A SECOND ORDER BACKWARD DIFFERENCE METHOD WITH VARIABLE STEPS FOR A PARABOLIC PROBLEM *

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Abstract.

The numerical solution of a parabolic problem is studied. The equation is discretized in time by means of a second order two step backward difference method with variable time step. A stability result is proved by the energy method under certain restrictions on the ratios of successive time steps. Error estimates are derived and applications are given to homogeneous equations with initial data of low regularity.

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1 Introduction.

In this paper we shall study the discretization in time of a parabolic problem by the two step backward difference method with variable step-size.

Let H and V be real Hilbert spaces with norms $\|\cdot\|$ and $|\cdot|$, respectively. We assume that V is continuously embedded in H, that is, $V \subset H$ with continuous inclusion $\|v\| \le \alpha |v|$, $v \in V$. We also denote the scalar product in H by (\cdot, \cdot) . Assume that a(t; u, v) is a V-elliptic bilinear form uniformly for $0 \le t \le T$. This means that for some c > 0, $a(t; v, v) \ge c|v|^2$, $0 \le t \le T$. We consider the problem of finding $u(t) \in V$ for $0 < t \le T$ such that

(1.1)
$$(u_t, v) + a(t; u, v) = (f, v), \quad v \in V, \ 0 < t \le T,$$
$$u(0) = u_0,$$

where u_0 is a given element in H, $f:[0,T] \to H$ and $u_t = du/dt$. Precise assumptions on the bilinear form will be stated in Section 2. Typically, the bilinear form will be defined by a second order elliptic partial differential operator or a discrete analogue of such an operator in which cases these assumptions will be satisfied.

In order to approximate the solution of this problem we introduce a sequence of time levels $\{t_n\}_{n=1}^N$, with $U_n \approx u(t_n)$, and let $k_n = t_n - t_{n-1}$ be the time step-size which in general will be variable. We shall further use the notation

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 $a_n(\cdot,\cdot)=a(t_n;\cdot,\cdot)$. If we replace the time derivative $u_t(t_n)$ in (1.1) by the difference quotient $\partial u(t_n)=k_n^{-1}(u(t_n)-u(t_{n-1}))$, we have the variable step backward Euler method

(1.2)
$$U_n \in V, \quad (\partial U_n, v) + a_n(U_n, v) = (f_n, v), \quad v \in V, \ t_1 \le t_n \le T, \\ U_0 = u_0,$$

where $f_n = f(t_n)$.

In this paper we study the discretization of (1.1) by means of a second order approximation to $u_t(t_n)$:

(1.3)
$$Du(t_n) = \left(1 + \frac{k_n}{k_{n-1}}\right) \frac{u(t_n) - u(t_{n-1})}{k_n} - \frac{k_n}{k_{n-1}} \frac{u(t_n) - u(t_{n-2})}{k_n + k_{n-1}}.$$

Since D is a two step backward difference operator we will need two starting values. As above we take $U_0=u_0$ and U_1 is obtained by taking one step of the backward Euler method (1.2) so that the method reads: Find $U_n \in V, n \geq 1$ such that

$$(DU_n, v) + a_n(U_n, v) = (f_n, v), \quad v \in V, \ t_2 \le t_n \le T,$$

$$(\partial U_1, v) + a_1(U_1, v) = (f_1, v), \quad v \in V,$$

$$U_0 = u_0.$$

Single step methods for parabolic problems have been considered in many papers, cf. e.g., Thomée [21] and the references therein. Multistep methods with constant step-size for parabolic problems have been studied using spectral techniques by, e.g., Zlámal [22], Crouzeix and Raviart [6], Crouzeix [4], Le Roux [13], Palencia [18], Gonzáles and Palencia [8], Savaré [20] and Bramble, Pasciak, Sammon and Thomée [2]. McLean and Thomée [15] contains an energy analysis of the two step method considered here, with constant time step, applied to an integro-differential equation.

We turn now to a brief description of some results for variable step-size. In [14] M.-N. Le Roux studies parabolic equations $u_t + Au = f(t)$ in an abstract Hilbert space setting. The discretization schemes are given by

$$\sum_{i=0}^q (lpha_{in}+k_{n+i}eta_{in}A)U_{n+i} = \sum_{i=0}^q k_{n+i}eta_{in}f_{n+i}, \quad n\geq 0.$$

It is assumed that the operator A is independent of t, and that for some a > 0,

$$((A - aI)u, u) \in S_{\theta} = \{z \colon |\arg(z)| \le \theta\}.$$

Under the assumption that the scheme is strongly $A(\theta)$ -stable, it is shown that if the step-sizes satisfy

(1.5)
$$\delta k \le k_j \le k, \qquad |\gamma_j - 1| \le M \frac{k_{j-1}}{1 + |\log k_{j-1}|},$$

then the following error estimate holds:

$$(1.6) \quad \|u(t_n) - U_n\| \le C'(1 + |\log k|) \Big(e^{(CM - \mu)t_n} \max_{0 \le s \le q - 1} \|u(t_s) - U_s\|$$

$$+ k^p \int_0^{t_n} e^{(CM - \mu)(t_n - t)} \|u^{(p+1)}(t)\| dt \Big).$$

We remark that the two step backward difference method with constant step-size is strongly A-stable (i.e. $A(\pi/2)$ -stable). The proof, using spectral techniques, is by a perturbation argument from the case of constant step-size. The result in [14] applied to our situation differs from our Theorem 4.2 in two respects. First, in our result the k_n^2 appears together with a local norm of u_{ttt} , whereas in (1.6) k^2 (recall $k_j \leq k$) stands in front of a norm of u_{ttt} over the whole time interval. Second, the condition (1.5) on γ_j is considerably more restrictive than our condition on γ_j ; in fact, γ_j tends to 1 as k_{max} tends to 0.

Grigorieff [10] derives error estimates for the method (1.4) applied to the Banach space equation, $u_t + Au = 0$, with A time-independent. It is assumed that the spectrum of the operator is included in the sector S_{θ} for some $\theta < \pi/3$ and

$$||(zI - A)^{-1}|| \le C/|z|, \quad z \notin S_{\theta},$$

For the case of nonsmooth data he shows that there are constants $C, \sigma > 0$ such that, if $\gamma_n \le \gamma < (1 + \sqrt{3})/2 \approx 1.37$, then

$$(1.8) ||U_N - u(t_N)|| \le C \left((t_N - t_1)^{-3} \sum_{n=1}^{N-1} k_n^3 + \frac{k_1^2}{t_N^2} + \exp(-\sigma t_N/k) \right) ||v||,$$

where $k = \max_{1 \le n \le N} k_n$. In the case of smooth data he proves, under the same assumption on the step-size ratio, that

$$\|U_N - u(t_N)\| \le C \bigg((t_N - t_1)^{-1} \sum_{n=1}^{N-1} k_n^3 + Nk^2 \exp(-\sigma t_N/k) + k_1^2 \bigg) \|A^2 v\|.$$

Note also that the bounds in (1.8), (1.9) are minimal, for a fixed number of steps, when the step-size is constant so that these results do not show any advantage of using variable time steps. We also remark that a stability result similar to (1.10) is shown under the above condition on γ_i .

Palencia and García-Archilla [19] also study the equation $u_t + Au = 0$ in a Banach space setting with time independent operator. The multistep method considered is of the form

$$U_n=\sum_{j=0}^{q-1}=r_j(\gamma_n,\ldots,\gamma_{n-q+2},k_nA)U_{n-1-j},\quad n\geq q,$$

where r_j are rational functions in $(\gamma_n, \ldots, \gamma_{n-q+2}, z)$ defined on the spectrum of A. Under the assumption that the spectrum of the operator is included in

the sector S_{θ} for some $\theta \in (0, \pi/2)$, and the resolvent condition (1.7) holds together with the assumption of strong $A(\theta)$ -stability of the method, a stability bound is shown under the condition that $\lambda < \gamma_j < \lambda^{-1}$, for some $\lambda \in (0,1)$, depending on the method. The stability bound however contains the factor $\exp(C\sum_{j=1}^{N}|\gamma_j-1|)$. In the case of the two-step backward difference method it turns out that $\lambda=0$ which means that no condition on the step-size ratios γ_j is required. However, for the stability factor to be moderate, the γ_j should be close to 1 such as, e.g., in (1.5).

For multistep methods with variable steps for ordinary differential equations see, e.g., [7, 16, 5, 9].

The paper is organized as follows. In Section 2 we state the assumptions on the bilinear form a and collect some preliminary material. In Section 3 we prove stability for (1.2) and an error estimate which follows from this. These results are well known, but are included for clarity of presentation. Our main result is Lemma 4.1 where we prove that for any sequence $\{t_n\}$ satisfying $\gamma_n = k_n/k_{n-1} \le \gamma < (2 + \sqrt{13})/3 \approx 1.86$ we have, for the solution of (1.4),

(1.10)
$$||U_N|| \le Ce^{C\Gamma_N} \Big(||u_0|| + \sum_{n=1}^N k_n ||f_n|| \Big), \quad t_N \le T,$$

where $\Gamma_N = \sum_{n=2}^{N-2} [\gamma_n - \gamma_{n+2}]_+$ with $[x]_+$ the positive part of x. Note in particular that Γ_N is bounded if γ_n is monotone. We remark that since our analysis relies on the use of the scalar product, it is not clear whether our result also extends to the Banach space case. Further, we do not know if the method of proof also can yield results for, e.g., the higher order backward difference methods.

In Section 5 we consider the case that the bilinear form is given by a second order elliptic differential operator, and prove an error estimate for a fully discrete version of (1.4).

Variable time steps are particularly useful when the solution changes rapidly in certain regions of time. In Section 6 we consider the homogeneous parabolic problem when the initial value has low regularity. Nonsmooth data error estimates that are optimal for positive time have been shown in Le Roux [13] in the case that the time step is constant and the bilinear form is time independent. However, such an estimate deteriorates as $t \to 0$. Here it is shown that if the sequence of time steps is graded near the origin, then we may have stability and an optimal order (in terms of the number of time steps) estimate uniformly down to t = 0.

2 Preliminaries.

In this section we shall make precise the assumptions needed on the bilinear form a in (1.1) and also state a discrete version of Gronwall's lemma.

Motivated by the case in which a is associated with a second order elliptic partial differential operator, we shall make the following assumptions (see [11], [12]): There are positive constants c, λ and C such that

(i)
$$a(t; v, v) \ge c|v|^2 - \lambda ||v||^2$$
, for $v \in V$, $0 < t < T$,

(ii)
$$|a(t; v, w)| + |a'(t; v, w)| \le C|v||w|$$
, for $v, w \in V$, $0 \le t \le T$,

(iii)
$$|a(t; v, w) - a(t; w, v)| \le C|v|||w||$$
, for $v, w \in V$, $0 \le t \le T$.

Here $a'(t;\cdot,\cdot)=(d/dt)a(t;\cdot,\cdot)$.

To put this into context, consider the initial-boundary value problem

where the operator A(t) is defined by

$$A(t)u = -\sum_{i,j} \frac{\partial}{\partial x_j} \left(b_{ij}(x,t) \frac{\partial u}{\partial x_i} \right) + \sum_i b_i(x,t) \frac{\partial u}{\partial x_i} + b(x,t)u.$$

Here Ω is a bounded domain in \mathbf{R}^d with smooth boundary Γ , the b's are smooth functions on $\bar{\Omega} \times [0, T]$ and $\{b_{ij}\}$ symmetric and uniformly positive definite. With this operator we associate the bilinear form

$$(2.2) a(t; u, v) = \sum_{i,j} \int_{\Omega} b_{ij} \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} dx + \sum_{i} \int_{\Omega} b_i \frac{\partial u}{\partial x_i} v dx + \int_{\Omega} buv dx.$$

We use the Sobolev space of order k on Ω with the usual norms $\|u\|_{H^k(\Omega)} = \|u\|_k$ and we write $\|u\|$ instead $\|u\|_0$ for the L_2 norm of u. In the particular form of (1.1) with a given by (2.2) we have $H = L_2(\Omega)$ with $(u, v) = \int_{\Omega} uv \, dx$ and $V = H_0^1(\Omega) = \{ u \in H^1(\Omega) : u|_{\partial\Omega} = 0 \}$ with norm $|\cdot| = \|\cdot\|_1$.

Let us verify that the conditions (i), (ii) and (iii) hold in this case. Since the coefficients in a are smooth it is immediate that (ii) holds. To prove (i) we use that $\{b_{ij}\}$ is uniformly positive definite so that $\sum_{ij} b_{ij}(x) \xi_i \xi_j \geq c |\xi|^2$ for some positive constant c, independent of $x \in \Omega$. We find

$$a(t; v, v) = \sum_{i,j} \int_{\Omega} b_{ij} \frac{\partial v}{\partial x_i} \frac{\partial v}{\partial x_j} dx + \sum_{i} \int_{\Omega} b_i \frac{\partial v}{\partial x_i} v dx + \int_{\Omega} bv^2 dx$$
$$\geq c \int_{\Omega} |\nabla v|^2 dx + \int_{\Omega} (b - \frac{1}{2} \sum_{i} \frac{\partial b_i}{\partial x_i}) v^2 dx, \quad \text{for } v \in H_0^1(\Omega).$$

Recalling that $\|\nabla v\|$ and $\|v\|_1$ are equivalent norms on $H_0^1(\Omega)$, (i) is thus satisfied with $\lambda \geq \sup_{\Omega} (\frac{1}{2} \sum_i \partial b_i / \partial x_i - b)$. Since $b_{ij} = b_{ji}$, we have

$$\begin{split} |a(t;v,w)-a(t;w,v)| &= \left|\sum_i \left(\int_\Omega b_i \frac{\partial v}{\partial x_i} w \, dx - \int_\Omega b_i \frac{\partial w}{\partial x_i} v \, dx\right)\right| \\ &= \left|\sum_i \int_\Omega (2b_i \frac{\partial v}{\partial x_i} + \frac{\partial b_i}{\partial x_i} v) w \, dx\right| \leq C \|v\|_1 \|w\|, \quad \text{for } v,w \in H^1_0(\Omega), \end{split}$$

which proves (iii).

We note that if we consider this bilinear form on the members of a family of finite dimensional subspaces $V_h \subset V$ depending on a parameter h, the assumptions are satisfied with constants independent of h. See Section 5 for details.

In subsequent sections we shall need the following discrete version of Gronwall's lemma.

LEMMA 2.1. Assume that the sequence $\{w_n\}$ satisfies

(2.3)
$$w_n \le a_n + \sum_{k=0}^{n-1} b_k w_k, \quad n = 0, 1, \dots,$$

where $\{a_n\}$ is nondecreasing and $b_n \geq 0$. Then we have the following bound:

$$w_n \le a_n \exp\left(\sum_{k=0}^{n-1} b_k\right).$$

3 The backward Euler method.

In this section we shall prove stability for the backward Euler method (1.2) and use this to derive an error estimate. These results will be models for our study of the second order backward difference method.

We shall begin by proving the uniqueness and existence of a discrete solution to (1.2) and for this purpose write it as

$$(U_n, v) + k_n a_n(U_n, v) = k_n(f_n, v) + (U_{n-1}, v).$$

Given $U_{n-1} \in H$ we need to show that there exists $U_n \in V$ such that the above equation holds. Since $||v|| \leq \alpha |v|$ for $v \in V$, the right hand side is a bounded linear functional on V. Let

$$b_n(u,v) = (u,v) + k_n a_n(u,v).$$

Clearly $|b_n(u,v)| \leq C|u||v|$, $u,v \in V$. The existence and uniqueness of U_n will follow from Lax-Milgram's lemma (cf. [3]) if we can prove that b_n is V-elliptic. But by (i) we have

$$b_n(v, v) \ge ||v||^2 + ck_n|v|^2 - \lambda k_n||v||^2 \ge ck_n|v|^2$$
, if $\lambda k_n \le 1$.

We now prove a stability result for the solution of (1.2).

LEMMA 3.1. Assume that $\{U_n\}$ satisfies (1.2). Then, if $0 < k_n \le k < 1/(2\lambda)$, we have

$$||U_N|| \le C \Big(||u_0|| + \sum_{n=1}^N k_n ||f_n|| \Big), \quad t_N \le T.$$

The constant C depends on k, λ and T.

PROOF. Choosing $v = U_n$ in (1.2) and multiplying by k_n we obtain, with $\Delta U_n = U_n - U_{n-1}$,

$$(\Delta U_n, U_n) + k_n a_n(U_n, U_n) = k_n(f_n, U_n).$$

The first term on the left can be written

$$(\Delta U_n, U_n) = \frac{1}{2} \Delta ||U_n||^2 + \frac{1}{2} ||\Delta U_n||^2.$$

Hence using (i) we obtain

$$\frac{1}{2}\Delta \|U_n\|^2 + \frac{1}{2}\|\Delta U_n\|^2 + ck_n|U_n|^2 \le \lambda k_n\|U_n\|^2 + k_n\|f_n\|\|U_n\|.$$

If we drop the second and third terms on the left hand side and sum from 1 to N, we find

$$\|(1-2\lambda k_N)\|U_N\|^2 \leq \|U_0\|^2 + 2\lambda \sum_{n=1}^{N-1} k_n\|U_n\|^2 + 2\sum_{n=1}^N k_n\|f_n\|\|U_n\|.$$

Let $||U_M|| = \max_{0 \le n \le N} ||U_n||$ and apply the above inequality with N replaced by M. We get, for sufficiently small step-sizes k_n

$$||U_M||^2 \le C \left(||U_0|| + \sum_{n=1}^{M-1} k_n ||U_n|| + \sum_{n=1}^M k_n ||f_n|| \right) ||U_M||.$$

We can thus cancel the factor $||U_M||$ on both sides. Since $||U_N|| \le ||U_M||$ and $M \le N$ we obtain

$$||U_N|| \le C \left(||U_0|| + \sum_{n=1}^N k_n ||f_n|| + \sum_{n=1}^{N-1} k_n ||U_n|| \right).$$

The proof is finished by applying Lemma 2.1.

Using Lemma 3.1 we can now prove an error estimate.

THEOREM 3.2. Assume that $\{U_n\}$ satisfy (1.2) and u is a sufficiently smooth solution of (1.1). If $0 < k_n \le k < 1/(2\lambda)$ we have

$$\|u(t_N) - U_N\| \le C \sum_{n=1}^N k_n \int_{t_{n-1}}^{t_n} \|u_{tt}(s)\| \ ds, \quad t_N \le T.$$

The constant C depends on k, λ and T.

PROOF. Let $e_n = u(t_n) - U_n$. By linearity, (1.2) and (1.1),

$$\begin{split} (\partial e_n, v) + a_n(e_n, v) &= (\partial u(t_n), v) + a_n(u(t_n), v) - (\partial U_n, v) - a_n(U_n, v) \\ &= (\partial u(t_n), v) + a_n(u(t_n), v) - (f_n, v) \\ &= (\partial u(t_n) - u_t(t_n), v) \equiv (\tau_n, v). \end{split}$$

Applying Lemma 3.1 to $\{e_n\}$, with $e_0 = u_0 - U_0 = 0$, we find

$$||e_N|| \le C \sum_{n=1}^N k_n ||\tau_n||,$$

and by Taylor's formula,

$$\tau_n = -\frac{1}{k_n} \int_{t_{n-1}}^{t_n} (s - t_{n-1}) u_{tt}(s) \, ds,$$

which completes the proof.

REMARK 3.1. If we use a constant time step the error estimate becomes

$$||u(t_N) - U_N|| \le Ck \int_0^{t_N} ||u_{tt}(s)|| ds,$$

so that the error is O(k) if u is smooth.

4 The second order method.

In this section we shall study the two step method (1.4) mentioned in the introduction. We shall prove a stability result and a corresponding error estimate.

The proof of the existence and uniqueness of a solution to (1.4) is analogous to that of the backward Euler method and will not be given. We begin instead with a stability result for (1.4). Let $\gamma_n = k_n/k_{n-1}$, $n \geq 2$, and set $\gamma^* = (2+\sqrt{13})/3 \approx 1.86$. We also introduce the quantity $\Gamma_N = \sum_{n=2}^{N-2} [\gamma_n - \gamma_{n+2}]_+$, where $[x]_+$ denotes the positive part of x, and note that

$$\Gamma_N = \begin{cases} 0, & \text{if } \{\gamma_n\} \text{ is increasing,} \\ \gamma_2 + \gamma_3 - \gamma_{N-1} - \gamma_N, & \text{if } \{\gamma_n\} \text{ is decreasing.} \end{cases}$$

Below we shall assume that $\{\gamma_n\}$ is bounded. Then Γ_N is bounded if the number of changes in monotonicity in $\{\gamma_n\}$ is bounded. We have the following

LEMMA 4.1. Assume that $\{U_n\}$ satisfies (1.4). Let $\gamma_n \leq \gamma < \gamma^*$. Then for sufficiently small step-sizes k_n (restricted by γ and the constants in (i)-(iii)) we have

$$||U_N|| \le C(||u_0|| + \sum_{n=1}^N k_n ||f_n||), \quad t_N \le T.$$

Here C depends on γ, T, Γ_N , and the constants in (i)-(iii).

PROOF. We shall begin by writing the difference operator in (1.3) in a more convenient form. Let $\Delta_k U_n = U_n - U_{n-k}$, k = 1, 2. With $\omega_n = \frac{1}{1+\gamma_n}$ and $\psi_n = (\frac{\gamma_n}{1+\gamma_n})^2$, we may write

$$DU_n = \frac{1}{\omega_n k_n} (\Delta_1 U_n - \psi_n \Delta_2 U_n).$$

We choose $v = 2\omega_n k_n (U_n + \delta \Delta_1 U_n)$ in (1.4), where $\delta > 0$ is a parameter to be chosen below, to obtain

(4.1)
$$2\omega_n k_n (DU_n, U_n + \delta \Delta_1 U_n) + 2\omega_n k_n a_n (U_n, U_n + \delta \Delta_1 U_n)$$
$$= 2\omega_n k_n (f_n, U_n + \delta \Delta_1 U_n), \quad n \ge 2.$$

We shall now make several technical manipulations with the terms of this equation to arrive finally at the inequality

$$(4.2) ||U_N|| \le C(||U_0|| + \sum_{n=1}^N k_n(||f_n|| + ||U_n||)) + C \sum_{n=2}^{N-2} [\gamma_n - \gamma_{n+2}]_+ ||U_n||.$$

From this the proof is completed by an application of the discrete Gronwall lemma.

Expanding the first term on the left side of (4.1) we have

$$2\omega_{n}k_{n}(DU_{n}, U_{n} + \delta\Delta_{1}U_{n}) = 2(\Delta_{1}U_{n}, U_{n}) - 2\psi_{n}(\Delta_{2}U_{n}, U_{n}) + 2\delta\|\Delta_{1}U_{n}\|^{2} - 2\delta\psi_{n}(\Delta_{2}U_{n}, \Delta_{1}U_{n})$$

$$= I_{n}^{1} + I_{n}^{2} + I_{n}^{3} + I_{n}^{4}.$$

With the use of the identity

$$2(\Delta_k U_n, U_n) = \Delta_k ||U_n||^2 + ||\Delta_k U_n||^2,$$

we find

$$I_n^1 = \Delta_1 ||U_n||^2 + ||\Delta_1 U_n||^2,$$

$$I_n^2 = -\psi_n \Delta_2 ||U_n||^2 - \psi_n ||\Delta_2 U_n||^2.$$

Since $\Delta_2 U_n = \Delta_1 U_n + \Delta_1 U_{n-1}$ and hence

$$\|\Delta_2 U_n\|^2 \le 2\|\Delta_1 U_n\|^2 + 2\|\Delta_1 U_{n-1}\|^2,$$

we get

$$I_n^2 \ge -\psi_n \Delta_2 \|U_n\|^2 - 2\psi_n \|\Delta_1 U_n\|^2 - 2\psi_n \|\Delta_1 U_{n-1}\|^2.$$

In the same way, since

$$2(\Delta_1 U_n, \Delta_1 U_{n-1}) \le \|\Delta_1 U_n\|^2 + \|\Delta_1 U_{n-1}\|^2,$$

we find

$$I_n^4 = -2\delta\psi_n \|\Delta_1 U_n\|^2 - 2\delta\psi_n(\Delta_1 U_n, \Delta_1 U_{n-1})$$

$$\geq -3\delta\psi_n \|\Delta_1 U_n\|^2 - \delta\psi_n \|\Delta_1 U_{n-1}\|^2.$$

We therefore obtain from (4.3)

$$(4.4) \quad 2\omega_n k_n(DU_n, U_n + \delta \Delta_1 U_n) \\ \geq \Delta_1 \|U_n\|^2 - \psi_n \Delta_2 \|U_n\|^2 + A_n \|\Delta_1 U_n\|^2 - B_n \|\Delta_1 U_{n-1}\|^2,$$

where

(4.5)
$$A_n = 1 + 2\delta - (2 + 3\delta)\psi_n, \qquad B_n = (2 + \delta)\psi_n.$$

We proceed with the second term on the left in (4.1) and write, without the factor $\omega_n k_n$,

$$2a_n(U_n, U_n + \delta \Delta_1 U_n) = 2a_n(U_n, U_n) + 2\delta a_n(U_n, \Delta_1 U_n).$$

We consider the second term on the right without δ . The following identity holds.

$$\begin{aligned} 2a_n(U_n, \Delta_1 U_n) &= a_n((U_n + U_{n-1}) + (U_n - U_{n-1}), \Delta_1 U_n) \\ &= a_n(U_n + U_{n-1}, U_n - U_{n-1}) + a_n(\Delta_1 U_n, \Delta_1 U_n) \\ &= \Delta_1(a_n(U_n, U_n)) + (a_{n-1}(U_{n-1}, U_{n-1}) - a_n(U_{n-1}, U_{n-1})) \\ &+ (a_n(U_{n-1}, U_n) - a_n(U_n, U_{n-1})) + a_n(\Delta_1 U_n, \Delta_1 U_n), \end{aligned}$$

where we added and subtracted the term $a_{n-1}(U_{n-1}, U_{n-1})$ in the last step. Estimating the last three terms, using the mean value theorem and (i)–(iii), we now obtain

where

$$\bar{A}_n = (2+\delta)\omega_n, \qquad \bar{B}_n = \delta\omega_n\gamma_n.$$

From (4.1), (4.4) and (4.6) we thus obtain, for $n \ge 2$,

$$(4.7) \qquad (\Delta_{1} \|U_{n}\|^{2} - \psi_{n} \Delta_{2} \|U_{n}\|^{2}) + (A_{n} \|\Delta_{1} U_{n}\|^{2} - B_{n} \|\Delta_{1} U_{n-1}\|^{2}) + (\bar{A}_{n} k_{n} a_{n} (U_{n}, U_{n}) - \bar{B}_{n} k_{n-1} a_{n-1} (U_{n-1}, U_{n-1})) \leq C k_{n}^{2} |U_{n-1}|^{2} + C k_{n} |U_{n-1}| \|U_{n}\| + C k_{n} \|\Delta_{1} U_{n}\|^{2} + C k_{n} \|f_{n}\| (\|U_{n}\| + \|U_{n-1}\|),$$

or, with obvious notation,

$$I_n + II_n + III_n \le IV_n + V_n + VI_n + VII_n$$
.

We now sum this inequality from n=2 to N. Beginning with the left hand side we have

$$\sum_{n=2}^{N} I_n = \|U_N\|^2 - \|U_1\|^2 - \sum_{n=2}^{N} \psi_n \|U_n\|^2 + \sum_{n=0}^{N-2} \psi_{n+2} \|U_n\|^2$$

$$= (1 - \psi_N) \|U_N\|^2 - \psi_{N-1} \|U_{N-1}\|^2 - (1 - \psi_3) \|U_1\|^2 + \psi_2 \|U_0\|^2$$

$$- \sum_{n=2}^{N-2} (\psi_n - \psi_{n+2}) \|U_n\|^2.$$

Hence

(4.8)
$$\sum_{n=2}^{N} I_n \ge (1 - \psi_N) \|U_N\|^2 - \psi_{N-1} \|U_{N-1}\|^2 - \|U_1\|^2 - \sum_{n=2}^{N-2} [\psi_n - \psi_{n+2}]_+ \|U_n\|^2.$$

Moreover

$$(4.9) \qquad \sum_{n=2}^{N} II_n = \sum_{n=2}^{N-1} (A_n - B_{n+1}) \|\Delta_1 U_n\|^2 + A_N \|\Delta_1 U_N\|^2 - B_2 \|\Delta_1 U_1\|^2,$$

and

$$(4.10) \qquad \sum_{n=2}^{N} III_{n} = \sum_{n=2}^{N-1} (\bar{A}_{n} - \bar{B}_{n+1}) k_{n} a_{n}(U_{n}, U_{n}) \\ + \bar{A}_{N} k_{N} a_{N}(U_{N}, U_{N}) - \bar{B}_{2} k_{1} a_{1}(U_{1}, U_{1}).$$

We shall now show that if $\gamma_n \leq \gamma$ for all n, then $A_n - B_{n+1} \geq c_{\gamma}$ and $\bar{A}_n - \bar{B}_{n+1} \geq c_{\gamma}$ for some $c_{\gamma} > 0$. Assume first only that $\gamma_n \leq \gamma'$ for all n. Since A_n is a decreasing function of γ_n , and B_n is an increasing function of γ_n , we then have

$$A_n - B_{n+1} \ge 1 + 2\delta - (2 + 3\delta)(\frac{\gamma'}{1 + \gamma'})^2 - (2 + \delta)(\frac{\gamma'}{1 + \gamma'})^2$$
$$= 1 + 2\delta - 4(1 + \delta)(\frac{\gamma'}{1 + \gamma'})^2$$

and, for similar reasons,

$$\bar{A}_n - \bar{B}_{n+1} \ge \frac{2+\delta}{1+\gamma'} - \frac{\delta\gamma'}{1+\gamma'}.$$

Hence $A_n - B_{n+1} \ge 0$ if

$$\left(\frac{\gamma'}{1+\gamma'}\right)^2 \le \frac{1+2\delta}{4(1+\delta)},$$

and $\bar{A}_n - \bar{B}_{n+1} \ge 0$ if

$$(4.12) \gamma' \le 1 + \frac{2}{\delta}.$$

Replacing the inequalities by equalities gives $\gamma' = \gamma^* \equiv (2 + \sqrt{13})/3$, $\delta = (1 + \sqrt{13})/2$. Fixing δ in this way we also see that if $\gamma_n \leq \gamma < \gamma^*$ we have $A_n - B_{n+1} \geq c_{\gamma}$, $\bar{A}_n - \bar{B}_{n+1} \geq c_{\gamma}$.

With these choices we obtain from (4.9) and (4.10)

(4.13)
$$\sum_{n=2}^{N} II_n \ge -C(\|U_0\|^2 + \|U_1\|^2),$$

and, using (i),

(4.14)
$$\sum_{n=2}^{N} III_n \ge cc_{\gamma} \sum_{n=2}^{N-1} k_n |U_n|^2 - C \sum_{n=2}^{N} k_n ||U_n||^2 - Ck_1 |U_1|^2.$$

Using the inequality $2ab \le \epsilon a^2 + \epsilon^{-1}b^2$, with a suitable $\epsilon > 0$, it is clear that for sufficiently small step-sizes k_n , we have

(4.15)
$$\sum_{n=2}^{N} (IV_n + V_n) \le \frac{1}{2} cc_{\gamma} \sum_{n=1}^{N-1} k_n |U_n|^2 + C \sum_{n=2}^{N} k_n ||U_n||^2.$$

From (4.7), (4.8) and (4.13)–(4.15) together with obvious estimates for VI, VII we now obtain

$$(1 - \psi_{N}) \|U_{N}\|^{2} \leq \psi_{N-1} \|U_{N-1}\|^{2} + C(\|U_{0}\|^{2} + \|U_{1}\|^{2} + k_{1}|U_{1}|^{2})$$

$$+ C \sum_{n=2}^{N} k_{n} \|f_{n}\| (\|U_{n}\| + \|U_{n-1}\|) + C \sum_{n=1}^{N} k_{n} \|U_{n}\|^{2}$$

$$+ \sum_{n=2}^{N-2} [\psi_{n} - \psi_{n+2}]_{+} \|U_{n}\|^{2}.$$

If we put $v = U_1$ in the equation for U_1 in (1.4) and multiply by k_1 we easily get, using (i),

$$||U_1||^2 + k_1|U_1|^2 \le C(||U_0||^2 + k_1||f_1||||U_1|| + k_1||U_1||^2).$$

Since also

$$\frac{1}{1-\psi_N} \le C, \qquad \frac{\psi_{N-1}}{1-\psi_N} \le \bar{c} < 1,$$

and further $[\psi_n - \psi_{n+2}]_+ \leq C[\gamma_n - \gamma_{n+2}]_+$, we thus obtain from (4.16)

$$||U_N||^2 \leq \bar{c}||U_{N-1}||^2 + C\left(||U_0||^2 + \sum_{n=1}^N k_n||f_n||(||U_n|| + ||U_{n-1}||)\right)$$
$$+ C\sum_{n=2}^{N-2} [\gamma_n - \gamma_{n+2}]_+ ||U_n||^2 + C\sum_{n=1}^N k_n ||U_n||^2.$$

We now let M be such that $0 \le M \le N$ and $||U_M|| = \max_{0 \le n \le N} ||U_n||$, and consider the above inequality with N replaced by M. This allows us to cancel a

factor $||U_M||$ so that

$$\|U_M\| \le C(\|U_0\| + \sum_{n=1}^M k_n \|f_n\|) + C \sum_{n=2}^{M-2} [\gamma_n - \gamma_{n+2}]_+ \|U_n\| + C \sum_{n=1}^M k_n \|U_n\|.$$

Since $||U_N|| \le ||U_M||$ and $M \le N$ we have the same inequality with M replaced by N and this finishes the proof of (4.2) and thus of the lemma.

We now prove an error estimate analogous to Theorem 3.2.

THEOREM 4.2. Let u be a sufficiently smooth solution of the continuous problem (1.1) and $\{U_n\}$ the solution of (1.4). For sequences $\{t_n\}_1^N$ satisfying $0 < \underline{\gamma} \leq \gamma_n \leq \overline{\gamma} < (2 + \sqrt{13})/3$, and sufficiently small step-sizes k_n (restricted by $\overline{\gamma}$ and the constants in (i)-(iii)) we have

$$\|u(t_N) - U_N\| \le C \left(k_1 \int_0^{t_1} \|u_{tt}(s)\| ds + \sum_{n=1}^N k_n^2 \int_{t_{n-1}}^{t_n} \|u_{ttt}(s)\| ds\right), \quad t_N \le T,$$

where C depends on $\underline{\gamma}, \overline{\gamma}, T, \Gamma_N$, and the constants in (i)-(iii).

PROOF. Let $e_n = u(t_n) - U_n$. Then we have

$$(De_n, v) + a_n(e_n, v) = (Du(t_n) - u_t(t_n), v) \equiv (\tau_n, v), \quad \text{for } n \ge 2,$$

 $(\partial e_1, v) + a_1(e_1, v) = (\partial u(t_1) - u_t(t_1), v) \equiv (\tau_1, v).$

By Lemma 4.1, since $e_0 = 0$,

$$||e_N|| \leq C \sum_{n=1}^N k_n ||\tau_n||.$$

Using Taylor's formula we find, for $n \geq 2$,

$$k_n\tau_n = \frac{(1+\gamma_n)}{2} \int_{t_{n-1}}^{t_n} (s-t_{n-1})^2 u_{ttt}(s) \, ds - \frac{\gamma_n^2}{2(1+\gamma_n)} \int_{t_{n-2}}^{t_n} (s-t_{n-2})^2 u_{ttt}(s) \, ds,$$

and for τ_1 we have

$$k_1 au_1 = -\int_0^{t_1} su_{tt}(s)\,ds.$$

Thus taking norms and using obvious estimates finishes the proof.

REMARK 4.1. If we use constant steps the theorem can be formulated as

$$\left\|u(t_N)-U_N
ight\|\leq C\left(k\int_0^{t_1}\left\|u_{tt}
ight\|ds+k^2\int_0^{t_N}\left\|u_{ttt}
ight\|ds
ight).$$

Note that the right hand side is $O(k^2)$ if u is smooth.

5 The finite element method.

So far we have only considered the discretization in time of the abstract equation (1.1). We shall now briefly state and prove an error estimate for a totally discrete scheme for the parabolic problem (2.1) in Section 2.

We consider the problem to find $u(\cdot,t) \in H_0^1(\Omega)$ such that

(5.1)
$$(u_t, v) + a(t; u, v) = (f, v), \quad v \in H_0^1(\Omega), \ 0 < t \le T,$$

$$u(0) = u_0,$$

where the bilinear form a is given by (2.2). We now choose a family of finite dimensional subspaces $V_h \subset H^1_0(\Omega)$ with the approximation property

$$\inf_{\chi \in V_h} (\|v - \chi\| + h\|v - \chi\|_1) \le Ch^s \|v\|_s, \quad v \in H^s(\Omega) \cap H^1_0(\Omega), \ 1 \le s \le r.$$

The semi-discrete problem for (5.1) then becomes to find $u_h(\cdot,t) \in V_h$ such that

(5.2)
$$(u_{h,t},\chi) + a(t;u_h,\chi) = (f,\chi), \qquad \chi \in V_h, \ 0 < t \le T,$$

$$u_h(0) = u_{0,h},$$

where $u_{0,h}$ is an approximation of u_0 in V_h . We can now apply the time discretization procedure discussed in Section 4 to arrive at a totally discrete scheme for (5.1): Find $U_n \in V_h$, $n \ge 1$ such that

(5.3)
$$(DU_{n}, \chi) + a_{n}(U_{n}, \chi) = (f_{n}, \chi), \quad \chi \in V_{h}, \ t_{2} \leq t_{n} \leq T,$$

$$(\partial U_{1}, \chi) + a_{1}(U_{1}, \chi) = (f_{1}, \chi), \qquad \chi \in V_{h},$$

$$U_{0} = u_{0,h}.$$

We define a new bilinear form \tilde{a} by

$$\tilde{a}(t; u, v) = a(t; u, v) + \lambda(u, v).$$

By (i) this form becomes $H^1_0(\Omega)$ -elliptic. Hence, by Lax–Milgram's lemma, we can introduce $R_h(t):H^1_0(\Omega)\to V_h$ defined by

$$\tilde{a}(t; R_h(t)u, \chi) = \tilde{a}(t; u, \chi), \qquad \chi \in V_h.$$

 $(R_h \text{ is often called the elliptic projection or Ritz projection in the case that } a \text{ is symmetric.})$ We will need to know the following facts about R_h , which we state without proof (see [11]).

Lemma 5.1. Let $\rho = u - R_h u$. Then

$$\|\rho\| \le Ch^r \|u\|_r,$$

 $\|\rho_t\| \le Ch^r (\|u\|_r + \|u_t\|_r).$

We shall demonstrate the following theorem.

Theorem 5.2. Let u be a sufficiently smooth solution of (5.1) and $\{U_n\}$ the solution of the fully discrete problem (5.3). Under the same assumptions as in Theorem 4.2 we have

$$\|u(t_N) - U_N\| \le C \Big(\|u_0 - u_{0,h}\| + h^r \|u_0\|_r + h^r \int_0^{t_N} \|u_t\|_r ds + k_1 \int_0^{t_1} \|u_{tt}\| ds + \sum_{n=1}^N k_n^2 \int_{t_{n-1}}^{t_n} \|u_{ttt}\| ds \Big), \quad t_N \le T.$$

PROOF. With R_n being shorthand notation for $R_h(t_n)$, we write

$$e_n = u_n - U_n = (u_n - R_n u_n) + (R_n u_n - U_n) = \rho_n + \theta_n.$$

Making use of Lemma 5.1 we find

$$\|
ho_N\| \leq Ch^r \|u_N\|_r \leq Ch^r (\|u_0\|_r + \int_0^{t_N} \|u_t\|_r \, ds).$$

To estimate $\|\theta_N\|$ we shall use Lemma 4.1. By the definition of R_n we have $a_n(\rho_n, \chi) + \lambda(\rho_n, \chi) = 0$, so that for $n \geq 2$

$$(D\theta_{n}, \chi) + a_{n}(\theta_{n}, \chi) = (DR_{n}u_{n} - u_{t}(t_{n}), \chi) + a_{n}(R_{n}u_{n} - u_{n}, \chi)$$

$$= (DR_{n}u_{n} - Du_{n} + Du_{n} - u_{t}(t_{n}), \chi) - a_{n}(\rho_{n}, \chi)$$

$$= (-D\rho_{n}, \chi) + (\tau_{n}, \chi) + \lambda(\rho_{n}, \chi),$$

where $\tau_n = Du_n - u_t(t_n)$. For n = 1 we find similarly

$$(\partial \theta_1, \chi) + a_1(\theta_1, \chi) = -(\partial \rho_1, \chi) + (\tau_1, \chi) + \lambda(\rho_1, \chi),$$

where $\tau_1 = \partial u(t_1) - u_t(t_1)$. Lemma 4.1 now gives

$$\|\theta_N\| \le C \left(\|\theta_0\| + \left(k_1 \|\partial \rho_1\| + \sum_{n=2}^N k_n \|D\rho_n\| \right) + \sum_{n=1}^N k_n \|\tau_n\| + \sum_{n=1}^N k_n \|\rho_n\| \right)$$

$$\equiv C \left(\|\theta_0\| + J_N^1 + J_N^2 + J_N^3 \right).$$

Since ∂ and D are approximations of the time-derivative, we find by invoking Lemma 5.1

$$egin{aligned} J_N^1 & \leq C \int_0^{t_N} \|
ho_t\| \, ds \leq C h^r \int_0^{t_N} (\|u\|_r + \|u_t\|_r) \, ds \ & \leq C h^r (\|u_0\|_r + \int_0^{t_N} \|u_t\|_r \, ds). \end{aligned}$$

The term J_N^2 is estimated exactly as in Theorem 4.2 and using Lemma 5.1 again we see that

$$\|J_N^3 \le Ch^r \sum_{n=1}^N k_n \|u_n\|_r \le Ch^r (\|u_0\|_r + \int_0^{t_N} \|u_t\|_r \, ds),$$

and $\|\theta_0\|$ is bounded as follows:

$$\|\theta_0\| \le \|R_0u_0 - u_0\| + \|u_0 - u_{0,h}\| \le Ch^r \|u_0\|_r + \|u_0 - u_{0,h}\|.$$

Together these estimates complete the proof.

6 Nonsmooth data.

In this section we shall analyze the error estimates in a particular case in which the solution is nonsmooth near t=0 and discuss how one can then choose the time steps.

Consider the homogeneous problem

(6.1)
$$u_t + Au = 0, \quad 0 < t \le T, \qquad u(0) = u_0,$$

where A is an unbounded operator on a H, selfadjoint, positive definite and independent of time. The weak form of (6.1) is an equation of type (1.1) with $f \equiv 0$. The following regularity result is known and easily shown by spectral representation of the solution:

(6.2)
$$||u(t)||_s \le Ct^{-(s-q)/2} ||u_0||_q, \quad 0 \le q \le s,$$

where $||u||_s = ||A^{s/2}u||$. We remark that, when $A = -\Delta$, the Laplacian, then $||u||_s$ is equivalent to the Sobolev norm of u of order s provided u satisfies certain boundary conditions (cf. [21]). Combining (6.1) and (6.2) gives

(6.3)
$$\left\| \frac{\partial^k u}{\partial t^k} \right\| = \|A^k u\| = \|u\|_{2k} \le Ct^{-k+q/2} \|u_0\|_q, \quad 0 \le q \le 2k.$$

Below we shall assume that we have low initial regularity, that is, we assume that $\|u_0\|_q < \infty$ only for small q > 0. Applying (6.3) to the error estimate for the backward Euler method in Theorem 3.2 we run into a problem if q is small because we need to evaluate the integral $\int_0^{t_1} \|u_{tt}(s)\| ds$, and the integrand then is of the order $O(t^{-2+q/2})$ which is nonintegrable at zero. However, we recall from the proof of Theorem 3.2 that this integral comes from estimating $k_1\|\tau_1\|$. Without this estimate we get

$$\|k_1\| au_1\| = \left\|\int_0^{t_1} su_{tt}\,ds
ight\| \leq C\int_0^{t_1} s^{-1+q/2}\,ds \leq Ct_1^{q/2}.$$

Hence, for the backward Euler method we find

$$\|u(t_n) - U_n\| \le C \left(t_1^{q/2} + \sum_{j=2}^n k_j \int_{t_{j-1}}^{t_j} t^{-2+q/2} dt\right) \le C \left(t_1^{q/2} + \sum_{j=1}^{n-1} k_j^2 t_j^{-2+q/2}\right).$$

Suppose that for a given initial value we want to compute the approximate solution in the interval (0,T] with N time steps. Let us choose the time levels t_n

according to $t_n = T(n/N)^{\beta}$, $\beta \ge 1$. Here $\beta = 1$ corresponds to constant step-size. Then $k_n = t_n - t_{n-1} \le T\beta N^{-1} (n/N)^{\beta-1}$. We thus have, for $0 \le n \le N$,

$$\|u(t_n) - U_n\| \le C \left(N^{-\beta q/2} + N^{-1} \sum_{j=1}^{N-1} \frac{1}{N} \left(\frac{j}{N}\right)^{-2+\beta q/2}\right)$$
 $\le \begin{cases} CN^{-\beta q/2}, & \beta q < 2, \\ CN^{-1} \log N, & \beta q = 2, \\ CN^{-1}, & \beta q > 2. \end{cases}$

We see that the error bound is of order $O(N^{-1})$ if we choose $\beta > 2/q$. We note that if q > 2 it will suffice to use constant steps in order to have an optimal order error estimate. Note also that our above estimate holds uniformly on $0 \le t_n \le T$. We remark that if we are satisfied with an estimate for $0 < \delta \le t_n \le T$, we can use the nonsmooth data error estimate with a constant time step (cf. [12], [13])

$$||u(t_n) - U_n|| \le C \frac{k}{t_n} ||v|| = Cn^{-1}, \quad t_n = nk.$$

We shall now consider the two step method. To be able to use the error estimate in Theorem 4.2 we must show that the assumptions on γ_n made there are fulfilled. For a fixed $\beta \geq 1$ we have

$$\gamma_n = \frac{k_n}{k_{n-1}} = \frac{n^{\beta} - (n-1)^{\beta}}{(n-1)^{\beta} - (n-2)^{\beta}} \to 1, \text{ as } n \to \infty,$$

which means that $\gamma_n \leq \gamma < (2+\sqrt{13})/3$ for $n \geq \bar{n}$, with \bar{n} independent of N. Although it is required in Lemma 4.1 that this holds for all $n \geq 2$, the above condition is in fact sufficient for stability and thus for the error estimate to hold. This is clear since by Lemma 4.1 we have stability starting from $n = \bar{n}$, and by choosing $v = U_n$ in (1.4), it is easy to see that the norm of the first \bar{n} approximations computed are also bounded as in Lemma 4.1, with the stability constant independent of N. We observe also that $\Gamma_N = \sum_{n=2}^{N-2} [\gamma_n - \gamma_{n+2}]_+$ is bounded because $\{\gamma_n\}$ is decreasing. Hence, we may apply Theorem 4.2 to obtain, with C independent of N,

$$||u(t_n) - U_n|| \leq C \left(t_1^{q/2} + t_2^{q/2} + \sum_{j=2}^n k_j^2 \int_{t_{j-1}}^{t_j} t^{-3+q/2} dt \right)$$

$$\leq C \left(t_1^{q/2} + t_2^{q/2} + \sum_{j=1}^{n-1} k_j^3 t_j^{-3+q/2} \right),$$

or with our special choice of time steps, for $0 \le n \le N$,

$$egin{array}{lll} \|u(t_n) - U_n\| & \leq & Cigg(N^{-eta = q/2} + N^{-2} \sum_{j=1}^{N-1} rac{1}{N} (rac{j}{N})^{-3 + eta q/2}igg) \ & \leq & igg\{ egin{array}{lll} CN^{-eta q/2}, & eta q < 4, \ CN^{-2} \log N, & eta q = 4, \ CN^{-2}, & eta q > 4. \end{array}
ight. \end{array}$$

Here we have a uniform $O(N^{-2})$ error bound if we take $\beta > 4/q$. The nonsmooth data error estimate for the two step method in case of constant step-size reads (cf. [13])

$$||u(t_n) - U_n|| \le C \frac{k^2}{t_n^2} ||v|| = Cn^{-2}, \quad t_n = nk.$$

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