

A HIGH ORDER PARALLEL METHOD FOR TIME DISCRETIZATION OF PARABOLIC TYPE EQUATIONS BASED ON LAPLACE TRANSFORMATION AND QUADRATURE

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Abstract. We consider the discretization in time of a parabolic equation, using a representation of the solution as an integral along a smooth curve in the complex left half plane. The integral is then evaluated to high accuracy by a quadrature rule. This reduces the problem to a finite set of elliptic equations, which may be solved in parallel. The procedure is combined with finite element discretization in the spatial variables. The method is also applied to some parabolic type evolution equations with memory.

Key Words. Parabolic type, Laplace transform, parallel method and high order quadrature.

1. Introduction

In this paper we present a survey of recent work on an approach to time discretization of some equations of parabolic type based on Laplace transformation and quadrature. Following work by Sheen, Sloan, and Thomée [7], [8], we first introduce our method for an abstract parabolic equation, and then apply the method to the heat equation and its spatial discretization by finite elements, which produces a fully discrete scheme. We then describe work in McLean and Thomée [3] concerning application of the method to an evolution equation with a memory term of fractional integral type, and finally preview ongoing work by McLean, Sloan, and Thomée [5], where the method is used for a parabolic integro-differential equation with a memory term of convolution type. Our presentation here will be sketchy, and we refer to the original papers for details.

We consider the approximate solution of a parabolic problem of the form

$$(1.1) \quad u_t + Au = f(t), \text{ for } t > 0, \quad \text{with } u(0) = u_0,$$

where u_0 and $f(t)$ are given. Having in mind the case that A is a second order elliptic differential operator with Dirichlet boundary conditions in a spatial domain Ω , we consider the problem in the framework of a Banach space \mathbb{B} . We assume that A is a closed operator in \mathbb{B} such that $-A$ generates a bounded analytic semigroup $E(t) = e^{-At}$. More precisely, we assume that the spectrum $\sigma(A)$ of A is contained in a sector of the right half plane, and that that the resolvent $(zI + A)^{-1}$ of $-A$ satisfies

$$(1.2) \quad \|(zI + A)^{-1}\| \leq M(1 + |z|)^{-1}, \text{ for } z \in \Sigma_\delta = \{z : |\arg z| < \delta\},$$

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with $\delta \in (\pi/2, \pi)$ and M independent of z . When A is symmetric and positive definite in a Hilbert space, δ can be chosen as an arbitrary number in $(\pi/2, \pi)$, and $M = O((\pi - \delta)^{-1})$. Here we shall consider δ and M fixed. For the elliptic differential operator case and $\mathbb{B} = C_0(\bar{\Omega})$, (1.2) was shown in Stewart [9].

The first step in our approach is to represent the solution $u(t)$ as a contour integral of the form

$$(1.3) \quad u(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{zt} w(z) dz,$$

where $w(z)$ is the Laplace transform of u ,

$$(1.4) \quad w(z) = \hat{u}(z) = \int_0^{\infty} e^{-zt} u(t) dt, \text{ for } \operatorname{Re} z \geq x_0,$$

with $x_0 \in \mathbb{R}$, and where initially Γ is an appropriately chosen line Γ_0 in the complex plane parallel to the imaginary axis. In (1.3), $u(t)$ is then just the inverse Laplace transform of $w(z)$. For our purposes, however, assuming that $w(z)$ may be continued analytically in an appropriate way, we shall want to take for Γ a deformed contour in the set Σ_{δ} in (1.2), which behaves asymptotically as a pair of straight lines in the left half plane, with slopes $\pm\sigma \neq 0$, say, so that the factor e^{zt} decays exponentially as $|z| \rightarrow \infty$ on Γ .

For concreteness, we take

$$(1.5) \quad \Gamma = \{z : z = \varphi(y) + i\sigma y, y \in \mathbb{R}\} \subset \Sigma_{\delta}, \quad \varphi(y) = \gamma - \sqrt{y^2 + \nu^2},$$

for suitable positive parameters γ, ν , and σ . The curve Γ is then the left-hand branch of a hyperbola, which crosses the real axis at $\alpha = \varphi(0) = \gamma - \nu$. Some of the constants below will depend on the parameters of Γ .

Taking Laplace transforms in (1.1), we obtain the transformed equation

$$(1.6) \quad (zI + A)w(z) = u_0 + \hat{f}(z),$$

and thus $w(z)$ may be written formally as

$$(1.7) \quad w(z) = (zI + A)^{-1}(u_0 + \hat{f}(z)), \text{ for } z \in \Gamma.$$

We assume that the Laplace transform $\hat{f}(z)$ has an analytic continuation from Γ_0 to our deformed contour Γ , so that all singularities of $\hat{f}(z)$ lie to the left of Γ . The same property will then apply to $w(z)$ in (1.7).

Using our assumptions on A, Γ , and $\hat{f}(z)$, one may use this representation of $u(t)$ to show the following stability and smoothness estimate.

Theorem 1.1. *We have for the solution $u(t)$ of (1.1), for $j, k \geq 0$,*

$$\|A^j u^{(k)}(t)\| \leq Ct^{-k} e^{\alpha t} (\|u_0\| + \|\hat{f}\|_{\Gamma}), \text{ for } t > 0, \quad \text{where } \|\hat{f}\|_{\Gamma} = \sup_{z \in \Gamma} |\hat{f}(z)|.$$

In terms of the analytic semigroup $E(t)$ we have for the solution of (1.1)

$$u(t) = E(t)u_0 + \int_0^t E(t-s)f(s) ds, \text{ for } t \geq 0.$$

Since $\|E(t)\| \leq C_0$ for $t \geq 0$ and for some $C_0 \geq 1$, one has the stability property

$$(1.8) \quad \|u(t)\| \leq C_0(\|u_0\| + \int_0^t \|f(s)\| ds), \text{ for } t \geq 0.$$

With the deformed contour represented as in (1.5), the integral (1.3) can be written as an infinite integral with respect to the real variable y ,

$$(1.9) \quad u(t) = \int_{-\infty}^{\infty} v(t, y) dy, \quad \text{with } v(t, y) = \frac{1}{2\pi i} e^{z(y)t} w(z(y)) z'(y),$$

where $z(y) = \varphi(y) + i\sigma y$. Because of the assumed behavior of $\operatorname{Re} z(y) = \varphi(y)$, the integrand in this integral decays exponentially for large $|y|$ when $t > 0$.

Our approximate solution will now be defined by approximating the integral by means of a quadrature scheme,

$$(1.10) \quad U_N(t) = \sum_{j=-N+1}^{N-1} \omega_j v(t, y_j) = \sum_{j=-N+1}^{N-1} \tilde{\omega}_j e^{z_j t} w(z_j),$$

where $z_j = z(y_j)$, $\tilde{\omega}_j = z'(y_j)\omega_j/(2\pi i)$, with certain quadrature points $y_j \in R$ and nonnegative weights ω_j . In Section 2 we shall consider in more detail one particular scheme, obtained by mapping the infinite integral to $(-1, 1)$, and then applying the trapezoidal rule to the resulting finite integral.

By (1.6), the values of the Laplace transform $w(z)$ needed in (1.10) satisfy

$$(1.11) \quad (z_j I + A)w(z_j) = u_0 + \hat{f}(z_j), \quad j = -N+1, \dots, N-1.$$

A central feature of our method is that the $2N-1$ values $w(z_j) \in \mathbb{B}$ in (1.10) can be computed in parallel, since (1.11) can be solved independently for each value of j . We remark that in the special case that $w(\bar{z}) = \overline{w(z)}$, such as, e.g., when \mathbb{B} is a Hilbert space and A positive definite, and if we choose the function $\varphi(y)$ to be even, then $\tilde{\mu}_{-j} = \overline{\tilde{\mu}_j}$ and $z_{-j} = \bar{z}_j$, so that (1.10) may be written as

$$U_N(t) = \frac{1}{N\tau} \tilde{\omega}_0 w(z_0) + 2\operatorname{Re} \left(\frac{1}{N\tau} \sum_{j=0}^{N-1} \tilde{\omega}_j e^{z_j t} w(z_j) \right),$$

The number of elliptic problems in (1.11) is then approximately halved.

We emphasize that $\hat{f}(z_j)$ denotes the value at z_j of the Laplace transform obtained by analytic continuation from the one defined in (1.4). For the scalar case examples of functions $f(t)$ for which $\hat{f}(z)$ may be determined analytically on suitable contours Γ are linear combinations of functions of the form $P(t)e^{-\lambda t}$ where $\operatorname{Re} \lambda \geq 0$ and $P(t)$ is a polynomial. In fact, for $f(t) = t^l e^{-\lambda t}$, we have $\hat{f}(z) = l!(\lambda + z)^{-l-1}$ for $z \neq -\lambda$, thus with a pole in the left half plane. In applications to partial differential equations, where f may depend also on a spatial variable x one may consider functions of the form $P(x, t)e^{-\lambda(x)t}$ where $P(x, t)$ is a polynomial in t , and linear combinations of such functions.

To solve (1.1) approximately to a given tolerance, it suffices in view of the stability result (1.8) to solve the problem approximately for a sufficiently close approximation of $f(t)$. We remark that in the case that the solution of a parabolic problem is needed only for a restricted time interval $[0, T]$, we may then replace the inhomogeneous term $f(t)$ by a function $F(t)$ of the above form which is a good approximation of $f(t)$ on $[0, T]$.

2. Time discretization by quadrature

In this section we first develop a quadrature formula for an integral over the real axis R with values in \mathbb{B} , by making a transformation to the finite interval $(-1, 1)$ and then applying the trapezoidal rule. Under appropriate conditions this

quadrature formula has a high order of accuracy. We then apply this formula to our representation (1.9) of the solution of the parabolic problem.

To define our quadrature formula we thus set $y = y(\eta)$, where $y(\eta)$ is a smooth increasing function mapping $(-1, 1)$ onto R , to obtain, for $v \in C(R; \mathbb{B})$,

$$(2.1) \quad J(v) = \int_{-\infty}^{\infty} v(y) dy = \int_{-1}^1 V(\eta) d\eta, \quad \text{where } V(\eta) = v(y(\eta))y'(\eta).$$

Specifically, with τ a positive parameter, we choose $y(\eta)$ to be the function

$$(2.2) \quad y(\eta) = \tau^{-1}\chi(\eta), \quad \text{where } \chi(\eta) = \log((1 + \eta)/(1 - \eta)).$$

In our application τ will be a scaling parameter in t , in that our approximate solution will be accurate of order essentially t/τ . Applying the composite trapezoidal rule with spacing $1/N$ to the integral over $(-1, 1)$, and assuming $V(\pm 1) = 0$, we now define

$$Q_{N,\tau}(v) = \frac{1}{N} \sum_{j=-N+1}^{N-1} V(\eta_j) = \frac{1}{N\tau} \sum_{j=-N+1}^{N-1} \mu_j v(y_j),$$

where $\eta_j = j/N$, $y_j = y(\eta_j) = \tau^{-1}\chi(\eta_j)$, $\mu_j = \chi'(\eta_j) = 2/(1 - \eta_j^2)$. This formula is of arbitrarily high order of accuracy, as expressed in the following lemma.

Lemma 2.1. *For any $r \geq 1$ we have, assuming that the $v^{(j)}(y)$ have the appropriate asymptotic behavior, that*

$$\|Q_{N,\tau}(v) - J(v)\| \leq \frac{C_r}{(N\tau)^r} \int_{-\infty}^{\infty} e^{r\tau|y|} \sum_{j=0}^r \|v^{(j)}(y)\| dy.$$

The proof uses the following easy consequence of the Euler-Maclaurin summation formula: Assume that the function $V \in W_1^r((-1, 1); \mathbb{B})$ is such that $V(\pm 1) = V^{(2k-1)}(\pm 1) = 0$ for $2k - 1 \leq r - 2$. Then

$$\left\| \frac{1}{N} \sum_{j=-N+1}^{N-1} V(\eta_j) - \int_{-1}^1 V(\eta) d\eta \right\| \leq \frac{C_r}{N^r} \int_{-1}^1 \|V^{(r)}(\eta)\| d\eta.$$

This is then applied to $V(\eta) = v(y(\eta))y'(\eta)$.

We are now in a position to apply our quadrature scheme to our representation (1.9) of the solution of (1.1), and define the approximation to $u(t)$ by

$$(2.3) \quad U_{N,\tau}(t) = Q_{N,\tau}(v(t, \cdot)) = \frac{1}{N\tau} \sum_{j=-N+1}^{N-1} \tilde{\mu}_j e^{z_j t} w(z_j), \quad \tilde{\mu}_j = \frac{1}{2\pi i} z'(y_j) \mu_j,$$

where $w(z)$ is defined by (1.7) and $z_j = z(y_j) = \varphi(y_j) + i\sigma y_j$. Note that $\max_{|j| \leq N-1} |z_j| = O(\log N)$.

We first note the following stability estimate. Here and below we write

$$(2.4) \quad L(t) = 1 + \log_+(1/t).$$

Theorem 2.2. *We have, for $U_{N,\tau}(t)$ defined by (2.3),*

$$\|U_{N,\tau}(t)\| \leq C e^{\gamma t} ((N\tau)^{-1} + L(t)) (\|u_0\| + \|\hat{f}\|_{\Gamma}), \quad \text{for } t > 0.$$

For the proof one uses that, by (1.2) and (1.7),

$$\|w(z_j)\| \leq C(1 + |y_j|)^{-1}(\|u_0\| + \|\widehat{f}\|_\Gamma),$$

and that, since $Re z_j = \varphi(y_j) \leq \gamma - |y_j|$,

$$\|U_{N,\tau}(t)\| \leq Ce^{\gamma t} \frac{1}{N\tau} \sum_{j=-N+1}^{N-1} \mu_j e^{-|y_j|t} (1 + |y_j|)^{-1} (\|u_0\| + \|\widehat{f}\|_\Gamma).$$

The term with $j = 0$ in the sum equals 2 and the contribution from $(N\tau)^{-1}$ times the remaining terms is bounded by

$$C \int_0^\infty e^{-ty} (1 + y)^{-1} dy \leq CL(t).$$

We have the following error estimate.

Theorem 2.3. *For any $r \geq 1$ and $\mu > \gamma$ we have*

$$\|U_{N,\tau}(t) - u(t)\| \leq \frac{C_r}{(N\tau)^r} e^{\mu t} L(t - r\tau) (\|u_0\| + \max_{k \leq r} \|\widehat{f}^{(k)}\|_\Gamma), \text{ for } t > r\tau.$$

In the proof one recalls from (1.9) and (2.3) that

$$U_{N,\tau}(t) - u(t) = Q_{N,\tau}(v(t, \cdot)) - J(v(t, \cdot)).$$

To apply Lemma 2.1, one uses (1.2) and the Leibniz rule applied to (1.7) to show that

$$\|w^{(j)}(z)\| \leq C(1 + |z|)^{-1} (\|u_0\| + \max_{k \leq j} \|\widehat{f}^{(k)}(z)\|), \text{ for } z \in \Gamma,$$

and hence, from the definition of $v(t, \cdot)$ in (1.9),

$$\|v^{(j)}(t, y)\| \leq C(1 + t^r) e^{t\varphi(y)} (1 + |y|)^{-1} (\|u_0\| + \max_{k \leq r} \|\widehat{f}^{(k)}\|_\Gamma), \text{ for } j \leq r, y \in R.$$

Since $(1 + t^r) e^{t\varphi(y)} \leq C e^{t(\mu - |y|)}$, the assumptions of Lemma 2.1 are then seen to be satisfied if $t > r\tau$, and hence

$$\|U_{N,\tau}(t) - u(t)\| \leq \frac{C}{(N\tau)^r} e^{\mu t} \int_{-\infty}^\infty \frac{e^{-|y|(t-r\tau)}}{1 + |y|} dy (\|u_0\| + \max_{k \leq r} \|\widehat{f}^{(k)}\|_\Gamma).$$

Bounding the integral appropriately shows the theorem.

3. Application to the finite element method for the heat equation

We now apply our above results to the discretization in both space and time of an initial-boundary value problem for the heat equation,

$$(3.1) \quad \begin{aligned} u_t - \Delta u &= f(t) & \text{in } \Omega, & \quad \text{with } u(\cdot, t) = 0 & \text{on } \partial\Omega \text{ for } t > 0, \\ u(\cdot, 0) &= u_0 & \text{in } \Omega, \end{aligned}$$

where Ω is a bounded convex domain in R^2 with smooth boundary $\partial\Omega$ and Δ denotes the Laplacian. Since our present work is developed in a Banach space context, we consider (3.1) in the Banach space $C_0(\bar{\Omega})$, and illustrate our theory by deriving error estimates in the maximum-norm $\|v\| = \sup_{x \in \Omega} |v(x)|$.

Let V_h denote standard piecewise linear finite element spaces defined on a family of quasi-uniform triangulations of Ω and vanishing on $\partial\Omega$. A spatially semidiscrete problem corresponding to (3.1) is to find $u_h(t) \in V_h$ such that, with (\cdot, \cdot) the inner product in $L_2(\Omega)$,

$$(u_{h,t}, \chi) + (\nabla u_h, \nabla \chi) = (f, \chi), \text{ for all } \chi \in V_h, t > 0, \quad \text{with } u_h(0) = P_h u_0,$$

where $P_h : L_2(\Omega) \rightarrow V_h$ is the orthogonal projection with respect to (\cdot, \cdot) . With $\Delta_h : V_h \rightarrow V_h$ the discrete Laplacian defined by

$$(\Delta_h \psi, \chi) = -(\nabla \psi, \nabla \chi), \text{ for all } \psi, \chi \in V_h,$$

this problem may also be written as

$$u_{h,t} - \Delta_h u_h = P_h f, \text{ for } t > 0, \quad \text{with } u_h(0) = P_h u_0.$$

This problem is of the form (1.1) when V_h , equipped with the maximum-norm, is considered as a Banach space. Recall that P_h is bounded in maximum-norm.

It was shown in Bakaev, Thomée, and Wahlbin [1] that a maximum-norm resolvent estimate for Δ_h of the form (1.2) holds, uniformly in h , or that for any $\delta \in (\pi/2, \pi)$ there is a $M \geq 1$ such that

$$\|(zI - \Delta_h)^{-1}\| \leq M(1 + |z|)^{-1}, \text{ for } z \in \Sigma_\delta.$$

The fully discrete solution obtained by application of our method to (3.1) is thus defined from (2.3) by

(3.2)

$$U_{N,h,\tau}(t) = \frac{1}{N\tau} \sum_{j=-N+1}^{N-1} \tilde{\mu}_j e^{z_j t} w_h(z_j), \quad w_h(z) = (zI - \Delta_h)^{-1} P_h(u_0 + \hat{f}(z)).$$

To find $U_{N,h,\tau}(t)$ it is thus required to solve the $2N - 1$ discrete elliptic problems

$$(\nabla w_h(z_j), \nabla \chi) + z_j (w_h(z_j), \chi) = (u_0 + \hat{f}(z_j), \chi), \text{ for all } \chi \in V_h, \quad |j| \leq N - 1.$$

To estimate the error in $U_{N,h,\tau}(t)$ we note that by Theorem 2.3 we obtain, uniformly in h , with C depending on r, τ , and t ,

$$(3.3) \quad \|U_{N,h,\tau}(t) - u_h(t)\| \leq CN^{-r} (\|u_0\| + \max_{k \leq r} \|\hat{f}^{(k)}\|_\Gamma), \text{ for } t > r\tau.$$

The remaining part of the error is bounded by the following maximum-norm error estimate for the semidiscrete problem.

Lemma 3.1. *We have for small h ,*

$$\|u_h(t) - u(t)\| \leq Ch^2 \log^2(1/h) t^{-1} e^{\gamma t} (\|u_0\| + \|\hat{f}\|_\Gamma), \text{ for } t > 0.$$

This result is a nonsmooth data error estimate in that it requires no regularity of data with respect to the spatial variable x , at the expense of the factor t^{-1} on the right. For solutions which are smoother in x , this factor and one of the factors $\log(1/h)$ can be removed. When the Banach space is the Hilbert space $L_2(\Omega)$ the factors $\log(1/h)$ are superfluous.

Together (3.3) and Lemma 3.1 show the following error bound for the fully discrete solution.

Theorem 3.2. *Let $u(t)$ be the solution of (3.1), and let $U_{N,h,\tau}(t)$ be the approximation defined by (3.2). Then, with C independent of N and h , but depending on t and τ , we have, for $t > \tau r$,*

$$\|U_{N,h,\tau}(t) - u(t)\| \leq \frac{C}{N^r} \left(\|u_0\| + \max_{k \leq r} \|\hat{f}^{(k)}\|_\Gamma \right) + Ch^2 \log^2 \frac{1}{h} \left(\|u_0\| + \|\hat{f}\|_\Gamma \right).$$

4. An evolution equation with a memory term of fractional integral type

In this section we apply our method to an initial value problems of the form

$$(4.1) \quad u_t + \int_0^t \beta(t-s)Au(s) ds = f(t), \quad \text{for } t > 0, \quad \text{with } u(0) = u_0,$$

where A is as above and the kernel in the memory term is the weakly singular function

$$\beta(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}, \quad \text{with } 0 < \alpha < 1.$$

This time we find for the Laplace transform $w(z) = \widehat{u}(z)$ of the solution $u(t)$

$$(zI + \widehat{\beta}(z)A)w(z) = u_0 + \widehat{f}(z),$$

so that, since $\widehat{\beta}(z) = z^{-\alpha}$,

$$(4.2) \quad w(z) = \widehat{E}(z)(u_0 + \widehat{f}(z)), \quad \text{where } \widehat{E}(z) = z^\alpha(z^{1+\alpha}I + A)^{-1}.$$

Our assumptions on A now imply that $(z^{1+\alpha}I + A)^{-1}$ is analytic for $z \in \Sigma_\theta$ with $\theta = \delta/(1+\alpha)$ where we suppose $\theta > \pi/2$.

We assume that the initial data u_0 belongs to \mathbb{B} and that the inhomogeneous term $f : [0, \infty) \rightarrow \mathbb{B}$ is such that its Laplace transform $\widehat{f}(z)$ may be continued analytically to Σ_θ . It follows then from (4.2) that $w(z)$ is analytic there and

$$\|w(z)\| = \|\widehat{E}(z)(u_0 + \widehat{f}(z))\| \leq C(1+|z|)^{-1}(\|u_0\| + \|\widehat{f}(z)\|), \quad \text{for } z \in \Sigma_\theta,$$

and that, with Γ as in (1.7), with $\Gamma \subset \Sigma_\theta$,

$$(4.3) \quad u(t) = \frac{1}{2\pi i} \int_\Gamma e^{tz} w(z) dz, \quad \text{for } t > 0.$$

This time we have the following stability and regularity result.

Theorem 4.1. *Let $u(t)$ be the solution of (4.1). Then, for $j = 0, 1$, $k \geq 0$, we have, with $\Gamma_\theta = \partial\Sigma_\theta$,*

$$\|A^j u^{(k)}(t)\| \leq C_k t^{-k-j(\alpha+1)}(\|u_0\| + \|\widehat{f}\|_{\Gamma_\theta}), \quad \text{for } t > 0.$$

In [3] we considered in addition to the quadrature scheme described in Section 2 also a truncated trapezoidal rule applied to R without first transforming it to a finite interval. For this we extend the function $\varphi(y)$ used in (1.5) to define Γ as an analytic function in an open strip $\mathcal{S}_r = \{\zeta = y + ip; |p| < r\}$ around the real axis. With τ a positive parameter. the scheme is then defined by

$$(4.4) \quad Q_{N,\tau}(v) = k \sum_{j=-N+1}^{N-1} v(jk) \approx J(v) = \int_{-\infty}^{\infty} v(y) dy, \quad \text{where } k = \sqrt{\frac{2\pi r}{\tau N}}.$$

We have the following lemma.

Lemma 4.2. *Assume that $v(\zeta)$ is analytic in \mathcal{S}_r , and that*

$$\|v(\zeta)\| \leq K e^{-t|y|}/(1+|y|), \quad \text{for } \zeta \in \mathcal{S}_r.$$

where K is a positive constant and t a positive parameter. Then

$$\|Q_{N,\tau}(v) - J(v)\| \leq CK L(t) e^{-\sqrt{2\pi r r N} \min(1,t/\tau)}, \quad \text{for } t > 0.$$

To show this one introduces $Q_\infty(v) = k \sum_{j=-\infty}^{\infty} v(jk)$ for $k > 0$ and observes as in McNamee, Stenger and Whitney [6, Section 5.5] that the meromorphic function $\cot(\pi y/k)$ has simple poles at $y = jk$ for integer j , with residue k/π , and thus

$$Q_\infty(v) = \frac{1}{2\pi i} \int_{\partial \mathcal{S}_r} v(\zeta) \pi \cot\left(\frac{\pi \zeta}{k}\right) d\zeta,$$

and that this implies, with $L(t)$ as in (2.4),

$$\|Q_\infty(v) - J(v)\| \leq \frac{e^{\pi r/k}}{2 \sinh(\pi r/k)} \|v\|_{L_1(\partial \mathcal{S}_r; \mathbb{B})} \leq CKL(t)e^{-2\pi r/k}.$$

One then notes that

$$\|Q_{N,\tau}(v) - Q_\infty(v)\| \leq k \sum_{|j| \geq N+1} \|v(jk)\| \leq CK e^{-tNk}, \text{ for } t \geq \tau.$$

Choosing k as in (4.4) yields the desired result.

As in the case of a parabolic equation, for the discretization in time we write (4.3) as an integral with respect to the real parameter y ,

$$(4.5) \quad u(t) = \int_{-\infty}^{\infty} v(t, y) dy, \quad \text{where } v(t, y) = \frac{1}{2\pi i} e^{z(y)t} w(z(y)) z'(y).$$

Applying (4.4), our approximate solution to (4.1) is

$$U_{N,\tau}(t) = Q_{N,\tau}(v(t, \cdot)) = k \sum_{j=-N}^N \tilde{\mu}_j e^{z_j t} w(z_j), \quad \tilde{\mu}_j = \frac{z'(jk)}{2\pi i}, \quad z_j = z(jk),$$

where the $w(z_j)$ are the solutions of the $2N + 1$ elliptic problems

$$(z_j^{1+\alpha} I + A)w(z_j) = z_j^\alpha (u_0 + \hat{f}(z_j)), \text{ for } |j| \leq N.$$

Here $\max_{|j| \leq N} |z_j| = O(\sqrt{N})$.

To apply Lemma 4.2 one now shows that the function $v(t, \cdot)$ in (4.5), extended to the strip \mathcal{S}_r , satisfies

$$\|v(t, \zeta)\| \leq C e^{\mu t} (\|u_0\| + \|\hat{f}\|_{\mathcal{N}_r}) e^{-t|y|} / (1 + |y|), \text{ for } \zeta = y + ip \in \mathcal{S}_r,$$

where $\mathcal{N}_r = \{z(\zeta) = \varphi(\zeta) + i\sigma\zeta : \zeta \in \mathcal{S}_r\} \subset \Sigma_\theta$. This leads to the following:

Theorem 4.3. *There exist positive constants r , μ , and C , such that*

$$\|U_{N,\tau}(t) - u(t)\| \leq C e^{\mu t} L(t) e^{-\sqrt{2\pi r \tau N} \min(1, t/\tau)} (\|u_0\| + \|\hat{f}\|_{\mathcal{N}_r}), \text{ for } t > 0.$$

As for the parabolic equation studied earlier, the time discretization method may be combined with spatial discretization by finite elements. Now the maximum-norm error in the spatially semidiscrete solution $u_h(t)$ is bounded by

$$\|u_h(t) - u(t)\| \leq Ch^2 \log^2(1/h) e^{\mu t} (1 + t^{-1-\alpha}) (\|u_0\| + \|\hat{f}\|_\Gamma), \text{ for } t > 0,$$

and for the corresponding fully discrete method we find, for fixed positive t ,

$$\|U_{N,\tau,h}(t) - u(t)\| \leq C(t, u_0, f) (e^{-\sqrt{2\pi r \tau N}} + h^2 \log^2(1/h)).$$

5. A parabolic integro-differential equation

In this section we apply our technique to the initial-value problem

$$(5.1) \quad u_t + Au + \int_0^t \beta(t-s)Au(s) ds = f(t), \quad \text{for } t > 0, \quad \text{with } u(0) = u_0.$$

As before A is assumed to be as in (1.2), and $\beta(t)$ is now an integrable function satisfying some technical assumptions given below.

Taking Laplace transforms in (5.1), we now formally obtain

$$(5.2) \quad (zI + (1 + \widehat{\beta}(z))A)w(z) = u_0 + \widehat{f}(z).$$

We shall assume that $\widehat{f}(z)$, $\widehat{\beta}(z)$, and $(1 + \widehat{\beta}(z))^{-1}$ are bounded analytic on and to the right of Γ . On Γ we have, in particular,

$$(zI + (1 + \widehat{\beta}(z))A)^{-1} = (1 + \widehat{\beta}(z))^{-1}(\tilde{z}(z)I + A)^{-1}, \quad \text{where } \tilde{z}(z) = z/(1 + \widehat{\beta}(z)),$$

provided $-\tilde{z}(z) \notin \sigma(A)$. The solution of (5.2) for $z \in \Gamma$ may then be written

$$w(z) = \widehat{E}(z)(u_0 + \widehat{f}(z)), \quad \text{with } \widehat{E}(z) = (1 + \widehat{\beta}(z))^{-1}(\tilde{z}(z)I + A)^{-1}.$$

Setting $\tilde{\Gamma} = \{\tilde{z}(z), z \in \Gamma\}$, we note that if $\tilde{\Gamma} \subset \Sigma_\delta$, which we assume in the sequel, then

$$\|\widehat{E}(z)\| \leq \frac{1}{|1 + \widehat{\beta}(z)|} \frac{M}{1 + |\tilde{z}(z)|} = \frac{M}{|1 + \widehat{\beta}(z)| + |\tilde{z}(z)|} \leq \frac{C}{1 + |z|}, \quad \text{for } z \in \Gamma.$$

As for the parabolic equation we may represent the solution of (5.1) as

$$(5.3) \quad u(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} w(z) dz = \frac{1}{2\pi i} \int_\Gamma e^{zt} \widehat{E}(z)(u_0 + \widehat{f}(z)) dz, \quad \text{for } t > 0.$$

We illustrate the assumption that $\tilde{\Gamma} \subset \Sigma_\delta$ by considering the special case $\beta(t) = \kappa e^{-\eta t}$, with κ real and $\eta \geq 0$, in which case

$$\widehat{\beta}(z) = \frac{\kappa}{z + \eta}, \quad \frac{1}{1 + \widehat{\beta}(z)} = \frac{z + \eta}{z + \eta + \kappa}, \quad \text{and } \tilde{z}(z) = \frac{z(z + \eta)}{z + \eta + \kappa}.$$

We note first that if $\eta + \kappa < 0$, then the requirement that $(1 + \widehat{\beta}(z))^{-1}$ be analytic on and to the right of Γ means that Γ must pass to the right of $-\eta - \kappa$. If $\eta + \kappa \geq 0$ then this is satisfied automatically, since we always require Γ to pass to the right of 0. To consider the constraints needed to ensure that $\tilde{\Gamma} \subset \Sigma_\delta$, we restrict ourselves to the case when (1.2) holds for arbitrary $\delta \in (\frac{1}{2}\pi, \pi)$, which is the case, for example, if A is positive definite and \mathbb{B} a Hilbert space. We are then led to the question of determining for which $z \in \mathcal{C} \setminus R_-$ we can have $\tilde{z}(z) \in R_-$, where R_- is the negative real axis. One may show that Γ can be chosen as any curve of the form (1.5) which avoids the circle $(x + \eta + \kappa)^2 + y^2 = \kappa(\eta + \kappa)$.

Using (5.3) one shows easily stability and smoothness of the solution.

Theorem 5.1. *For the solution $u(t)$ of (5.1) we have, for $j = 0, 1$ and $k \geq 0$,*

$$\|A^j u^{(k)}(t)\| \leq C_0 e^{\alpha t} t^{-k-j} (\|u_0\| + \|\widehat{f}\|_\Gamma), \quad \text{for } t > 0, \quad \text{where } \alpha = \varphi(0).$$

This time, following López-Fernandes and Palencia [2], before we apply quadrature to the integral representation of the solution, we make a change of variables $y \rightarrow \nu \sinh y$ in (1.5) and write

$$\Gamma = \{z : z = Z(y) = \gamma - \nu \cosh y + i\sigma\nu \sinh y, \quad y \in R\}.$$

With $\alpha = \arcsin(1/\sqrt{1 + \sigma^2})$, $\lambda = \nu\sqrt{1 + \sigma^2}$ we have

$$z = Z(y) = \gamma - \lambda(\sin \alpha \cosh y - i \cos \alpha \sinh y) = \gamma - \lambda \sin(\alpha + iy).$$

The solution is thus represented as

$$u(t) = \int_{-\infty}^{\infty} v(t, y) dy, \quad \text{where } v(t, y) = \frac{1}{2\pi i} e^{Z(y)t} w(Z(y)) Z'(y).$$

We now apply the quadrature rule

$$(5.4) \quad Q_N(v) = k \sum_{j=-N}^N v(jk) \approx J(v) = \int_{-\infty}^{\infty} v(y) dy, \quad \text{with } k = \log N/N,$$

Lemma 5.2. *Assume $v(\zeta)$ analytic, with*

$$\|v(\zeta)\| \leq K e^{-\kappa \cosh y}, \quad \text{for } \zeta \in \mathcal{S}_r = \{\zeta = y + ip, |p| < r\}.$$

We then have, with $L(\kappa)$ as defined by (2.4),

$$\|Q_N(v) - J(v)\| \leq CKL(\kappa)(e^{-2\pi r N/\log N} + e^{-\kappa N/2}).$$

In the same way as earlier we define our approximate solution to (5.1) as

$$(5.5) \quad U_N(t) = Q_N(v(t, \cdot)) = k \sum_{j=-N}^N \tilde{\mu}_j e^{Z_j t} w(Z_j), \quad \tilde{\mu}_j = \frac{Z'(jk)}{2\pi i},$$

where $Z_j = Z(jk)$ and $w(Z_j)$ are defined by

$$(\tilde{Z}_j I + A)w(Z_j) = (1 + \hat{\beta}(Z_j))^{-1}(u_0 + \hat{f}(Z_j)), \quad \tilde{Z}_j = \tilde{z}(Z_j), \quad \text{for } |j| \leq N,$$

We note that $\max_{|j| \leq N} |Z_j| = O(N)$ and $\max_{|j| \leq N} |\tilde{Z}_j| = O(N)$. Setting $\mathcal{N}_r = \{Z(\zeta) = \gamma - \lambda \sin(\alpha - p + iy) : \zeta = y + ip \subset \mathcal{S}_r\}$ one may show that for μ and r appropriate

$$\|v(t, \zeta)\| \leq C e^{\mu t} (\|u_0\| + \|\hat{f}\|_{\mathcal{N}_r}) e^{-t \sin(\alpha - r) \cosh h}.$$

With $\tilde{\mathcal{N}}_r = \{\tilde{z}(z) : z \in \mathcal{N}_r\}$, Lemma 5.2 will show the following error estimate.

Theorem 5.3. *Let $u(t)$ be the solution of (5.1) and let $U_N(t)$ be its approximation defined by (5.5). Assume that $\mathcal{N}_r \cup \tilde{\mathcal{N}}_r \subset \Sigma_\delta$. Then, under the appropriate assumptions on $\hat{f}(z)$, we have, with $c > 0$,*

$$\|U_N(t) - u(t)\| \leq C e^{\mu t} L(t)(e^{-2\pi r N/\log N} + e^{-ctN})(\|u_0\| + \|\hat{f}\|_{\mathcal{N}_r}), \quad \text{for } t > 0.$$

For any fixed positive t this error bound is of order $O(e^{-2\pi r N/\log N})$.

As earlier our time discretization method may be applied in the case that $A = -\Delta$ to a spatially semidiscrete problem to yield a fully discrete scheme, this time with an error bound of order $O(e^{-2\pi r N/\log N} + h^2 \log^2(1/h))$ for fixed positive t .

6. Numerical example

In this section we give a numerical example for a parabolic equation, employing our method. In order to be able to illustrate the behavior of the time discretization methods unpolluted by a spatial discretization, we consider just the scalar problem ($\mathbb{B} = R$)

$$(6.1) \quad u_t + u = 1 + t + e^{-2t}, \quad \text{for } t > 0, \quad \text{with } u(0) = 1,$$

which has the exact solution

$$u(t) = 1 + t + e^{-t} - e^{-2t}.$$

Even though the three different quadrature formulas were used above for different equations, they can all be applied to a parabolic equation, and we illustrate this below in Tables 1, 2, and 3 for (6.1). We use

$$\Gamma = \{z = 2 - \sqrt{y^2 + 1} + 2iy\}, \quad \tau = .5.$$

In Table 4 we include also, for comparison, the standard Crank-Nicolson method. The calculations were made by Bill McLean, whose help is gratefully acknowledged.

t	$N = 10$	$N = 20$	$N = 40$	$N = 80$
0.4	2.50E-2	1.84E-2 (0.44)	2.11E-3 (3.13)	5.12E-4 (2.04)
0.8	4.24E-3	1.16E-3 (1.87)	7.77E-5 (3.90)	2.68E-5 (1.53)
1.2	6.98E-4	2.69E-4 (1.38)	2.42E-5 (3.47)	7.47E-10 (14.98)
1.6	5.49E-4	1.29E-4 (2.09)	3.25E-6 (5.31)	2.14E-8 (7.25)
2.0	6.14E-5	1.76E-5 (1.80)	3.25E-7 (5.76)	2.42E-10 (10.39)
2.4	4.80E-4	4.57E-6 (6.72)	3.38E-8 (7.08)	2.29E-11 (10.53)
2.8	1.69E-4	6.42E-6 (4.72)	1.44E-8 (8.81)	2.66E-12 (12.40)
3.2	4.61E-4	4.65E-6 (6.63)	1.44E-8 (8.34)	3.17E-12 (12.15)
3.6	8.27E-4	5.55E-6 (7.22)	1.48E-8 (8.55)	3.22E-12 (12.16)
4.0	2.99E-3	7.12E-6 (8.71)	1.50E-8 (8.89)	3.25E-12 (12.18)

Table 1. Errors in the first quadrature rule.

t	$N = 10$	$N = 20$	$N = 40$	$N = 80$
0.4	4.89E-3	3.45E-3 (0.50)	3.41E-4 (3.34)	7.36E-4 (-1.11)
0.8	3.12E-4	1.40E-4 (1.15)	1.01E-4 (0.48)	2.07E-5 (2.28)
1.2	4.57E-4	1.57E-6 (8.19)	1.09E-6 (0.52)	4.09E-7 (1.42)
1.6	6.54E-4	9.06E-7 (9.50)	1.46E-6 (-0.69)	9.36E-8 (3.96)
2.0	5.75E-4	1.44E-6 (8.64)	2.42E-7 (2.58)	1.28E-8 (4.24)
2.4	4.56E-4	1.46E-6 (8.29)	3.44E-8 (5.41)	6.46E-10 (5.73)
2.8	5.89E-4	6.20E-7 (9.89)	6.60E-9 (6.55)	1.31E-10 (5.65)
3.2	8.87E-4	1.04E-7 (13.06)	1.99E-9 (5.71)	2.58E-11 (6.27)
3.6	1.98E-3	2.65E-7 (12.86)	7.43E-10 (8.48)	2.39E-12 (8.28)
4.0	7.58E-3	5.95E-8 (16.96)	2.65E-10 (7.81)	4.44E-15 (15.87)

Table 2. Errors in the second quadrature rule.

t	$N = 10$	$N = 20$	$N = 40$	$N = 80$
0.4	1.06E-2	2.67E-4 (5.31)	7.32E-6 (5.19)	6.53E-10 (13.45)
0.8	1.24E-3	4.67E-6 (8.05)	1.35E-9 (11.76)	1.78E-15 (19.53)
1.2	2.75E-4	2.45E-7 (10.13)	9.29E-13 (18.01)	0.00E+0 (∞)
1.6	7.58E-5	4.88E-9 (13.92)	2.66E-15 (20.80)	8.88E-16 (1.58)
2.0	1.06E-5	2.38E-8 (8.80)	5.55E-14 (18.71)	4.44E-16 (6.97)
2.4	5.26E-5	2.67E-8 (10.95)	1.57E-13 (17.38)	0.00E+0 (∞)
2.8	1.38E-5	4.58E-8 (8.24)	1.44E-13 (18.28)	8.88E-16 (7.34)
3.2	1.56E-4	2.53E-7 (9.27)	9.50E-14 (21.34)	1.78E-15 (5.74)
3.6	3.35E-4	3.57E-7 (9.88)	2.54E-12 (17.10)	8.88E-16 (11.48)
4.0	1.25E-4	1.39E-6 (6.49)	3.62E-12 (18.55)	1.78E-15 (10.99)

Table 3. Errors in the third quadrature rule.

t	$N = 10$	$N = 20$	$N = 40$	$N = 80$
0.40	2.06E-02	5.03E-03 (2.03)	1.25E-03 (2.01)	3.13E-04 (2.00)
0.80	2.21E-02	5.43E-03 (2.03)	1.35E-03 (2.01)	3.38E-04 (2.00)
1.20	1.80E-02	4.43E-03 (2.02)	1.10E-03 (2.01)	2.76E-04 (2.00)
2.00	8.98E-03	2.23E-03 (2.01)	5.55E-04 (2.00)	1.39E-04 (2.00)
2.40	5.94E-03	1.48E-03 (2.01)	3.69E-04 (2.00)	9.21E-05 (2.00)
2.80	3.83E-03	9.56E-04 (2.00)	2.39E-04 (2.00)	5.97E-05 (2.00)
3.20	2.42E-03	6.07E-04 (1.99)	1.52E-04 (2.00)	3.80E-05 (2.00)
3.60	1.50E-03	3.80E-04 (1.99)	9.51E-05 (2.00)	2.38E-05 (2.00)
4.00	9.21E-04	2.34E-04 (1.98)	5.87E-05 (1.99)	1.47E-05 (2.00)

Table 4. Errors for the Crank-Nicolson time stepping method.

References

- [1] N. Yu. Bakaev, V. Thomée and L. B. Wahlbin. Maximum-norm estimates for resolvents of elliptic finite element operators, *Math. Comp.* 72 (2003), 1597–1610.
- [2] M. López-Fernandez and C. Palencia, On the numerical inversion of the Laplace transform of certain holomorphic mappings. *Manuscript*.
- [3] W. McLean and V. Thomée, Numerical solution of an evolution equation with a positive-type memory term, *J. Austral. Math. Soc. Ser. B* 35 (1993), 23–70.
- [4] W. McLean, V. Thomée and L. B. Wahlbin, Discretization with variable time steps of an evolution equation with a positive-type memory term, *J. Comput. Appl. Math.* 69 (1996) 49–69.
- [5] W. McLean, I. H. Sloan and V. Thomée, Time discretization via Laplace transformation of an integrodifferential equation of parabolic type. *Under preparation*.
- [6] J. McNamee, F. Stenger and E. L. Whitney, Whittaker’s cardinal function in retrospect, *Math. Comp.* 25 (1971), 141–154.
- [7] D. Sheen, I. H. Sloan and V. Thomée, A parallel method for time-discretization of parabolic problems based on contour integral representation and quadrature, *Math. Comp.* 69 (1999), 177–195.
- [8] D. Sheen, I. H. Sloan and V. Thomée, A parallel method for time-discretization of parabolic equations based on Laplace transformation and quadrature, *IMA J. Numer. Anal.* 23 (2004), 269–299.
- [9] H. B. Stewart, *Generation of analytic semigroups by strongly elliptic operators*, Trans. Amer. Math. Soc. 199 (1974), 141–161.

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