t_i + k_{i+1}$ with $k_{i+1} := k_i^{\mathrm{new}}$, otherwise we set $k_i := k_i^{\mathrm{new}}$ and recompute U_i at the new t_i.

As with (4.4) the quadrature approximation to the residual and its norm can also cause side-effects in (6.3) related to "stepping over" singularities in the data, thus we augment the rule (6.3) with (4.6) so as to prevent this. Also, the efficiency issue that led to (4.7) is relevant here as well and so we again need to limit the ratio k_i^{new}/k_i. This time we assume that $E_{\mathrm{CN}}(i,p) = O(k_i^2)$. Now, if $k_i^{\mathrm{new}} > k_i$ (and we are therefore marching forward) we define $\alpha \in (0,1]$ by $E_{\mathrm{CN}}(i,p) = \alpha\mathcal{E}$ and then choose k_i^{new} so as to bring α to unity. That is:

$$O\big((k_i^{\mathrm{new}})^2\big) = \mathcal{E} = O(k_i^2/\alpha) \Longrightarrow k_i^{\mathrm{new}} = \frac{k_i}{\sqrt{\alpha}}. \tag{6.4}$$

This, along with (4.6), (4.7) and (6.3) defines the adaptive criteria implemented in the numerical experiments below.

k	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,\infty)$	$\widehat{E}_{\mathrm{CN}}(N,2)$	$N = T/k$
0.4	2.063(+2)	9.827(+2)	5.479(+2)	30
0.2	2.613(+1)	3.280(+2)	1.866(+2)	60
0.1	6.493(+0)	9.343(+1)	5.353(+1)	120
0.05	1.605(+0)	2.514(+1)	1.446(+1)	240
0.025	4.012(−1)	6.537(+0)	3.767(+0)	480
0.0125	1.002(−1)	1.668(+0)	9.619(−1)	960
0.00625	2.506(−2)	4.213(−1)	2.431(−1)	1920
0.003125	6.264(−3)	1.059(−1)	6.111(−2)	3840
0.0015625	1.566(−3)	2.654(−2)	1.532(−2)	7680

Table 6.4 Results of solving P2 with the Crank-Nicolson variant in the constant time step mode; $C_1^s := 1.16$.

$\mathcal{E}$	$p=\infty$			$p=2$		
	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,\infty)$	work ratio	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,2)$	work ratio
256	1.858(+1)	2.050(+2)	18/23	2.860(+1)	1.891(+2)	16/21
128	9.959(+0)	1.039(+2)	21/25	1.996(+1)	1.024(+2)	18/22
64	6.094(+0)	5.866(+1)	28/32	9.640(+0)	5.438(+1)	24/30
32	3.470(+0)	2.994(+1)	35/40	7.169(+0)	3.070(+1)	30/36
16	1.756(+0)	1.513(+1)	47/55	3.782(+0)	1.598(+1)	38/44
8	9.718(−1)	7.631(+0)	61/67	1.771(+0)	7.733(+0)	50/57
4	5.204(−1)	3.954(+0)	82/91	9.432(−1)	3.902(+0)	65/74
2	2.754(−1)	1.977(+0)	112/122	4.942(−1)	1.982(+0)	87/96
1	1.434(−1)	9.898(−1)	154/167	2.566(−1)	9.785(−1)	121/134
0.5	7.372(−2)	4.989(−1)	210/224	1.307(−1)	4.986(−1)	163/176
0.25	3.769(−2)	2.495(−1)	293/312	6.653(−2)	2.493(−1)	226/244
0.125	1.913(−2)	1.249(−1)	408/433	3.363(−2)	1.246(−1)	313/337
0.0625	9.679(−3)	6.249(−2)	569/601	1.695(−2)	6.242(−2)	439/469
0.03125	4.880(−3)	3.125(−2)	798/841	8.521(−3)	3.123(−2)	613/652

Table 6.5 Results of solving P2 with the Crank-Nicolson variant in the adaptive mode: $C_1^s := 1.16$, $k_{\mathrm{init}} = 1.0$.

The numerical tests that follow are again based upon (4.8) in the context of problems P2, P3 and P5, given by the data in Table 4.1, but before these are presented we discuss the numerical determination of the stability constants, C_1^s. An examination of the proof of Theorem 5.2 reveals that the *a posteriori* error bound requires knowledge only of the strong initial-data-stability of the dual problem, and so, referring to Table 4.1, we use P1 to numerically determine a suitable value for C_1^s for P2 and P3, and use P4 to do the same for P5. Now, according to Remark 2.1 the dual problem relevant to (4.8) is actually (4.8) itself with $f := 0$. Thus we can compute a numerical solution to (4.8) for a given U_0 and, from Theorem 2.1, set $C_1^s := (1+\epsilon)\|U'\|_{L_1^h(\mathcal{J})}/|U(0)|$, where ϵ is a user-specified parameter which increases from zero as the degree of confidence the user has in the discrete dual solution decreases. In the tests below we always take $\epsilon \approx 0$.

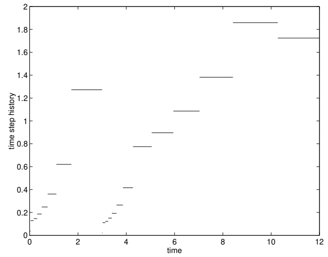

Figure 6.1 Evolution of the time steps when solving P2 in the adaptive mode for $\mathcal{E} = 128$ and $p = \infty$.

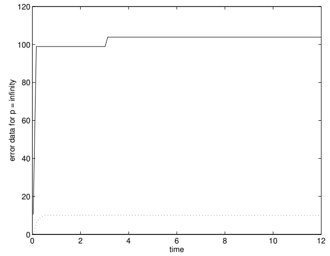

Figure 6.2 Evolution of the nodal error, e, and estimator, $E_{\mathrm{CN}}(i,\infty)$, when solving P2 for $\mathcal{E} = 128$, $k_{\mathrm{init}} = 1.0$.

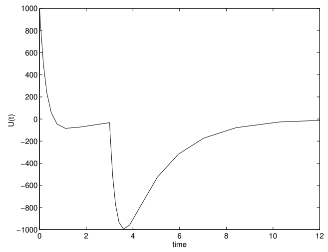

Figure 6.3 Evolution of the approximate solution to P2 for $\mathcal{E} = 128$ and $p = \infty$.

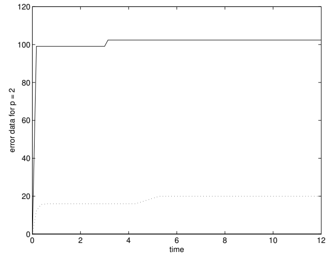

Figure 6.4 Evolution of the nodal error, e, and estimator, $E_{\mathrm{CN}}(i,2)$, when solving P2 for $\mathcal{E} = 128$, $k_{\mathrm{init}} = 1.0$.

It seems that the safest way to arrive at a satisfactory value for C_i^s is to perform several "cheap" computations and look for some evidence of convergence in the computed values. This is done for P1 in Table 6.1. Here (5.3) has been implemented, for the dual problem, in the constant time step mode for various values of $U_0 = u_0$. Recall from Section 4 that the exact value for C_1^s is $1.159\ldots$, it is clear that even on the coarse mesh ($k = 0.4$) the numerical calculation of C_1^s in the manner just described is accurate and reliable. That the computed value is independent of U_0 is not a surprise since, up to machine accuracy, U_0 changes the solution only up to a multiplicative constant.

For the problem P4 this approach is not so pleasing. we require C_1^s for P4 so that we can use it later in the numerical tests with P5. Table 6.2 shows the calculated value of $\|U'\|_{L_1^h(\mathcal{J})}/|U_0|$ again derived from (5.3) in the constant time step mode. It is immediately evident that it is not possible to get a value, in which one has confidence, for C_1^s by performing only cheap computations with constant time step. In fact the numerical solutions for $k = 0.4$ and $k = 0.2$ were hopelessly oscillatory (this is why columns for these values are not included in Table 6.2), and even for $k = 0.1$ these oscillations were still very marked in a visual inspection of the numerical solution. Clearly the computed value of C_1^s depends crucially upon *every* value of U' occuring on $\mathcal{J}$, and therefore oscillatory errors are completely unacceptable when solving the dual problem. Because we have an exact solution to P4 we can infer the source of these errors: the exact solution decreases rapidly from u_0 to a minimum at

k	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,\infty)$	$\widehat{E}_{\mathrm{CN}}(N,2)$	$N=T/k$
0.4	6.188(+2)	1.762(+3)	7.882(+2)	30
0.2	3.526(+1)	3.557(+2)	2.023(+2)	60
0.1	8.452(+0)	1.020(+2)	5.842(+1)	120
0.05	2.092(+0)	2.748(+1)	1.580(+1)	240
0.025	5.217(−1)	7.147(+0)	4.118(+0)	480
0.0125	1.303(−1)	1.824(+0)	1.052(+0)	960
0.00625	3.258(−2)	4.606(−1)	2.658(−1)	1920
0.003125	8.145(−3)	1.158(−1)	6.682(−2)	3840
0.0015625	2.036(−3)	2.902(−2)	1.675(−2)	7680

Table 6.6 Results of solving P3 with the Crank-Nicolson variant in the constant time step mode; $C_1^s := 1.16$.

$\mathcal{E}$	$p=\infty$			$p=2$		
	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,\infty)$	work ratio	$e_{\mathrm{CN}}(t_N)$	$\widehat{E}_{\mathrm{CN}}(N,2)$	work ratio
256	2.041(+1)	2.443(+2)	43/73	4.103(+1)	2.008(+2)	35/51
128	1.013(+1)	9.685(+1)	53/83	1.550(+1)	9.745(+1)	43/73
64	5.958(+0)	5.543(+1)	69/100	1.004(+1)	5.370(+1)	60/92
32	3.334(+0)	3.198(+1)	87/112	5.402(+0)	2.986(+1)	76/106
16	1.837(+0)	1.540(+1)	124/153	3.029(+0)	1.583(+1)	102/129
8	9.800(−1)	7.600(+0)	165/196	1.858(+0)	7.998(+0)	129/158
4	5.191(−1)	3.850(+0)	217/248	9.578(−1)	3.967(+0)	170/202
2	2.709(−1)	1.947(+0)	299/331	4.676(−1)	1.980(+0)	236/269
1	1.387(−1)	9.815(−1)	408/441	2.389(−1)	9.786(−1)	319/353
0.5	7.100(−2)	4.972(−1)	566/599	1.257(−1)	4.924(−1)	435/469
0.25	3.636(−2)	2.477(−1)	788/823	6.504(−2)	2.478(−1)	608/644
0.125	1.875(−2)	1.245(−1)	1099/1137	3.328(−2)	1.242(−1)	841/877
0.0625	9.588(−3)	6.239(−2)	1541/1582	1.692(−2)	6.246(−2)	1179/1219
0.03125	4.874(−3)	3.121(−2)	2165/2209	8.556(−3)	3.115(−2)	1654/1696

Table 6.7 Results of solving P3 with the Crank-Nicolson variant in the adaptive mode: $C_1^s := 1.16$, $k_{\mathrm{init}} = 1.0$.

$t = 0.0766\ldots$, and so time steps larger than this make it impossible for the discrete scheme to effectively capture this feature.

In general we will, of course, not have the exact solution to the dual problem at hand and so we need to devise a strategy for dealing with this kind of situation. In this case a visual inspection of the solution for $k = 0.4$, 0.2 and 0.1 suggests that the oscillations are spurious and that the dual solution decays to zero long before $t_i = T = 12$. This implies that, in Table 6.2, we could reduce T and still get the seemingly reliable value of $C_1^s = 1.094$ at the smaller time steps. The dual computation is then cheaper due to the fewer time levels, and to the fewer calculations required in the history term at each time level. However, in practice we cannot expect this type of behaviour to always be present, what we really want to do is to solve the dual problem adaptively. Of course for this we need a value for C_1^s and this is precisely what we

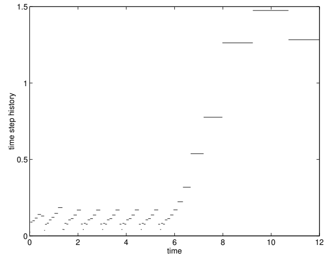

Figure 6.5 Evolution of the time steps when solving P3 in the adaptive mode for $\mathcal{E} = 64$ and $p = \infty$.

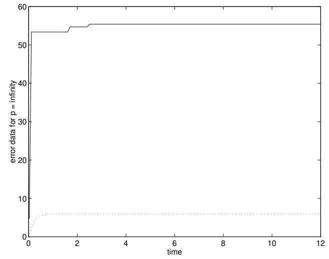

Figure 6.6 Evolution of the nodal error, e, and estimator, $E_{\mathrm{CN}}(i,\infty)$, when solving P3 for $\mathcal{E} = 64$, $k_{\mathrm{init}} = 1.0$.

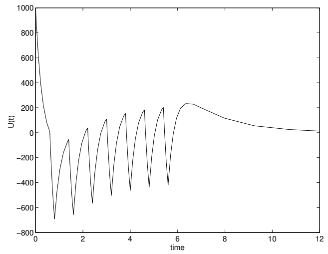

Figure 6.7 Evolution of the approximate solution to P3 for $\mathcal{E} = 64$ and $p = \infty$.

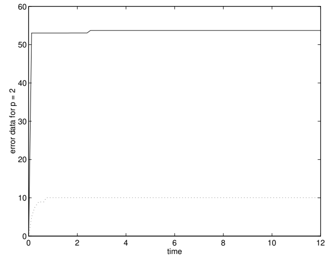

Figure 6.8 Evolution of the nodal error, e, and estimator, $E_{\mathrm{CN}}(i,2)$, when solving P3 for $\mathcal{E} = 64$, $k_{\mathrm{init}} = 1.0$.

are trying to find. What we suggest here is that C_1^s be found recursively, beginning with a cheap constant time step computation for a sequence of decreasing time steps. This would then produce a sequence of stability constants and the most pessimistic of these constants could then be used to provide an adapted solution which would itself produce a constant. This new constant could be used again, and so on until the computed values for C_1^s have “converged”.

Applying this approach to problem P4 we infer from the first two columns of Table 6.2 that $C_1^s = 5.926 \approx 6$ is an appropriately pessimistic value and so we use this for an adaptive solution. The results are shown in Table 6.3, and are given in the form $C_1^s : i$ where: C_1^s is the new adaptively calculated value of C_1^s, and i is the total number of solutions to the discrete problem required to solve adaptively. Again, in terms now of the scaled tolerance $\widehat{\mathcal{E}}$ the results are independent of the value set for U_0, and from the last two columns, where C_1^s seems to have converged, we now have a seemingly reliable value as $C_1^s \approx 1.1$. Also, since $T/276 \approx 0.05$, the number of solutions required for $\widehat{\mathcal{E}} = 1$ corresponds roughly to those required for constant time stepping with $k = 0.05$.

Having now established the values $C_1^s = 1.16$ for P2 and P3, and $C_1^s = 1.1$ for P5, we now close this section with the numerical solution of these problems using, this time, the practical Crank-Nicolson variant. We remark here only that Tables 6.4 to 6.9 and Figures 6.1 to 6.12 are each direct analogues of their counterparts in Section

k	$e_{\rm CN}(t_N)$	$\widehat{E}_{\rm CN}(N,\infty)$	$\widehat{E}_{\rm CN}(N,2)$	$N = T/k$
0.1*	1.076(+3)	1.218(+4)	6.523(+3)	120
0.05*	5.802(+2)	4.639(+3)	2.572(+3)	240
0.025	2.096(+2)	1.654(+3)	9.351(+2)	480
0.0125	5.133(+1)	5.355(+2)	3.059(+2)	960
0.00625	1.179(+1)	1.580(+2)	9.073(+1)	1920
0.003125	2.890(+0)	4.348(+1)	2.504(+1)	3840
0.0015625	7.193(−1)	1.145(+1)	6.604(+0)	7680

Table 6.8 Results of solving P5 with the Crank-Nicolson variant in the constant time step mode; $C_1^s := 1.1$ (* numerical solutions highly oscillatory).

$\mathcal{E}$	$p = \infty$			$p = 2$		
	$e_{\rm CN}(t_N)$	$\widehat{E}_{\rm CN}(N,\infty)$	work ratio	$e_{\rm CN}(t_N)$	$\widehat{E}_{\rm CN}(N,2)$	work ratio
256	1.880(+1)	2.560(+2)	96/147	3.483(+1)	2.559(+2)	91/130
128	1.074(+1)	1.268(+2)	108/158	1.877(+1)	1.279(+2)	105/150
64	5.997(+0)	6.398(+1)	127/171	9.563(+0)	6.347(+1)	107/133
32	3.320(+0)	3.199(+1)	155/210	5.355(+0)	3.196(+1)	164/252
16	1.799(+0)	1.600(+1)	188/232	2.935(+0)	1.600(+1)	174/235
8	9.643(−1)	7.998(+0)	241/292	1.680(+0)	7.994(+0)	213/281
4	5.099(−1)	3.875(+0)	296/327	8.764(−1)	3.999(+0)	287/386
2	2.669(−1)	1.989(+0)	395/433	4.779(−1)	1.971(+0)	327/380
1	1.384(−1)	9.918(−1)	524/563	2.472(−1)	9.995(−1)	411/454
0.5	7.125(−2)	4.943(−1)	714/761	1.299(−1)	4.972(−1)	561/615
0.25	3.660(−2)	2.494(−1)	976/1028	6.712(−2)	2.493(−1)	754/813
0.125	1.892(−2)	1.250(−1)	1347/1414	3.424(−2)	1.247(−1)	1038/1114
0.0625	9.690(−3)	6.248(−2)	1864/1951	1.736(−2)	6.241(−2)	1429/1518
0.03125	4.932(−3)	3.125(−2)	2594/2703	8.758(−3)	3.121(−2)	1979/2084

Table 6.9 Results of solving P5 with the Crank-Nicolson variant in the adaptive mode: $C_1^s := 1.1$, $k_{\rm init} = 1.0$.

4, and so we refer back to the explanatory remarks made at the end of that section.

7. Incorporation of quadrature errors. In this section we begin to examine how the *a posteriori* error estimates, and the resulting adaptive algorithms, may be adjusted to incorporate the errors introduced by the "variational crimes" of replacing the inner products and Volterra operator by numerical quadrature rules. To keep this section short we build only on the analysis of the backward Euler variant, in the case $p = \infty$, and its practical realization as discussed above in Sections 3 and 4. Also, for simplicity, we restrict ourselves to the case where σ = constant in (1.1) and we make some further assumptions on the data.

Assumptions 7.1. *To incorporate quadrature-error estimates we strengthen Assumptions 1.1.*

(i) σ = *constant.*

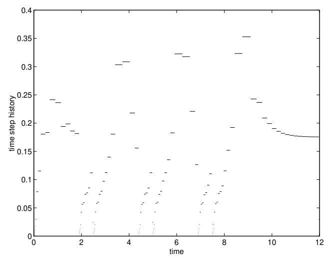

Figure 6.9 Evolution of the time steps when solving P5 in the adaptive mode for $\mathcal{E} = 32$ and $p = \infty$.

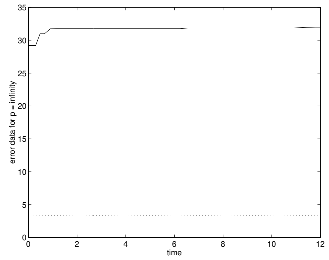

Figure 6.10 Evolution of the nodal error, e, and estimator, $E_{\rm CN}(i,\infty)$, when solving P5 for $\mathcal{E} = 32$, $k_{\rm init} = 1.0$.

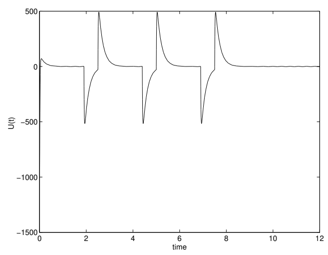

Figure 6.11 Evolution of the approximate solution to P5 for $\mathcal{E} = 32$ and $p = \infty$.

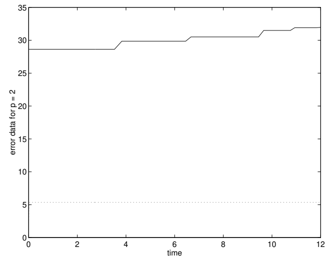

Figure 6.12 Evolution of the nodal error, e, and estimator, $E_{\rm CN}(i,2)$, when solving P5 for $\mathcal{E} = 32$, $k_{\rm init} = 1.0$.

(ii) $d^n f/dt^n \in L_\infty(\mathcal{J})$ *for some integer* $n > 0$.

(iii) $\partial^n\phi/\partial t^n$, $\partial^n\phi/\partial s^n \in L_\infty(\mathcal{J}\times\mathcal{J})$ *and* $d^n\phi(t,t)/dt^n \in L_\infty(\mathcal{J})$ *for some integers* $n \geq 1$.

Assumptions 3.1 are retained unchanged. ■

From Section 4 we see that the quadrature rules used to form the practical algorithm are the midpoint, trapezoid and three-point Simpson rules, thus we will need the following standard error bounds.

Lemma 7.1. *Let a and b be real numbers such that $k := b - a > 0$. Also let $I : w \to \int_a^b w(t)\,dt$ be a definite integral operator defined for all functions $w \in L_1(a,b)$. The following quadrature estimates apply. If $I_M : w \to \mathbb{R}$ represents a midpoint rule approximation to I then*

$$|Iw - I_M w| \leq \min\left\{ Q_n^M k^n \|w^{(n)}\|_{L_1(a,b)} : n = 1, 2 \right\},$$

where the Q_n^M are constants. If I_T is the trapezoidal rule approximation to I then

$$|Iw - I_T w| \leq \min\left\{ Q_n^T k^n \|w^{(n)}\|_{L_1(a,b)} : n = 1, 2 \right\},$$

where the Q_n^T are also constants. Finally, if I_S is the three-point Simpson rule approximation to I then

$$|Iw - I_S w| \le \min\left\{Q_n^S k^n \|w^{(n)}\|_{L_1(a,b)} : n = 1,2,3,4\right\},$$

where the Q_n^S are, again, constants. ∎

To study the quadrature errors we note first that the computed solution, call it $W \in V_0^h$, actually satisfies, in place of (3.4),

$$(A_h W, v)_h := (\sigma W, v) - (\Lambda_h W, v)_M + \sum_{i=0}^{N-1} v_i^+ [\![W_i]\!] = (f, v)_S, \tag{7.1}$$

where: $(\cdot,\cdot)_M$, $(\cdot,\cdot)_S$ represent composite midpoint and Simpson "inner products" and the discrete Volterra operator, Λ_h, is given by a composite Simpson rule using the time stepping partition of $\mathcal{J}$. Setting $\theta := U - W$ we have the following quadrature-error representation.

Lemma 7.2. *The Galerkin and computed approximations, U and W, are related by*

$$(\sigma\theta, v) - \Delta_M(\Lambda U, v) - \big((\Lambda - \Lambda_h)U, v\big)_M - (\Lambda_h\theta, v)_M + \sum_{i=0}^{N-1} v_i^+ [\![\theta_i]\!] = \Delta_S(f, v) \quad \forall v \in V_0^h,$$

where $\Delta_M(\Lambda U, v) := (\Lambda U, v) - (\Lambda U, v)_M$ and $\Delta_S(f, v) := (f, v) - (f, v)_S$.

Proof. Note first that $[\![U_i]\!] - [\![W_i]\!] = [\![(U - W)_i]\!]$ and

$$(\Lambda U, v) - (\Lambda_h W, v)_M = \Delta_M(\Lambda U, v) + \big((\Lambda - \Lambda_h)U, v\big)_M + (\Lambda_h\theta, v)_M.$$

Subtracting (7.1) from (3.4) gives

$$(\sigma U, v) - (\Lambda U, v) + \sum_{i=0}^{N-1} v_i^+ [\![U_i]\!] - (\sigma W, v) + (\Lambda_h W, v)_M - \sum_{i=0}^{N-1} v_i^+ [\![W_i]\!] = (f, v) - (f, v)_S,$$

from which the result follows immediately. ∎

Drawing on the stability results for the dual problem in Lemma 3.3 we assume the following.

Lemma 7.3. *Suppose that the analogues of Lemmas 3.2 and 3.3 hold for the discrete Galerkin forward problem with quadrature, (7.1), then there is a non-decreasing weak stability factor, $S_1(t)$, such that U satisfies $\|U\|_{L_\infty(0,t)} \le S_1(t)(|u_0| + \|f\|_{L_\infty(0,t)})$, for all $t \in \mathcal{J}$.* ∎

Our first main result is a computable bound on θ. To ease the notation a little we recall I, I_M, I_T and I_S from Lemma 7.1 and write $Iw|_{(a,b)}$ instead of just Iw so we may easily denote integrals over different intervals. An exact analogue of this notation will also be used for I_M, I_T and I_S.

Theorem 7.1. *Let Assumptions 1.1, 3.1 and 7.1 hold. Then $\theta = U - W$ satisfies the a posteriori error bound*

$$\begin{aligned}
\|\theta\|_{L_\infty(0,t_j)} \le S_1^2(t_j)\Bigg(&\max_{1\le i\le j}\min\Bigg\{Q_1^M k_i^2\left(\|\phi\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i\|\phi_t\|_{L_\infty(\mathcal{J}_i\times(0,t_i))}\right),\\
&Q_2^M k_i^3\left(\left\|\frac{d\phi}{dt}\right\|_{L_\infty(\mathcal{J}_i)} + \|\phi_t\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i\|\phi_{tt}\|_{L_\infty(\mathcal{J}_i\times(0,t_i))}\right)\Bigg\}\\
&+ t_j K \min_{1\le q\le 4}\left\{Q_q^S \max_{1\le n\le i\le j}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_n)}\right\}\right\}\Bigg)\\
&\times\left(|u_0| + \|f\|_{L_\infty(0,t_j)}\right)\\
&+ S_1(t_j)\max_{1\le i\le j}\min_{1\le q\le 4}\left\{Q_q^S k_i^{q+1}\left\|\frac{d^q f}{dt^q}\right\|_{L_\infty(\mathcal{J}_i)}\right\},
\end{aligned}$$

for all $t \in \overline{\mathcal{J}_j}$ and for all $j \in \{1,\dots,N\}$. Here: the subscript s^q denotes q-fold s-differentiation, $S_1(t)$ comes from Lemma 7.3, $d\phi/dt = d\phi(t,t)/dt$ and the constants Q_q^M, Q_q^S come from Lemma 7.1.

Proof. Pick an arbitrary $j \in \{1,\dots,N\}$ and in Lemma 7.2 choose $v = 1$ on $\mathcal{J}_j$ and $v = 0$ elsewhere, Lemma 7.2 then gives

$$\begin{aligned}
\int_{t_{j-1}}^{t_j}\sigma\theta\,dt - \left[\int_{t_{j-1}}^{t_j}\Lambda U\,dt - k_j\Lambda U(t_{j-1/2})\right] + k_j(\Lambda - \Lambda_h)U(t_{j-1/2})&\\
-k_j\Lambda_h\theta(t_{j-1/2}) + \theta_j = \theta_{j-1} + (If - I_S f)|_{\mathcal{J}_j}&.
\end{aligned}$$

Defining

$$\widetilde{S}_j := \int_{t_{j-1}}^{t_j}\sigma(t)\,dt, \qquad \widetilde{F}_j := k_j I_S\phi(t_{j-1/2},\cdot)|_{(t_{j-1},t_{j-1/2})},$$

$$\widetilde{H}_j(\theta) := k_j\sum_{n=1}^{j-1} I_S\phi(t_{j-1/2},\cdot)|_{\mathcal{J}_n}\theta_n,$$

with $\widetilde{H}_1(\theta) := 0$, and

$$\Delta(k_j, U) := k_j(\Lambda - \Lambda_h)U(t_{j-1/2}) - \left[\int_{t_{j-1}}^{t_j}\Lambda U\,dt - k_j\Lambda U(t_{j-1/2})\right],$$

(which is motivated by the quadrature rule:

$$k_j\Lambda_h\theta(t_{j-1/2}) = k_j\sum_{n=1}^{j-1} I_S\phi(t_{j-1/2},\cdot)|_{\mathcal{J}_n}\theta_n + k_j I_S\phi(t_{j-1/2},\cdot)|_{(t_{j-1},t_{j-1/2})})$$

we get by setting $\widetilde{G}_j := (1 - \widetilde{F}_j + \widetilde{S}_j)^{-1}$ that (compare (3.12))

$$\theta_j := \widetilde{G}_j\left(\theta_{j-1} - \Delta(k_j, U) + (If - I_S f)|_{\mathcal{J}_j} + \widetilde{H}_j(\theta)\right) \qquad \text{for } j = 1,\dots,N.$$

Assuming analogues to Lemmas 3.2 and 3.3 and using the linearity of the problem, with $\theta_0 = 0$, we then have

$$\|\theta\|_{L_\infty(0,t_j)} \leq S_1(t_j) \max_{1\leq i\leq j} \{|\Delta(k_i, U) - (If - I_S f)|_{\mathcal{J}_i}|\}.$$

Taking the norm term-by-term we get firstly, by Lemma 7.1, that

$$\begin{aligned}\max_{1\leq i\leq j} |(If - I_S f)|_{\mathcal{J}_i}| &\leq \max_{1\leq i\leq j} \min_{1\leq q\leq 4} \left\{ Q_q^S k_i^q \left\| f^{(q)} \right\|_{L_1(\mathcal{J}_i)} \right\} \\ &\leq \max_{1\leq i\leq j} \min_{1\leq q\leq 4} \left\{ Q_q^S k_i^{q+1} \left\| f^{(q)} \right\|_{L_\infty(\mathcal{J}_i)} \right\}.\end{aligned}$$

Recalling the definition of $\Delta(k_j, U)$ we have secondly that

$$\begin{aligned}k_j \left|(\Lambda - \Lambda_h)U(t_{j-1/2})\right| &\leq k_j \min_{1\leq q\leq 4} \left\{ Q_q^S \sum_{n=1}^{j} k_n^q \left\|\phi_{s^q}(t_{j-1/2}, \cdot)\right\|_{L_\infty(\mathcal{J}_n)} \|U\|_{L_1(\mathcal{J}_n)} \right\}, \\ &\leq k_j \min_{1\leq q\leq 4} \left\{ Q_q^S \max_{1\leq n\leq j} \left\{ k_n^q \left\|\phi_{s^q}\right\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)} \right\} \right\} \|U\|_{L_1(0,t_j)}, \\ &\leq S_1(t_j) t_j k_j \min_{1\leq q\leq 4} \left\{ Q_q^S \max_{1\leq n\leq j} \left\{ k_n^q \left\|\phi_{s^q}\right\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)} \right\} \right\} \\ &\quad \times \left(|u_0| + \|f\|_{L_\infty(0,t_j)}\right),\end{aligned}$$

where the subscript s^q denotes the q^{th} s-derivative and we used Lemmas 7.1 and 7.3. It follows immediately that

$$\begin{aligned}\max_{1\leq i\leq j} k_i \left|(\Lambda - \Lambda_h)U(t_{i-1/2})\right| \leq \min_{1\leq q\leq 4} &\left\{ Q_q^S \max_{1\leq n\leq i\leq j} \left\{ k_n^q \left\|\phi_{s^q}\right\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_n)} \right\} \right\} \\ &\times S_1(t_j) t_j K \left(|u_0| + \|f\|_{L_\infty(0,t_j)}\right).\end{aligned}$$

Thirdly, from Lemma 7.1,

$$\left| \int_{t_{j-1}}^{t_j} \Lambda U \, dt - k_j \Lambda U(t_{j-1/2}) \right| \leq \min_{q=1,2} \left\{ Q_q^M k_j^q \left\|(\Lambda U)_{t^q}\right\|_{L_1(\mathcal{J}_j)} \right\},$$

and we have for $t \in \mathcal{J}_j$ that for $q = 1$,

$$\begin{aligned}\|(\Lambda U)_t\|_{L_1(\mathcal{J}_j)} &= \left\| \phi(t,t)U(t) + \int_0^t \phi_t(t,s)U(s)\, ds \right\|_{L_1(\mathcal{J}_j)}, \\ &\leq k_j \|\phi\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)} \|U\|_{L_\infty(\mathcal{J}_j)} + k_j \left\| \int_0^t \phi_t(t,s)U(s)\, ds \right\|_{L_\infty(\mathcal{J}_j)}, \\ &\leq k_j \|\phi\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)} \|U\|_{L_\infty(\mathcal{J}_j)} + k_j t_j \|\phi_t\|_{L_\infty(\mathcal{J}_j\times(0,t_j))} \|U\|_{L_\infty(0,t_j)},\end{aligned}$$

since, for $q = 1$,

$$\begin{aligned}\left\| \int_0^t \phi_t(t,s)U(s)\, ds \right\|_{L_\infty(\mathcal{J}_j)} &\leq \left\| \, \|\phi_t(t,\cdot)\|_{L_\infty(0,t)} \|U\|_{L_1(0,t)} \right\|_{L_\infty(\mathcal{J}_j)} \\ &\leq \|\phi_t\|_{L_\infty(\mathcal{J}_j\times(0,t_j))} \|U\|_{L_1(0,t_j)}.\end{aligned}$$

While, for $q = 2$,

$$\begin{aligned}\|(\Lambda U)_{tt}\|_{L_1(\mathcal{J}_j)} &= \left\| U(t)\frac{d\phi}{dt}(t,t) + \phi_t(t,t)U(t) + \int_0^t \phi_{tt}(t,s)U(s)\, ds \right\|_{L_1(\mathcal{J}_j)} \\ &\leq k_j \left(\left\| \frac{d\phi}{dt} \right\|_{L_\infty(\mathcal{J}_j)} + \|\phi_t\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)} + t_j \|\phi_{tt}\|_{L_\infty(\mathcal{J}_j\times(0,t_j))} \right) \|U\|_{L_\infty(0,t_j)}.\end{aligned}$$

Therefore, using the stability estimate: $\|U\|_{L_\infty(0,t_j)} \leq S_1(t_j)(|u_0| + \|f\|_{L_\infty(0,t_j)})$, we find that

$$\begin{aligned}\max_{1\leq i\leq j} \left| \int_{t_{i-1}}^{t_i} \Lambda U\, dt - k_i \Lambda U(t_{i-1/2}) \right| &\leq S_1(t_j) \left(|u_0| + \|f\|_{L_\infty(0,t_j)}\right) \times \\ \max_{1\leq i\leq j} \min &\left\{ Q_1^M k_i^2 \left(\|\phi\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i \|\phi_t\|_{L_\infty(t_i\times(0,t_i))} \right), \right. \\ &\left. Q_2^M k_i^3 \left(\left\| \frac{d\phi}{dt} \right\|_{L_\infty(\mathcal{J}_i)} + \|\phi_t\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i \|\phi_{tt}\|_{L_\infty(\mathcal{J}_i\times(0,t_i))} \right) \right\}.\end{aligned}$$

Putting these bounds together we obtain

$$\begin{aligned}&\max_{1\leq i\leq j} |\Delta(k_i, U) + (If - I_S f)|_{\mathcal{J}_i}| \\ &\leq \max_{1\leq i\leq j} \left\{ k_i \left|(\Lambda - \Lambda_h)U(t_{i-1/2})\right| + \left| \int_{t_{i-1}}^{t_i} \Lambda U\, dt - k_i \Lambda U(t_{i-1/2}) \right| + |(I - I_S)f|_{\mathcal{J}_i}| \right\} \\ &\leq S_1(t_j) \left(|u_0| + \|f\|_{L_\infty(0,t_j)}\right) \left(t_j K \min_{1\leq q\leq 4} \left\{ Q_q^S \max_{1\leq n\leq i\leq j} \left\{ k_n^q \|\phi_{s^q}\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_n)} \right\} \right\} \right. \\ &\quad + \max_{1\leq i\leq j} \min \left\{ Q_1^M k_i^2 \left(\|\phi\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i \|\phi_t\|_{L_\infty(\mathcal{J}_i\times(0,t_i))} \right), \right. \\ &\quad \left.\left. Q_2^M k_i^3 \left(\left\| \frac{d\phi}{dt} \right\|_{L_\infty(\mathcal{J}_i)} + \|\phi_t\|_{L_\infty(\mathcal{J}_i\times\mathcal{J}_i)} + t_i \|\phi_{tt}\|_{L_\infty(\mathcal{J}_i\times(0,t_i))} \right) \right\} \right) \\ &\quad + \max_{1\leq i\leq j} \min_{1\leq q\leq 4} \left\{ Q_q^S k_i^{q+1} \|f^{(q)}\|_{L_\infty(\mathcal{J}_i)} \right\}.\end{aligned}$$

This completes the proof. ■

With this computable bound on $U - W$ at our disposal the next task is to build on Theorem 3.1 and provide an *a posteriori* error bound for the computed error $u - W$. Toward this we begin with the following estimate for the Galerkin residual.

Lemma 7.4. *Let Assumptions 1.1, 3.1 and 7.1 hold, then*

$$\begin{aligned}
&k_j\|f-\sigma U+\Lambda U\|_{L_\infty(\mathcal{J}_j)}+|U_j-U_{j-1}| \\
&\quad\le k_j\|f-\sigma W+\Lambda_h W\|_{L_\infty(\mathcal{J}_j)}+|W_j-W_{j-1}| \\
&\qquad+\left(2+k_j\|\sigma\|_{L_\infty(\mathcal{J}_j)}+\frac{2k_jt_j}{3}\|\phi\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\right)\|\theta\|_{L_\infty(0,t_j)} \\
&\qquad+S_1(t_j)k_j\Bigg(\min_{1\le q\le 4}\left\{Q_q^S t_{j-1}\max_{1\le n\le j-1}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\}\right\} \\
&\qquad\qquad+\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}\right\}\Bigg)\left(|u_0|+\|f\|_{L_\infty(0,t_j)}\right).
\end{aligned}$$

where $\|\theta\|_{L_\infty(0,t_j)}$ is bounded by Theorem 7.1.

Proof. We begin with the following estimates:

$$k_j\|\sigma\theta\|_{L_\infty(\mathcal{J}_j)}\le k_j\|\sigma\|_{L_\infty(\mathcal{J}_j)}\|\theta\|_{L_\infty(\mathcal{J}_j)};\quad |\theta_j-\theta_{j-1}|\le 2\|\theta\|_{L_\infty(0,t_j)};$$

while for the Simpson-trapezoidal rule described in section 4,

$$\begin{aligned}
k_j\|\Lambda_h\theta\|_{L_\infty(\mathcal{J}_j)}&\le k_j\left\|\sum_{n=1}^{j-1}\frac{k_n}{6}\left(\phi(t,t_{n-1})+4\phi(t,t_{n-1/2})+\phi(t,t_n)\right)\theta_n\right\|_{L_\infty(\mathcal{J}_j)} \\
&\quad+k_j\left\|\frac{(t-t_{j-1})}{2}\big(\phi(t,t_{j-1})+\phi(t,t)\big)\theta_j\right\|_{L_\infty(\mathcal{J}_j)} \\
&\le\frac{2k_j}{3}\sum_{n=1}^{j-1}k_n\|\phi\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\|\theta\|_{L_\infty(0,t_j)}+\frac{k_j^2}{2}\|\phi\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}\|\theta\|_{L_\infty(0,t_j)} \\
&\le\frac{2k_jt_j}{3}\|\phi\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\|\theta\|_{L_\infty(0,t_j)}.
\end{aligned}$$

Also, from Lemma 7.1,

$$\begin{aligned}
&k_j\|(\Lambda-\Lambda_h)U\|_{L_\infty(\mathcal{J}_j)} \\
&\quad\le k_j\left\|(I-I_S)\phi(t,\cdot)U(\cdot)|_{(0,t_{j-1})}\right\|_{L_\infty(\mathcal{J}_j)}+k_j\left\|(I-I_T)\phi(t,\cdot)U(\cdot)|_{(t_{j-1},t)}\right\|_{L_\infty(\mathcal{J}_j)}, \\
&\quad\le k_j\left\|\min_{1\le q\le 4}\left\{Q_q^S\sum_{n=1}^{j-1}k_n^q\|\phi_{s^q}(t,\cdot)\|_{L_1(\mathcal{J}_n)}\|U\|_{L_\infty(\mathcal{J}_n)}\right\}\right\|_{L_\infty(\mathcal{J}_j)} \\
&\qquad+k_j\left\|\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}(t,\cdot)\|_{L_\infty(\mathcal{J}_j)}\|U\|_{L_\infty(\mathcal{J}_j)}\right\}\right\|_{L_\infty(\mathcal{J}_j)}, \\
&\quad\le k_j\Bigg(\min_{1\le q\le 4}\left\{Q_q^S\sum_{n=1}^{j-1}k_n^{q+1}\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\} \\
&\qquad\quad+\left\|\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}(t,\cdot)\|_{L_\infty(\mathcal{J}_j)}\right\}\right\|_{L_\infty(\mathcal{J}_j)}\Bigg)\|U\|_{L_\infty(0,t_j)}, \\
&\quad\le S_1(t_j)k_j\Bigg(\min_{1\le q\le 4}\left\{Q_q^S t_{j-1}\max_{1\le n\le j-1}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\}\right\} \\
&\qquad\qquad+\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}\right\}\Bigg)\left(|u_0|+\|f\|_{L_\infty(0,t_j)}\right),
\end{aligned}$$

where we also used the stability estimate in Lemma 7.2. Putting these results together we now get, by adding and subtracting like quantities, that

$$\begin{aligned}
&k_j\|f-\sigma U+\Lambda U\|_{L_\infty(\mathcal{J}_j)}+|U_j-U_{j-1}| \\
&\quad\le k_j\|f-\sigma W+\Lambda_h W\|_{L_\infty(\mathcal{J}_j)}+|W_j-W_{j-1}| \\
&\qquad+k_j\|(\Lambda-\Lambda_h)U+\Lambda_h\theta-\sigma\theta\|_{L_\infty(\mathcal{J}_j)}+|\theta_j-\theta_{j-1}|, \\
&\quad\le k_j\|f-\sigma W+\Lambda_h W\|_{L_\infty(\mathcal{J}_j)}+|W_j-W_{j-1}| \\
&\qquad+\left(2+k_j\|\sigma\|_{L_\infty(\mathcal{J}_j)}+\frac{2k_jt_j}{3}\|\phi\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\right)\|\theta\|_{L_\infty(0,t_j)} \\
&\qquad+S_1(t_j)k_j\Bigg(\min_{1\le q\le 4}\left\{Q_q^S t_{j-1}\max_{1\le n\le j-1}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\}\right\} \\
&\qquad\qquad+\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}\right\}\Bigg)\left(|u_0|+\|f\|_{L_\infty(0,t_j)}\right).
\end{aligned}$$

This is the desired result. ■

We can now state the fully practical *a posteriori* error estimate.

Theorem 7.2. *Let Assumptions 1.1, 3.1 and 7.1 hold, then the distance between the exact solution, u, to (1.1) and the computed approximation, W, satisfies the following a posteriori error estimate,*

$$\begin{aligned}
\|u-W\|_{L_\infty(0,t_i)}&\le C_1^s\max_{1\le j\le i}\left\{k_j\|r^h(W)\|_{L_\infty(\mathcal{J}_j)}+|W_j-W_{j-1}|\right\} \\
&\quad+c_i\Big(S_1(t_i)(1+C_1^s\Phi_4^i)(\Phi_1^i+\Phi_2^i)+C_1^s\Phi_3^i\Big)\left(|u_0|+\|f\|_{L_\infty(0,t_i)}\right) \\
&\quad+c_i(1+C_1^s\Phi_4^i)F^i,
\end{aligned}$$

where $r^h(W):=f-\sigma W+\Lambda_h W$, and:

$$\begin{aligned}
\Phi_1^i&:=\max_{1\le j\le i}\min\Bigg\{Q_1^M k_j\left(\|\phi\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}+t_j\|\phi_t\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\right), \\
&\qquad Q_2^M k_j^2\left(\left\|\frac{d\phi}{dt}\right\|_{L_\infty(\mathcal{J}_j)}+\|\phi_t\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}+t_j\|\phi_{tt}\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\right)\Bigg\}, \\
\Phi_2^i&:=t_i\min_{1\le q\le 4}\left\{Q_q^S\max_{1\le n\le j\le i}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\}\right\}, \\
\Phi_3^i&:=\max_{1\le j\le i}\Bigg\{\min_{1\le q\le 4}\left\{Q_q^S t_{j-1}\max_{1\le n\le j-1}\left\{k_n^q\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_n)}\right\}\right\} \\
&\qquad+\min_{q=1,2}\left\{Q_q^T k_j^{q+1}\|\phi_{s^q}\|_{L_\infty(\mathcal{J}_j\times\mathcal{J}_j)}\right\}\Bigg\}, \\
\Phi_4^i&:=\max_{1\le j\le i}\left\{2+k_j\|\sigma\|_{L_\infty(\mathcal{J}_j)}+\frac{2k_jt_j}{3}\|\phi\|_{L_\infty(\mathcal{J}_j\times(0,t_j))}\right\}, \\
F^i&:=\max_{1\le j\le i}\min_{1\le q\le 4}\left\{Q_q^S k_j^q\left\|\frac{d^qf}{dt^q}\right\|_{L_\infty(\mathcal{J}_j)}\right\},
\end{aligned}$$

with $c_i:=KS_1(t_i)$.

Proof. Firstly we recall Theorem 7.1 to obtain

$$\|\theta\|_{L_\infty(0,t_i)} \leq c_i S_1(t_i)\left(\Phi_1^i + \Phi_2^i\right)\left(|u_0| + \|f\|_{L_\infty(0,t_i)}\right) + c_i F^i.$$

Now we use this with the triangle inequality, Theorem 3.1 and Lemma 7.4 to obtain the following.

$$\begin{aligned}
\|u - W\|_{L_\infty(0,t_i)} &\leq \|u - U\|_{L_\infty(0,t_i)} + \|\theta\|_{L_\infty(0,t_i)}\\
&\leq C_1^s \max_{1\leq j\leq i}\left\{k_j\|f - \sigma U + \Lambda U\|_{L_\infty(\mathcal{J}_j)} + |U_j - U_{j-1}|\right\} + \|\theta\|_{L_\infty(0,t_i)},\\
&\leq C_1^s \max_{1\leq j\leq i}\left\{k_j\|f - \sigma W + \Lambda_h W\|_{L_\infty(\mathcal{J}_j)} + |W_j - W_{j-1}|\right\} + \|\theta\|_{L_\infty(0,t_i)}\\
&\quad + c_i C_1^s \Phi_3^i\left(|u_0| + \|f\|_{L_\infty(0,t_i)}\right) + C_1^s\Phi_4^i\|\theta\|_{L_\infty(0,t_i)},\\
&\leq C_1^s \max_{1\leq j\leq i}\left\{k_j\|r^h(W)\|_{L_\infty(\mathcal{J}_j)} + |W_j - W_{j-1}|\right\} + c_i C_1^s\Phi_3^i\left(|u_0| + \|f\|_{L_\infty(0,t_i)}\right)\\
&\quad + c_i S_1(t_i)(1 + C_1^s\Phi_4^i)(\Phi_1^i + \Phi_2^i)\left(|u_0| + \|f\|_{L_\infty(0,t_i)}\right) + c_i(1 + C_1^s\Phi_4^i)F^i.
\end{aligned}$$

This is the desired result. ■

Recalling from Assumption 3.1 that K is the maximum permitted time step for the scheme we see that the factor c_i in this bound can be used to attenuate the effect of $S_1^2(t_i)$ (from Theorem 7.1) to only $c_i S_1(t_i)$. The price of this damping is a lost power of the time step in the quadrature errors. Obviously if $S_1(t_i)$ does not grow "too fast" the introduction of c_i can be avoided and the estimate given above is then optimal.

Also, it appears that a similar analysis could be performed for the Crank-Nicolson variant, the additional requirement would be a strong discrete stability estimate for the Galerkin solution, from (5.3), since in this case $U' \neq 0$.

8. Concluding remarks. In this report we have presented two modern variants of classical finite difference discretization schemes for the ODE with memory: (1.1). The important point is that, once the finite element overhead of quadrature is accepted, these schemes are not significantly more expensive than their classical counterparts, and they come with rigorous *a posteriori* Galerkin-error estimates which can form the basis of rational adaptive solvers. In this final section we firstly want to make some observations concerning the numerical results in Sections 4 and 6, and then finish with some more general comments on the results presented above.

Looking first at the results for the backward Euler variant in Tables 4.2—7: we can compare the true errors with those estimated to find that in the constant time stepping mode the estimates are larger than the true errors by only a factor of around ten; in the adaptive mode they are only a factor of around four larger. This behaviour seems independent of the problem tested. Also, by comparing the "work ratio" columns in the tables of adapted results with the "$N = T/k$" columns in the corresponding fixed step tables, it is clear that the adaptive algorithms can generate approximate solutions with superior (and user-specified) accuracy for a smaller amount of computational effort. In particular, looking at the results for the problem P5 (Tables 4.6 and 4.7) we can see that constant time stepping over 7680 levels produces an error of 35, while adaptively solving over only 126 levels (166 solutions of the discrete equation) produces an error of 49. On the other hand, if we allow ourselves ≈ 8000 steps in the adaptive

solver we get an error of around $0.5 \ll 35$ (this is for $\mathcal{E} = 2$). Assuming that the error halves as the time step halves, to get this accuracy with a constant time step would require around $7680 \times 35/0.5 = 537600$ levels! Clearly an adaptive solver is *essential* for problems with rough solutions such as this.

Moving on now to the results for the Crank-Nicolson variant, Tables 6.4—6.9: we see that the estimators are, respectively, only around eighteen and seven times too large for constant and adaptive time stepping, and again these factors seem independent of the problem being solved. Why this is so (if it is) is not clear. On the face of it this scheme seems disproportionately more efficient than the backward Euler variant when the solution is smooth enough to allow it. For example: to get for P2 $\widehat{E}_{\text{CN}}(N,2) \approx 0.06$ takes 3840 constant time steps but only 469 adaptive ones. Also: to get for P5 $\widehat{E}_{\text{CN}}(N,2) \approx 8$ takes 7680 steps as against only 281. The *adaptive advantage* for P3 is not so dramatic but this is because the solution does not allow it—it is rough over most of $\mathcal{J}$ (see Figure 6.7). The scheme is not suited to solving in the constant time step mode because of the possible oscillatory nature of the discrete solution—recall the discussion in Section 6 concerning the calculation of the stability constant for P4. Also, we can note that for most values of $\mathcal{E}$ $\widehat{E}_{\text{CN}}(N,2)$ seems a more efficient estimator than $\widehat{E}_{\text{CN}}(N,\infty)$. This is clear from the values in the "work ratio" columns.

Thus the evidence is that both schemes furnish sharp and reliable error control, and that the Crank-Nicolson variant is potentially very efficient. The problem with the scheme (as in the classical case) is that when the data is rough the numerical solution can undergo severe oscillation. Perhaps the best way to use these schemes is in a combined algorithm which allows the possibility to switch schemes as the data (or numerical solution) changes its nature.

The Crank-Nicolson variant is not the only way to get a higher order scheme in this finite element framework. Perhaps more natural would be to take $r > 0$ in (3.2) and formulate the corresponding discontinuous Galerkin method (see e.g. [5] for $r = 0, 1$). Here, for discontinuous approximation by piecewise polynomials of degree r there are $r + 1$ unknowns to be solved for on each $\overline{\mathcal{J}}_i$. Therefore one has to solve an $r + 1$ square system at each time level. Would this scheme for $r = 1$ be cheaper overall than the mixed Euler–Crank-Nicolson algorithm discussed above? This will be an interesting question to explore at a later time.

We have mentioned before that implementing adaptive quadrature rules might obviate the need for the contingency rule (4.6). It is important to get this right because iterating a large number of times on each time level will kill off any adaptive advantage otherwise gained. Also, this adaptive quadrature could be employed if one lacks faith in the negligibilty of the quadrature errors.

Perhaps the thorniest issue associated with this overall approach to numerical analysis concerns the stability constants C_q^s. The only known way of obtaining these *a priori* for general problems of the generic type (1.1) is to perform a Gronwall-type summation. But then, as is well known, this can result in a constant which is vastly larger than necessary. It seems that the need to calculate this constant numerically, in order to get a sharp value, is the price of the error bounds. For our model problems we have shown in Section 6 that, with a little care, these constants can be calculated, rather accurately, for not too high a price. How expensive this process is is of course relative to $\mathcal{E}$. The smaller $\mathcal{E}$ becomes the cheaper, in terms of the share of computational effort, the process described around Tables 6.1—3 becomes.

Of course we recognise that for some problems, particularly nonlinear ones, C_q^s may be prohibitively difficult to determine with any real confidence, but even then, so long as its existence is proven, adaptive error control up to a multiplicative constant should still be be possible. Thus we can guide the shape of the function κ (see Theorem 5.1) but not its norm.

Also on the subject of the dual stability constant note that all five of the problems we have used (Table 4.1) have solutions that decay to zero as time increases. On an intuitive level it is then reasonable to expect that C_q^s be bounded independently of T. However, if the solution were, for example, to blow-up exponentially then in Theorems 3.1 and 5.2 C_1^s could be exponentially large in T. The effect might well be to force much smaller time steps in a neighbourhood of $T = 0$ than are really called for. A way around this could be to use "time dependent constants". Examining the proofs of these Theorems we see that to bound the errors at time t_i requires only the strong initial-data stability: $\|\chi'\|_{L_1(0,t_i)} \leq C_1^s|\chi(t_i)|$. Clearly it would be straightforward to keep track of how C_1^s evolves as t_i increases and use C_1^s as a *function*, as opposed to a constant, in the theorems.

Theorem 7.2 demonstrates that if the data $\{\sigma, \phi, f\}$ are piecewise smooth (with respect to the nodes $\{t_i\}$) then, for small enough time steps, the quadrature errors are negligible as compared to the Galerkin error. However, Theorem 7.2 furnishes a *computable* error bound and so, if desired, the quadrature-error estimates could be incorporated into the adaptive scheme. This appears to be particularly relevant to the case where $S_1(t_i)$ is growing "fast" and $d\phi/dt$ or ϕ_{tt} are not L_∞ functions. In this case the terms $\{\Phi_j^i\}_{1\leq j\leq 4}$ may be comparable in magnitude to the Galerkin error and could be adaptively managed by appropriate choices for the time steps.

We finish now with a collection of bulleted comments:

- Theorems 3.1 and 5.2 call only for L_1 strong stability of (2.1)—this is the weakest we could ask for.
- The numerical results do not in any way suggest that we are unjustified in ignoring the quadrature errors in the discrete solution.
- Quadrature requires extra smoothness than that assumed in Assumptions 1.1 and so if the data is rough more thought is needed for the quadrature replacements.
- Frequently when ϕ is rough it is simple enough (or has a simple enough rough part) to be integrated analytically. There is then no need for quadrature in the Φ terms (4.1) and (6.1).
- A clear disadvantage with these approximation schemes is the lack of smoothness of U. This implies that the sparse quadrature rules developed in [16] cannot be applied to alleviate the history storage and calculation time requirements of the algorithms. (Unless ϕ is smooth enough to allow repeated integration by parts.) However, recall the discussion in Section 1: the whole point of an adaptive algorithm is to in some sense optimize N, thus we do not expect these problems to be as pronounced, for most input data, in the adaptive scheme as they are in the constant step solution mode.

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