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NUMERICAL SOLUTION VIA LAPLACE TRANSFORMS OF A FRACTIONAL ORDER EVOLUTION EQUATION

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ABSTRACT. We consider the discretization in time of a fractional order diffusion equation. The approximation is based on a further development of the approach of using Laplace transformation to represent the solution as a contour integral, evaluated to high accuracy by quadrature. This technique reduces the problem to a finite set of elliptic equations with complex coefficients, which may be solved in parallel. Three different methods, using $2N+1$ quadrature points, are discussed. The first has an error of order $O\left(e^{-cN}\right)$ away from $t=0$, whereas the second and third methods are uniformly accurate of order $O\left(e^{-c\sqrt{N}}\right)$. Unlike the first and second methods, the third method does not use the Laplace transform of the forcing term. The basic analysis of the time discretization takes place in a Banach space setting and uses a resolvent estimate for the associated elliptic operator. The methods are combined with finite element discretization in the spatial variables to yield fully discrete methods.

1. Introduction. For $-1 < \alpha < 1$, we shall consider numerical, particularly time discretization, methods for an initial-value problem of the form

$$\partial_t u + \partial_t^{-\alpha} A u = f(t), \quad \text{for} \quad t > 0, \quad \text{with} \quad u(0) = u_0, \tag{1.1}$$

where $\partial_t = \partial/\partial t$, and where A is a sectorial linear operator in a complex Banach space $\mathcal{B}$.

In the applications we have in mind, A is a linear, second-order elliptic partial differential operator in some spatial variables (whose coefficients

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must be independent of t). If $\alpha = 0$, the problem (1.1) then reduces to a classical parabolic equation, providing, e.g., a macroscopic model of the density u of diffusing particles that undergo Brownian motion with mean-square displacement proportional to t. If $-1 < \alpha < 0$ then (1.1) instead models anomalous sub-diffusion, see Gorenflo, Mainardi, Moretti and Paradisi [**5**], Henry and Wearne [**6**], Metzler and Klafter [**16**], Yuste, Acado and Lindenberg [**27**], in which the mean-square displacement of the diffusing particles is proportional to $t^{1+\alpha}$. The case $0 < \alpha < 1$ is of interest for applications in viscoelasticity. Schneider and Wyss [**21**] describe (1.1) as a fractional diffusion equation if $-1 < \alpha < 0$ and as a fractional wave equation if $0 < \alpha < 1$.

Denoting the Laplace transform of u with respect to t by

$$\widehat{u}(z) = \mathcal{L}\{u(t)\} = \int_0^\infty e^{-zt} u(t)\, dt, \tag{1.2}$$

we find that the solution of (1.1) formally satisfies

$$(zI + z^{-\alpha}A)\widehat{u}(z) = g(z) := u_0 + \widehat{f}(z), \tag{1.3}$$

where I denotes the identity operator in the Banach space $\mathcal{B}$. This equation serves as an implicit definition of $\partial_t^{-\alpha}$. Equivalently, since

$$\mathcal{L}\{t^{\mu-1}/\Gamma(\mu)\} = z^{-\mu}, \qquad \text{for} \quad \mu > 0,$$

we may interpret the fractional order time derivative ($\alpha < 0$) or integral ($\alpha > 0$) in the Riemann–Liouville sense,

$$(\partial_t^{-\alpha} u)(t) := \begin{cases} \partial_t \displaystyle\int_0^t \frac{(t-s)^\alpha}{\Gamma(1+\alpha)}\, u(s)\, ds, & \text{if} \quad -1 < \alpha < 0, \\ \displaystyle\int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}\, u(s)\, ds, & \text{if} \quad 0 < \alpha < 1. \end{cases}$$

Thus, (1.1) is an integro-differential equation for $\alpha \neq 0$, and so the problem is non-local in time.

Instead of using time stepping for the numerical solution, as was done for the case $0 < \alpha < 1$, e.g., in [**10, 11, 13, 15, 17, 19**], our approach is to represent the solution of (1.1) as an inverse Laplace transform, which is then approximated by quadrature. Developed first for parabolic problems ($\alpha = 0$) in Sheen, Sloan and Thomée [**22, 23**], such an approach is even more attractive for problems as occurring in (1.1) with $\alpha \neq 0$, involving convolution integrals in time, see López-Fernandez, Palencia and Schädle [**8**], McLean and Thomée [**14**] and McLean, Sloan and Thomée [**12**]. Our present paper also covers the case $-1 < \alpha < 0$, which has received less attention from a numerical point of view; see, however, some generalizations of the implicit (Langlands and Henry [**7**]) and explicit (Yuste and Acedo [**26**]) Euler method, and an example (Weideman [**25**]) in the context of numerical inversion of Laplace transforms.

In Section 2, we will outline three time discretization methods of the type mentioned above. In each method, we must solve $2N + 1$ elliptic problems, one for each quadrature point. The first is based on the ideas of [**8**] and achieves a convergence rate of order $O(e^{-cN})$ for t in a compact interval $[t_0, T]$, with $0 < t_0 < T < \infty$. For the second and third methods, the error is of order $O(e^{-c\sqrt{N}})$ but the convergence is uniform on $[0, T]$. The third method, unlike the first two, does not require the Laplace transform of the inhomogenous term f, but has the disadvantage that the source terms in the elliptic problems depend on t. Gavrilyuk and Makarov [**4**] considered a scheme of the second type for the special case of a parabolic PDE ($\alpha = 0$).

We set out the details of our error analysis in Section 3. Subsequent parts of the paper proceed to consider the application of our methods for time discretization to the design of fully discrete schemes for the case of equation (1.1) when $A = -\Delta$, where Δ is the Laplacian in a smooth (or convex) bounded domain $\Omega \subset \mathbb{R}^d$, under homogeneous Dirichlet boundary conditions.

In Section 4 we show nonsmooth and smooth data error estimates for the spatially-discrete, continuous-time problem. Subsequently, in Section 5, we combine the separate error estimates for the space and time discretizations to bound the error for fully discrete solutions.

Finally, in Section 6 we present the results of some simple numerical experiments, illustrating our theoretical results.

2. Preliminaries. We begin this section by stating some technical assumptions. We require that A is a closed, densely defined linear operator in a complex Banach space $\mathcal{B}$, and that the spectrum of A lies in the interior of a closed sector in $\mathbb{C}$ of the form

$$\Sigma_\varphi = \{z \neq 0 : \ |\arg z| \leq \varphi\} \cup \{0\}, \quad \text{with } 0 < \varphi < (1-\alpha)\,\frac{\pi}{2}. \tag{2.1}$$

In addition, we assume that for some constant $M \geq 1$ the operator A satisfies the resolvent estimate

$$\|(zI - A)^{-1}\| \leq \frac{M}{1+|z|}, \quad \text{for } z \in \overline{\mathbb{C} \setminus \Sigma_\varphi}, \tag{2.2}$$

or, equivalently,

$$\|(zI + A)^{-1}\| \leq \frac{M}{1+|z|}, \quad \text{for } z \in \Sigma_{\pi-\varphi}, \tag{2.3}$$

where $\|\cdot\|$ also denotes the operator norm induced by the norm in $\mathcal{B}$. From (1.3), it follows that

$$\widehat{u}(z) = \widehat{\mathcal{E}}(z) g(z), \qquad \text{where} \quad \widehat{\mathcal{E}}(z) := z^\alpha (z^{1+\alpha} I + A)^{-1}, \tag{2.4}$$

and from (2.3) we obtain, for any $\overline{\beta} < \pi$ with $\frac{1}{2}\pi < \overline{\beta} \leq (\pi-\varphi)/(1+\alpha)$,

$$\|\widehat{\mathcal{E}}(z)\| \leq \frac{M|z|^\alpha}{1+|z|^{1+\alpha}} \leq \frac{M}{|z|}, \quad \text{for } \ z \in \Sigma_{\overline{\beta}}, \tag{2.5}$$

since $z^{1+\alpha} \in \Sigma_{\pi-\varphi}$ for $z \in \Sigma_{\overline{\beta}}$; note that $(\pi-\varphi)/(1+\alpha) > \frac{1}{2}\pi$ by (2.1).

For any $\omega > 0$, let Γ_0 be the line $\operatorname{Re} z = \omega$, with $\operatorname{Im} z$ increasing, and recall the Laplace inversion formula

$$u(t) = \frac{1}{2\pi i} \int_{\Gamma_0} e^{zt} \widehat{u}(z)\, dz, \quad \text{for } \ t > 0. \tag{2.6}$$

Now let Γ be any curve in the sector $\Sigma_{\overline{\beta}}$ which is homotopic with Γ_0, and assume that the Laplace transform $\widehat{f}(z)$, defined according to (1.2), may be continued as an analytic function to the closed subdomain of $\Sigma_{\overline{\beta}}$

to the right of Γ and including Γ. Deforming the contour of integration in (2.6), we may then write

$$u(t) = \frac{1}{2\pi i}\int_\Gamma e^{zt} w(z)\,dz, \quad \text{where } w(z) = \widehat{\mathcal{E}}(z)g(z). \tag{2.7}$$

Taking $f \equiv 0$ in (1.3), so that $g(z) = u_0$ in (2.4), we see that the solution operator for the homogeneous case of problem (1.1) is given by

$$\mathcal{E}(t)u_0 = \frac{1}{2\pi i}\int_\Gamma e^{zt}\widehat{\mathcal{E}}(z)u_0\,dz. \tag{2.8}$$

For the inhomogeneous case, the inverse Laplace transform of $\widehat{\mathcal{E}}(z)\widehat{f}(z)$ is the convolution of $\mathcal{E}(t)$ and $f(t)$, so one may show the Duhamel formula

$$u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t-s)f(s)\,ds. \tag{2.9}$$

By the argument in [**14**, Theorems 2.1 and 2.2] one may establish the stability and smoothing property

$$\|A^\sigma \mathcal{E}^{(k)}(t)u_0\| \le CMt^{-\sigma(1+\alpha)-k}\|u_0\|, \tag{2.10}$$

for $t > 0$, $0 \le \sigma \le 1$ and $k \ge 0$. In particular, by the case $\sigma = k = 0$, it follows from (2.9) that the continuous problem (1.1) is stable in the sense that

$$\|u(t)\| \le CM\left(\|u_0\| + \int_0^t \|f(s)\|\,ds\right), \quad \text{for} \quad t \ge 0. \tag{2.11}$$

For our numerical methods we thus select an integration contour Γ in (2.7), such that $\widehat{f}(z)$, and thus also $g(z)$, is analytic on and to the right of Γ, and then apply a quadrature formula to (2.7). To make this more precise, we assume that $\widehat{f}$ is analytic in $\Sigma_\beta^\omega := \omega + \Sigma_\beta \subset \Sigma_{\overline{\beta}}$, with $\omega \ge 0$, $\frac{1}{2}\pi < \beta \le \overline{\beta} < \pi$, and we choose Γ to be a curve with parametric representation of the form

$$z(\xi) := \omega + \lambda(1 - \sin(\delta - i\xi)), \quad \text{for } \xi \in \mathbb{R}, \tag{2.12}$$

where the constants λ and δ satisfy

$$\lambda > 0 \quad \text{and} \quad 0 < \delta < \beta - \tfrac{1}{2}\pi. \tag{2.13}$$

Writing $z = x + iy$ we find that Γ is the left branch of the hyperbola

$$\left(\frac{x-\omega-\lambda}{\lambda\sin\delta}\right)^2 - \left(\frac{y}{\lambda\cos\delta}\right)^2 = 1, \tag{2.14}$$

which cuts the real axis at the point $z = \omega + \lambda(1 - \sin\delta)$ and has asymptotes $y = \pm(x - \omega - \lambda)\cot\delta$. Thus, the conditions (2.13) ensure that Γ lies in the sector Σ_β^ω and crosses into the left half-plane. The same family of contours was used in [**14**], with a different parametrization.

Using (2.12) in (2.7) we may represent $u(t)$ as an integral in ξ,

$$\begin{gathered} u(t) = \int_{-\infty}^{\infty} v(\xi, t)\, d\xi, \\ \text{where} \quad v(\xi, t) = \frac{1}{2\pi i}\, e^{z(\xi)t} w\big(z(\xi)\big) z'(\xi). \end{gathered} \tag{2.15}$$

The factor $e^{z(\xi)t}$ has modulus $e^{\mathrm{Re}\, z(\xi)t} = e^{\omega t} e^{\lambda t(1-\sin\delta\cosh\xi)}$, showing that as a function of ξ, the integrand exhibits a very rapid, double-exponential, decay as $|\xi| \to \infty$, for any fixed $t > 0$.

2.1. *First method.* For our first approximation method, we choose a quadrature step $k > 0$ and apply an equal weight quadrature rule

$$Q_N(v) := k \sum_{j=-N}^{N} v(\xi_j) \approx J(v) := \int_{-\infty}^{\infty} v(\xi)\, d\xi, \quad \textit{with} \;\; \xi_j := jk. \tag{2.16}$$

Setting $z_j := z(\xi_j)$, $z_j' := z'(\xi_j)$, we then obtain an approximate solution to our problem of the form

$$U_N(t) := Q_N(v(\cdot, t)) = \frac{k}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} w(z_j)\, z_j'. \tag{2.17}$$

To compute $U_N(t)$ we must then solve the $2N + 1$ "elliptic" equations

$$(z_j^{1+\alpha} I + A) w(z_j) = z_j^\alpha g(z_j), \quad \text{for} \quad |j| \le N. \tag{2.18}$$

These equations are independent and hence may be solved in parallel. We remark that the $w(z_j)$ determine the approximate solutions (2.17) for all $t > 0$. In practice, however, the accuracy of the approximation $U_N(t) \approx u(t)$ deteriorates as $t \to 0$ or $t \to \infty$. Notice that the numerical solution (2.17)depends on the choice of the curve Γ, even though the representation (2.7) does not.

To analyze the quadrature error, we extend the parametric representation (2.12) of Γ to a conformal mapping

$$z = \Phi(\zeta) = \omega + \lambda(1 - \sin(\delta - i\zeta)), \tag{2.19}$$

which transforms the strip $Y_r = \{\, \zeta : |\operatorname{Im}\zeta| \le r \,\}$ with $r > 0$ onto the set $S_r = \{\, \Phi(\zeta) : \zeta \in Y_r \,\} \supset \Gamma$. In fact, Φ maps the line $\operatorname{Im}\zeta = \eta$ to the left branch of the hyperbola

$$\left(\frac{x - \omega - \lambda}{\lambda \sin(\delta + \eta)}\right)^2 - \left(\frac{y}{\lambda \cos(\delta + \eta)}\right)^2 = 1, \tag{2.20}$$

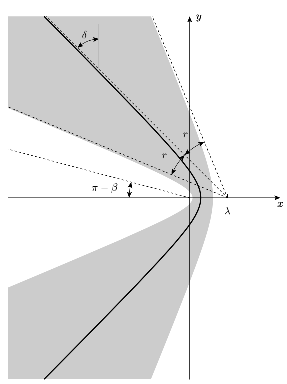

FIGURE 1. The region S_r (shaded) and the contour Γ for the case $\omega = 0$.

so S_r is bounded on the left by the left branch of the hyperbola corresponding to $\operatorname{Im}\zeta = r$ and on the right by the hyperbola branch corresponding to $\operatorname{Im}\zeta = -r$. To ensure that $S_r \subset \Sigma_\beta^\omega$ and that $\operatorname{Re} z \to -\infty$ if $|z| \to \infty$ with $z \in S_r$, we require $0 < \delta - r < \delta + r < \beta - \frac{1}{2}\pi$, see Figure 1, or equivalently that

$$0 < r < \min\bigl(\delta, \beta - \tfrac{1}{2}\pi - \delta\bigr). \tag{2.21}$$

We introduce the notation

$$\|g\|_{X,Z} := \sup_{z\in Z} \|g(z)\|_X, \quad \text{for } X \subseteq \mathcal{B} \text{ and } Z \subseteq \mathbb{C}, \tag{2.22}$$

which we abbreviate by $\|g\|_Z$ if $X = \mathcal{B}$. In Section 3 below, following recent work of López-Fernandez, Palencia and Schädle [**9**], we shall see that with a specific quadrature step in (2.16) satisfying $k \propto 1/N$ and with λ appropriately chosen, depending on N, then we have, with $\mu > 0$,

$$\|U_N(t) - u(t)\| \le CMe^{-\mu N}\bigl(\|u_0\| + \|\widehat{f}\|_{\Sigma_\beta^\omega}\bigr), \quad 0 < t_0 \le t \le T. \tag{2.23}$$

An error bound of order $O(e^{-cN/\log N})$, for t bounded away from 0, was derived in López-Fernandez and Palencia [**8**] for $0 < \alpha < 1$, and the same argument was also applied in McLean, Sloan and Thomée [**12**] for a related integro-differential equation of parabolic type. In this case, the contour of integration Γ was fixed, independent of N, but both parameters ω and λ in (2.12) were used to accommodate the singularities of $\widehat{f}(z)$. In [**14**], we treated (1.1) in the case $0 < \alpha < 1$ using two other quadrature rules with points on the hyperbola (2.14), and obtained error bounds of order $O(e^{-c\sqrt{N}})$ and $O(N^{-ct})$, respectively, with $c > 0$, for t bounded away from zero.

2.2. *Second method.* For the case $\alpha = 0$ of a parabolic partial differential equation, Gavrilyuk and Makarov [**4**] modified the integrand in the representation formula (2.7) in a way that gave $O(e^{-c\sqrt{N}})$ convergence, uniformly down to $t = 0$, provided the data possess some "spatial" regularity. A similar modification works when $\alpha \neq 0$: If we define

$$F(t) := \int_0^t f(s)\,ds \quad \text{and} \quad \mathcal{F}(t) = u_0 + F(t),$$

then $\mathcal{L}\{\mathcal{F}(t)\} = z^{-1}\big(u_0 + \widehat{f}(z)\big) = z^{-1}g(z)$, so we may write

$$u(t) = \mathcal{F}(t) + \frac{1}{2\pi i}\int_\Gamma e^{zt}\widehat{\mathcal{E}}^0(z)g(z)dz, \quad \widehat{\mathcal{E}}^{\,0}(z) := \widehat{\mathcal{E}}(z) - z^{-1}I. \tag{2.24}$$

The point of this modification is that if $g(z)$ possesses some spatial regularity, then $\|\widehat{\mathcal{E}}^0(z)g(z)\|$ decays more quickly than $\|\widehat{\mathcal{E}}(z)g(z)\|$ as $|z| \to \infty$ for $z \in \Gamma$.

Setting

$$w^0(z) := \widehat{\mathcal{E}}^0(z)g(z) = w(z) - z^{-1}g(z), \tag{2.25}$$

and using the parametric representation (2.12) of Γ, with λ appropriately chosen in the modified integral in (2.24), we now have

$$u(t) = \mathcal{F}(t) + \int_{-\infty}^{\infty} v^0(\xi, t)\, d\xi, \quad v^0(\xi, t) := \frac{1}{2\pi i} e^{z(\xi)t} w^0(z(\xi))\, z'(\xi).$$

Applying again the quadrature rule (2.16) we obtain our second approximate solution to (1.1),

$$U_N^0(t) := \mathcal{F}(t) + \frac{k}{2\pi i}\sum_{j=-N}^{N} e^{z_j t} w^0(z_j)\, z_j'. \tag{2.26}$$

Once again, to compute this approximate solution, we must first obtain the values of $w(z_j)$ for $|j| \le N$ by solving the "elliptic" equations (2.18), and then use (2.25) to find the $w^0(z_j)$. The approximate solution $U_N^0(t)$ is then determined by (2.26) for all $t \ge 0$.

To define the "spatial" regularity we introduce a scale of Banach spaces $\mathcal{B}^\sigma$ with norms $\|\cdot\|_\sigma$ for $\sigma \ge 0$ by

$$\mathcal{B}^\sigma := \{\, v \in \mathcal{B} : A^\sigma v \in \mathcal{B}\,\} \quad \text{and} \quad \|v\|_\sigma = \|v\|_{\mathcal{B}^\sigma} = \|A^\sigma v\|.$$

For our modified method (2.26), with the quadrature step chosen in a specific way such that $k \propto 1/\sqrt{N}$, and with $0 < \sigma \le 1$ and $\|g\|_{\sigma,Z} = \|g\|_{\mathcal{B}^\sigma,Z}$, cf. (2.22), we prove

$$\|U_N^0(t) - u(t)\| \le CM\, e^{-c\sqrt{N}}\big(\|u_0\|_\sigma + \|\widehat{f}\|_{\sigma,\Sigma_\beta^\omega}\big), \quad 0 \le t \le T. \tag{2.27}$$

In practice, it is important to minimize the spatial regularity requirements for the inhomogeneous term so that we avoid imposing unwanted restrictions on the boundary values of $f(t)$. Fortunately, we may rely instead on regularity in time, as reflected in the decay of the Laplace transform $\widehat{f}(z)$ as $|z| \to \infty$. Defining

$$\|g\|_{\sigma,\nu,Z} = \sup_{z\in Z}\big((1+|z|)^{\nu}\|g(z)\|_{\sigma}\big), \quad \text{for } \sigma,\ \nu \geq 0, \tag{2.28}$$

we will show that if $(1+\alpha)\sigma_0 + \nu \geq (1+\alpha)\sigma,\ \sigma_0 \geq 0$, then the error estimate (2.27) may be replaced by

$$\|U_N^0(t) - u(t)\| \leq CM\, e^{-c\sqrt{N}}\big(\|u_0\|_{\sigma} + \|\widehat{f}\|_{\sigma_0,\nu,\Sigma_\beta^\omega}\big), \quad 0 \leq t \leq T. \tag{2.29}$$

For example, if $f(t) = e^{-t}v$, then $\widehat{f}(z) = (1+z)^{-1}v$ so that $\|\widehat{f}\|_{1,\Sigma_\beta^\omega} < \infty$ requires $Av \in \mathcal{B}$, whereas $\|\widehat{f}\|_{0,1,\Sigma_\beta^\omega} < \infty$ only requires $v \in \mathcal{B}$.

2.3. *Third method.* A serious restriction in the application of these two schemes is that they require the Laplace transform $\widehat{f}(z)$ to exist, to be computable for each z on the contour Γ, and to be such that the norms of $\widehat{f}(z)$ indicated above are finite. We remark that using the stability estimate (2.11), one can see that it suffices that the given $f(t)$ may be approximated sufficiently well by a function $\widetilde{f}(t)$ which has the above properties; such approximation is discussed in [**23**].

We therefore consider a third alternative, based on the application of Duhamel's formula (2.9), which does not have the disadvantages mentioned above. Substituting the integral representation (2.8) into (2.9), we find that

$$\begin{aligned} u(t) &= \frac{1}{2\pi i}\int_{\Gamma} e^{zt}\widehat{\mathcal{E}}(z)u_0\,dz + \int_0^t \frac{1}{2\pi i}\int_{\Gamma} e^{z(t-s)}\widehat{\mathcal{E}}(z)f(s)\,dz\,ds \\ &= \frac{1}{2\pi i}\int_{\Gamma}\widehat{\mathcal{E}}(z)g(z,t)\,dz, \\ g(z,t) &:= e^{zt}u_0 + \int_0^t e^{z(t-s)}f(s)\,ds. \end{aligned} \tag{2.30}$$

This means that, compared to (2.7), we have restricted the integration in the definition of $\widehat{f}(z)$ to $(0,t)$, which is consistent with the fact that

$u(t)$ only depends on f over this interval. Note that we have included the factor e^{zt} in the definition of $g(z,t)$ to avoid floating-point overflow when $\operatorname{Re} z$ is large and negative. Since

$$\frac{1}{2\pi i}\int_\Gamma z^{-1} g(z,t)\,dz = \operatorname*{res}_{z=0} \frac{g(z,t)}{z} = g(0,t) = \mathcal{F}(t),$$

it follows that

$$u(t) = \mathcal{F}(t) + \frac{1}{2\pi i}\int_\Gamma \widehat{\mathcal{E}}^0(z) g(z,t)\,dz,$$

which is similar to (2.24). Setting $w(z,t) := \widehat{\mathcal{E}}(z) g(z,t)$ and

$$\widetilde{w}(z,t) := \widehat{\mathcal{E}}^0(z) g(z,t) = w(z,t) - z^{-1} g(z,t), \tag{2.31}$$

and using once again the parametric representation (2.12) for Γ, we obtain

$$u(t) = \mathcal{F}(t) + \int_{-\infty}^{\infty} \tilde{v}(\xi,t)\,d\xi, \quad \text{where} \quad \tilde{v}(\xi,t) = \frac{1}{2\pi i}\widetilde{w}\big(z(\xi),t\big) z'(\xi).$$

The quadrature rule (2.16) now gives our third approximate solution

$$\widetilde{U}_N(t) := \mathcal{F}(t) + \frac{k}{2\pi i}\sum_{j=-N}^{N} \widetilde{w}(z_j,t) z_j', \tag{2.32}$$

where the $\widetilde{w}(z_j,t)$ may be obtained by first solving the equations

$$(z_j^{1+\alpha} I + A) w(z_j,t) = z_j^\alpha g(z_j,t), \quad \text{for } |j| \le N, \tag{2.33}$$

and then using (2.31). In contrast to the elliptic equations (2.18) arising in the previous two schemes, the right hand sides in (2.33), and hence also the solutions, may now depend on t. This is the price we pay to obtain a scheme requiring only $f(t)$ and not its Laplace transform $\widehat{f}(z)$. Fortunately, the equations (2.33) are independent both for different j and for different t, so not only can we solve each system of $2N+1$ equations in parallel, but we may also solve the systems for different t in parallel.

For our third scheme (2.32) we prove that with a $k \propto 1/\sqrt{N}$, and if $\sigma_0 + (1+\alpha)^{-1} \geq \sigma$, then

$$\|\widetilde{U}_N(t) - u(t)\| \leq CM\, e^{-c\sqrt{N}}\Big(\|u_0\|_\sigma + \|f(0)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0}\, ds\Big), \quad \text{for } 0 \leq t \leq T, \tag{2.34}$$

i.e., the convergence rate is the same as in (2.29) but with no requirement that $\widehat{f}(z)$ exist and be bounded for $z \in \Sigma_\beta^\omega$.

The error in approximating $f(t)$ by a function $\widetilde{f}(t)$, for instance by some interpolation process, which makes $g(z,t)$ defined in (2.30) more easily computable, may again be handled by the stability estimate (2.11).

2.4. *Fully-discrete schemes.* Suppose now that $A = -\Delta$ in (1.1), where Δ is the Laplacian in a smooth (or convex) bounded domain $\Omega \subset \mathbb{R}^d$, under homogeneous Dirichlet boundary conditions. We then first discretize (1.1) in the spatial variables by piecewise linear finite elements, which results in an initial boundary value problem of the form (1.1) in the finite element space, where now $A = A_h = -\Delta_h$, with Δ_h the discrete Laplacian. To define a fully discrete solution we may then apply one of our above time discretization methods to this spatially semidiscrete problem.

Thus, our initial value problem (1.1) now takes the form

$$\partial_t u - \partial_t^{-\alpha}\Delta u = f(t), \quad \text{for } t > 0, \quad \text{with } u(0) = u_0, \tag{2.35}$$

and we consider this equation in the Hilbert space $L_2 = L_2(\Omega)$ equipped with the usual norm $\|\cdot\|_{L_2}$. Since $A = -\Delta$ is positive definite, we have $\operatorname{spec}(A) \subset (0,\infty)$, and it is clear that Δ generates an analytic semigroup $e^{\Delta t}$, and that the resolvent estimate (2.2) holds for arbitrarily small φ. In particular, it follows that the stability and smoothness estimates (2.10) hold in this case.

To discretize in space only, we use a family of triangulations $\mathcal{T}_h = \{K\}$ of Ω indexed by h, the maximum diameter of the elements K. Let V_h

denote the corresponding space of continuous piecewise linear functions vanishing on $\partial\Omega$, and recall the approximation property

$$\inf_{\chi\in V_h}\left\{\|v-\chi\|_{L_2}+h\|\nabla(v-\chi)\|_{L_2}\right\}\le Ch^2\|v\|_{H^2}.$$

The spatially semidiscrete problem is then to find $u_h(t)\in V_h$ for $t\ge 0$, such that

$$(2.36)\qquad \begin{gathered}(\partial_t u_h,\chi)+(\partial_t^{-\alpha}\nabla u_h,\nabla\chi)=(f,\chi),\quad \forall\ \chi\in V_h,\ t\ge 0,\\ u_h(0)=u_{0h}.\end{gathered}$$

Here, as usual, $(\cdot,\cdot)$ denotes the inner product in $L_2(\Omega)$ and $u_{0h}\in V_h$ is a suitable approximation to u_0. Introducing the discrete Laplacian $\Delta_h : V_h\to V_h$ defined by

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

the problem (2.36) is equivalent to

$$(2.37)\quad \partial_t u_h-\partial_t^{-\alpha}\Delta_h u_h=P_hf(t),\quad \text{for } t\ge 0,\quad \text{with } u_h(0)=u_{0h},$$

where $P_h : L_2(\Omega)\to V_h$ is the orthogonal projector with respect to $(\cdot,\cdot)$. Since $-\Delta_h$ is positive definite, the resolvent estimate (2.2) again holds for arbitrarily small φ, with M independent of h. Thus, also the analogue of (2.10) applies to the solution operator $\mathcal{E}_h(t)$ of the spatially semidiscrete homogeneous equation.

In the analysis in Section 4 of the spatial discretization we show the nonsmooth and smooth data error estimates, with $u_{0h}=P_hu_0$,

$$\|u_h(t)-u(t)\|_{L_2}\le C^2t^{-1-\alpha}h^2(\|u_0\|_{L_2}+\|\widehat{f}\|_{L_2,\Sigma_\beta^\omega}),\quad \text{for } 0<t\le T,$$

and, for u_0 and f sufficiently smooth, but with $f(t)$ not necessarily satisfying any boundary conditions for $t>0$,

$$\|u_h(t)-u(t)\|_{L_2}\le C(u_0,f)h^2,\quad \text{for } 0\le t\le T.$$

Subsequently, in Section 5, we apply the error estimates (2.23), (2.29) and (2.34) for our time discretization methods to the spatially semidiscrete problem, in a way that yields error estimates for the corresponding fully discrete solutions.

We note that the problems (2.35) and (2.36) could also have been considered in the Banach space $\mathcal{C}_0(\Omega)$ of continuous functions, vanishing on $\partial\Omega$, equipped with the maximum-norm. In fact, the resolvent estimate (2.2) then holds for $A = -\Delta$ by Stewart [**24**], and for $A = -\Delta_h$, uniformly in h, in the case of quasiuniform triangulations, by Bakaev, Thomée and Wahlbin [**1**]. We shall not give the details here.

3. Time discretization. We begin by showing the nonsmooth data error estimate (2.23), which is based on an error bound for the quadrature rule (2.16). The analysis will depend on assuming that the integrand may be analytically continued into a strip Y_r around the real axis in the complex ζ-plane, and satisfies a certain boundedness property there.

The next lemma is essentially an improvement, used in [**9**], of [**8**, Theorem 2], cf. also [**12**], and shows that under appropriate conditions the quadrature error is of order $O(e^{-\mu N})$ as $N \to \infty$, with $\mu > 0$, for t bounded away from zero. For completeness we include a sketch of the proof. Here and below we write $\bar{r} = 2\pi r$ and $\ell(t) = \max\big(1, \log(1/t)\big)$.

Lemma 3.1. *Assume v is analytic in the strip $Y_r = \{\zeta : |\mathrm{Im}\,\zeta| \le r\}$, and that there exist positive V_η and γ_η, increasing in η, such that*

$$\|v(\zeta)\| \le V_\eta e^{-\gamma_\eta \cosh \xi} \quad \text{for} \;\; \zeta = \xi + i\eta \in Y_r. \tag{3.1}$$

Then, with $Q_N(v)$ and $J(v)$ as in (2.16), and if $k = b/N$, where b satisfies $b \cosh b = \bar{r}N/\gamma_0$, we have, for $k \le \bar{r}/\log 2$,

$$\|Q_N(v) - J(v)\| \le C V_r \ell(\gamma_{-r})\, e^{-\bar{r}N/b}. \tag{3.2}$$

Proof. Let $Q_\infty(v) = k \sum_{j=-\infty}^{\infty} v(jk)$. Using contour integration as in [**14**, Theorem 3.1] it can be shown that

$$\|Q_\infty(v) - J(v)\| \le \frac{e^{-\bar{r}/k}}{1 - e^{-\bar{r}/k}} \int_{-\infty}^{\infty} \big(\|v(\xi + ir)\| + \|v(\xi - ir)\|\big)\, d\xi, \tag{3.3}$$

so we have, since $e^{-\bar{r}/k} \le 1/2$ and $\bar{r}/k = \bar{r}N/b$,

$$\|Q_\infty(v) - J(v)\| \le \frac{4V_r e^{-\bar{r}/k}}{1 - e^{-\bar{r}/k}} \int_0^\infty e^{-\gamma_{-r}\cosh\xi}\, d\xi \le CV_r \ell(\gamma_{-r}) e^{-\bar{r}N/b},$$

where we have used, see [**8**], that the integral is bounded by $C\ell(\gamma_r)$. Estimating the remainder of the infinite sum, we have

$$\|Q_\infty(v) - Q_N(v)\| \le 2V_0 k \sum_{j=N+1}^{\infty} e^{-\gamma_0 \cosh(jk)} \le 2V_r \int_{Nk}^\infty e^{-\gamma_0 \cosh\xi}\, d\xi,$$

and, because $\gamma_0 \cosh(Nk) = \gamma_0 \cosh b = \bar{r}N/b$, we find, using the substitution $s = \cosh\xi - \cosh(Nk)$, that

$$\begin{aligned}\int_{Nk}^\infty e^{-\gamma_0\cosh\xi}\, d\xi &= e^{-\gamma_0\cosh(Nk)} \int_0^\infty \frac{e^{-\gamma_0 s}}{\sqrt{(s+\cosh(Nk))^2 - 1}}\, ds \\ &\le e^{-\bar{r}N/b} \int_0^\infty \frac{e^{-\gamma_0 s}}{\sqrt{s^2+2s}}\, ds \le Ce^{-\bar{r}N/b}\ell(\gamma_0).\end{aligned}$$

Since $\ell(t)$ is decreasing, this completes the proof of (3.2).

To apply Lemma 3.1 to our numerical method, recall the conformal mapping $\Phi : \zeta \mapsto z$ defined in (2.19), whose restriction to the real axis coincides with the parametric representation (2.12) of the integration contour $\Gamma \subset S_r = \Phi(Y_r)$. In the proof of our error estimate for $U_N(t)$ we shall need the following technical lemma for the behavior of $\Phi(\zeta)$.

Lemma 3.2. *If $\zeta = \xi + i\eta$, then we have, for $\zeta \in Y_r$,*

$$|\Phi(\zeta) - \omega| \ge \tfrac{1}{2}\lambda e^{|\xi|}\cos^2(\delta+\eta) \quad \textit{and} \quad \left|\frac{\Phi'(\zeta)}{\Phi(\zeta)-\omega}\right| \le \frac{2}{\cos(\delta+\eta)}.$$

Proof. We have, setting $\psi = \delta + \eta$ for brevity,

$$\begin{aligned}|\Phi(\zeta) - \omega|^2 &= \lambda^2 |1 - \sin(\psi - i\xi)|^2 \\ &= \lambda^2\big((1 - \sin\psi\, \cosh\xi)^2 + \cos^2\psi \sinh^2\xi\big) = \lambda^2(\cosh\xi - \sin\psi)^2.\end{aligned}$$

Hence

$$e^{-|\xi|}|\Phi(\zeta)-\omega| = \lambda e^{-|\xi|}(\cosh\xi - \sin\psi) = \tfrac{1}{2}\lambda(e^{-2|\xi|} - 2e^{-|\xi|}\sin\psi + 1)$$
$$= \tfrac{1}{2}\lambda\big((e^{-|\xi|} - \sin\psi)^2 + \cos^2\psi\big) \ge \tfrac{1}{2}\lambda\cos^2\psi.$$

Similarly

$$|\Phi'(\zeta)|^2 = \lambda^2|\cos(\psi - i\xi)|^2 = \lambda^2(\cosh^2\xi - \sin^2\psi), \tag{3.4}$$

and hence

$$\left|\frac{\Phi'(\zeta)}{\Phi(\zeta)-\omega}\right|^2 = \frac{\cosh^2\xi - \sin^2\psi}{(\cosh\xi - \sin\psi)^2} = \frac{\cosh\xi + \sin\psi}{\cosh\xi - \sin\psi}$$
$$\le \frac{1+\sin\psi}{1-\sin\psi} \le \frac{4}{\cos^2\psi}. \qquad \square$$

We are now ready for the proof of (2.23). We recall from (2.22) the notation $\|g\|_Z = \sup_{z\in Z}\|g(z)\|$.

Theorem 3.1. *Let u be the solution of* (1.1)*, with $\widehat{f}$ analytic in Σ_β^ω. Let $0 < t_0 < T$, $0 < \theta < 1$, and let $b > 0$ be defined by $\cosh b = 1/(\theta\tau\sin\delta)$, where $\tau = t_0/T$. Let r satisfy* (2.21) *so that $\Gamma \subset S_r \subset \Sigma_\beta^\omega$, and let the scaling factor be $\lambda = \theta\bar{r}N/(bT)$. Then we have, for the approximate solution $U_N(t)$ defined by* (2.17)*, with $k = b/N \le \bar{r}/\log 2$,*

$$\|U_N(t) - u(t)\| \le CM\, e^{\omega t}\ell(\rho_r N)e^{-\mu N}\big(\|u_0\| + \|\widehat{f}\|_{\Sigma_\beta^\omega}\big), \quad \textit{for } t_0 \le t \le T,$$

where $\mu = \bar{r}(1-\theta)/b$, $\rho_r = \theta\bar{r}\tau\sin(\delta - r)/b$, and $C = C_{\delta,r,\beta}$.

Proof. To apply Lemma 3.1 to the representation (2.15), we set

$$v(\zeta,t) = \frac{1}{2\pi i}e^{\Phi(\zeta)\,t}w(\Phi(\zeta))\Phi'(\zeta), \quad \text{for } \zeta \in Y_r. \tag{3.5}$$

Since $w(z) = \widehat{\mathcal{E}}(z)g(z)$, cf. (2.7), the resolvent estimate (2.5) and the inequality $|z| \ge c_\beta|z-\omega|$ for $z \in \Sigma_\beta^\omega$, with $c_\beta = \sin\beta > 0$, give

$$\|w(z)\| \le M|z|^{-1}\big\|g(z)\big\| \le CM|z-\omega|^{-1}\big\|g(z)\big\|, \quad \text{for } z \in \Sigma_\beta^\omega,$$

and so, since $\operatorname{Re}\Phi(\zeta) = \omega + \lambda(1 - \sin(\delta+\eta)\cosh\xi)$, we have

$$\|v(\zeta,t)\| \le CMe^{\omega t}\, e^{\lambda t(1-\sin(\delta+\eta)\cosh\xi)}\, \frac{|\Phi'(\zeta)|}{|\Phi(\zeta)-\omega|}\, \|g\|_{\Sigma_\beta^\omega}, \quad \text{for } \zeta \in Y_r.$$

Thus, using Lemma 3.2, we see that $v(\zeta,t)$ satisfies (3.1) with

$$\begin{aligned} V_\eta &= \frac{CM}{\cos(\delta+\eta)}\, e^{(\omega+\lambda)t}\|g\|_{\Sigma_\beta^\omega}, \\ \gamma_\eta &= \lambda t_0 \sin(\delta+\eta), \quad \text{for } t \ge t_0. \end{aligned} \tag{3.6}$$

With b and λ chosen as stated we have $b\cosh b = b/(\theta\tau\sin\delta) = bT\lambda/(\theta\lambda t_0\sin\delta) = \bar{r}N/\gamma_0$, and hence Lemma 3.1 yields

$$\|U_N(t) - u(t)\| \le CM\ell(\gamma_{-r})e^{\omega t}e^{\lambda T}e^{-\bar{r}N/b}\|g\|_{\Sigma_\beta^\omega}, \quad \text{for } t_0 \le t \le T.$$

Since $\lambda T - \bar{r}N/b = (\theta - 1)\bar{r}N/b = -\mu N$ and $\gamma_{-r} = \lambda t_0 \sin(\delta - r) = \theta\bar{r}\tau N\sin(\delta - r)/b = \rho_r N$, this shows the result stated. □

We remark that $\ell(\rho_r N) = 1$ for $N \ge 1/(\rho_r e)$ but that this lower bound is large for θ, τ and $\delta - r$ small, and also note that the constant $C_{\delta,r,\beta}$ is independent of θ, t_0 and T.

Although Theorem 3.1 implies stability in the sense that

$$\|U_N(t)\| \le C(\|u_0\| + \|\widehat{f}\|_{\Sigma_\beta^\omega}), \quad \text{for } t_0 \le t \le T,$$

numerical evaluation of the sum (2.17) is sensitive to perturbations in $w(z_j)$, cf. [**9**]. To illustrate this, assume that there are perturbations of $w(z_j)$ (in applications containing the errors in solving the elliptic equations (2.18)), which are bounded by ε in norm for all j. Then, using (3.4), the effect on $U_N(t)$ may be bounded by

$$\varepsilon\,\frac{k}{2\pi}\sum_{|j|\le N} |e^{\Phi(\xi_j)}\Phi'(\xi_j)| \le C\,\varepsilon\,\lambda\, e^{(\omega+\lambda)t}\, k \sum_{|j|\le N} \cosh\xi_j\, e^{-\gamma_0\cosh\xi_j}.$$

One may show (cf. [**9**], p. 1340) that the Riemann sum is bounded by C/γ_0, and since $\lambda/\gamma_0 \le C$ and $\lambda t \le \lambda T = (\theta\bar{r}/b)N$, for $t_0 \le t \le T$, the above error is bounded by $C\varepsilon e^{(\theta\bar{r}/b)N}$, which grows exponentially with N. The instability is weaker with a smaller θ, at the expense of the rate of convergence in Theorem 3.1, and may be removed by choosing $\theta = 1/N$: In this case $b = O(\log N)$ and the error of order $O(e^{-cN/\log N})$, with $c > 0$, cf. also [**8, 12**]. For a more sophisticated approach to choosing $\theta = O(1/N)$, see the discussion in [**9**, Section 4].

We shall now consider error estimates which hold uniformly down to $t = 0$, under some regularity assumptions on the data, for the modified approximation rules (2.26) and (2.32) based on the representations (2.24) and (2.30), respectively. We remark that it is not difficult to show that the result of Theorem 3.1 is valid also when the quadrature rule (2.16) is applied to the modified representation (2.24), i.e., the choice $k = b/N$ again leads to convergence of order $O(e^{-cN})$ for t bounded away from zero. We begin with a technical lemma.

Lemma 3.3. *If A satisfies the resolvent estimate* (2.2) *and if $0 \le \sigma \le 1$, then, with $\widehat{\mathcal{E}}^0(z)$ as defined in* (2.24), *we have*

$$\big\|\widehat{\mathcal{E}}^0(z)v\big\| \le \frac{C_\sigma M}{|z|(1+|z|^{1+\alpha})^\sigma}\|v\|_\sigma, \quad \textit{for } z \in \Sigma_{\overline{\beta}} \quad \textit{and } v \in \mathcal{B}^\sigma.$$

Proof. Setting $w = z^{1+\alpha}$, $\mathcal{R}(w) = (wI + A)^{-1}$, we have

$$\widehat{\mathcal{E}}^0(z) = (wI + A)^{-1}(z^\alpha I - z^{-1}(wI + A)) = -z^{-1}A^{1-\sigma}\mathcal{R}(w)A^\sigma,$$

and, using the interpolation inequality, cf. Pazy [**18**, p. 73],

$$\|v\|_{1-\sigma} \le C_\sigma \|v\|_0^\sigma \, \|v\|_1^{1-\sigma} = C_\sigma \|v\|^\sigma \, \|Av\|^{1-\sigma}, \tag{3.7}$$

we conclude

$$\begin{aligned}\big\|\widehat{\mathcal{E}}^0(z)v\big\| &= |z|^{-1}\big\|\mathcal{R}(w)A^\sigma v\big\|_{1-\sigma} \\ &\le C_\sigma |z|^{-1}\big\|\mathcal{R}(w)A^\sigma v\big\|^\sigma \big\|A\mathcal{R}(w)A^\sigma v\big\|^{1-\sigma}.\end{aligned}$$

If $z \in \Sigma_{\overline{\beta}}$, then (2.5) and the fact that $A\mathcal{R}(w) = I - w\mathcal{R}(w)$ give

$$\big\|\mathcal{R}(w)A^\sigma v\big\| \le \frac{M\|A^\sigma v\|}{1+|w|} \quad \text{and} \quad \big\|A\mathcal{R}(w)A^\sigma v\big\| \le CM\|A^\sigma v\|.$$

Together these estimates show the desired bound. □

The following lemma provides the modification of Lemma 3.1 appropriate to an assumed "single exponential" decay rate for the integrand.

Lemma 3.4. *Assume that v is bounded and analytic in Y_r, and that*

$$\|v(\zeta)\| \le V e^{-\gamma|\xi|}, \quad \textit{for } \zeta = \xi + i\eta \in Y_r, \quad \textit{with } \gamma > 0.$$

Then, with $Q_N(v)$ and $J(v)$ as in (2.16), we have, for $k = \sqrt{\bar{r}/(\gamma N)} \le \bar{r}/\log 2$,

$$\|Q_N(v) - J(v)\| \le C_r\, V\gamma^{-1}\, e^{-\sqrt{\bar{r}\gamma N}}. \tag{3.8}$$

Proof. By (3.3) we obtain, since $e^{-\bar{r}/k} \le 1/2$,

$$\|Q_\infty(v) - J(v)\| \le \frac{4Ve^{-\bar{r}/k}}{1 - e^{-\bar{r}/k}} \int_0^\infty e^{-\gamma\xi}\, d\xi \le 8\gamma^{-1}\, V e^{-\bar{r}/k},$$

whereas for the tail of the infinite sum,

$$\begin{aligned} \|Q_\infty(v) - Q_N(v)\| &\le 2Vk \sum_{j=N+1}^{\infty} e^{-\gamma\xi_j} \le 2V \int_{Nk}^{\infty} e^{-\gamma\xi}\, d\xi \\ &\le 2V\gamma^{-1} e^{-\gamma Nk}. \end{aligned}$$

The error bound (3.8) now follows by the triangle inequality, after choosing $\bar{r}/k = \gamma Nk$, i.e., as stated. □

We are now ready to show the convergence of order $O(e^{-c\sqrt{N}})$, uniformly down to $t = 0$, for our second approximation method (2.26). In order to reduce the demands for "spatial" regularity on the inhomogeneous term $f(t)$, we use the norms $\|\widehat{f}\|_{\sigma,\nu,Z}$ introduced in (2.28).

Theorem 3.2. *Let u be the solution of* (1.1), *with $\widehat{f}$ analytic in Σ_β^ω. Let $0 < \sigma \le 1$, set $\gamma = (1+\alpha)\sigma$, and let $\Gamma \subset S_r \subset \Sigma_\beta^\omega$ be defined by $\lambda = \gamma/(\kappa T)$, where $\kappa = 1 - \sin(\delta - r)$. Let $U_N(t)$ be the approximate solution* (2.26) *with $k = \sqrt{\bar{r}/(\gamma N)} \le \bar{r}/\log 2$. Then, if $\sigma_0,\ \nu \ge 0$ and $\sigma_0 + \nu(1+\alpha)^{-1} \ge \sigma$, we have, with $C = C_{\delta,r,\beta,\sigma,\sigma_0}$, for $0 \le t \le T$,*

$$\|U_N^0(t) - u(t)\| \le CM\gamma^{-1}T^\gamma e^{\omega t} e^{-\sqrt{\bar{r}\gamma N}} \,(\|u_0\|_\sigma + \|\widehat{f}\|_{\sigma_0,\nu,\Sigma_\beta^\omega}).$$

Proof. Define $v^0(\zeta,t)$ as $v(\zeta,t)$ in (3.5), but with w^0 in place of w, where $w^0(z)$ is defined by (2.25). By Lemma 3.3 we have, for $z \in \Sigma_\beta^\omega$,

$$\begin{aligned}\|w^0(z)\| \le \|\widehat{\mathcal{E}}^0(z)u_0\| + \|\widehat{\mathcal{E}}^0(z)\widehat{f}(z)\| &\le \frac{C_\sigma M}{|z|(1+|z|)^{(1+\alpha)\sigma}}\,\|u_0\|_\sigma \\ &\quad + \frac{C_{\sigma_0} M}{|z|\,(1+|z|)^{(1+\alpha)\sigma_0+\nu}}\ \ (1+|z|)^\nu \|\widehat{f}(z)\|_{\sigma_0} \\ &\le \frac{CM}{|z|^{1+\gamma}} G \le \frac{CM}{|z-\omega|^{1+\gamma}} G, \quad \text{where } G = \|u_0\|_\sigma + \|\widehat{f}\|_{\sigma_0,\nu,\Sigma_\beta^\omega},\end{aligned}$$

where we have used $(1+\alpha)\sigma_0 + \nu \ge (1+\alpha)\sigma = \gamma$ and $|z| \ge c_\beta |z-\omega|$ on Σ_β^ω. Hence, by Lemma 3.2, using also $1 - \sin(\delta+\eta)\cosh\xi \le \kappa$,

$$\begin{aligned}(3.9)\quad \|v^0(\zeta,t)\| &\le CM\, e^{\omega t} e^{\lambda t(1-\sin(\delta+\eta)\cosh\xi)}\, \frac{|\Phi'(\zeta)|}{|\Phi(\zeta)-\omega|^{1+\gamma}}\, G \\ &\le CM\, e^{\omega t} \frac{e^{\lambda\kappa T}}{\lambda^\gamma} e^{-\gamma|\xi|} G \le CM\, e^{\omega t}\gamma^{-\gamma} T^\gamma e^{-\gamma|\xi|} G, \quad \text{for } \zeta \in Y_r.\end{aligned}$$

Since $\gamma^{-\gamma}$ is bounded it follows by Lemma 3.4 that

$$\|U_N^0(t) - u(t)\| \le CM\, e^{\omega t}\gamma^{-1}\, T^\gamma\, e^{-\sqrt{\bar{r}\gamma N}}\, G, \quad \text{for } 0 \le t \le T.$$

Note that our choice of λ minimizes the ratio $e^{\lambda\kappa T}/\lambda^\gamma$. □

We remark that the contour Γ used in Theorem 3.2 depends on the parameter σ, i.e., on the regularity we wish to assume on the data. We also remark that in (3.9) we have simply disregarded the double exponential decay of the factor $e^{-\lambda t \sin(\delta+\eta)\cosh\xi}$ by using $\cosh\xi \ge 1$. See our later comments on the numerical results in Figure 2.

Under the choices of parameters made one may show a weak stability result for $U_N(t)$ in terms of data. In fact, similarly to (3.9) one finds

$$\|v^0(\xi,t)\| \le CM\, e^{\omega t}(\|u_0\| + \|\widehat{f}\|_{\Sigma_\beta^\omega}), \quad \text{for } \xi \in \mathbb{R},$$

and hence we have from (2.16), since $kN \le C\sqrt{N}$, for $t \ge 0$,

$$\begin{aligned}(3.10)\quad \|U_N^0(t)\| &\le \|\mathcal{F}(t)\| + \|Q_N(v^0(\cdot,t))\| \\ &\le \|u_0\| + \int_0^t \|f(s)\|\,ds + CMe^{\omega t}\sqrt{N}(\|u_0\| + \|\widehat{f}\|_{\Sigma_\beta^\omega}).\end{aligned}$$

In view of the exponential decay factors $e^{-\mu N} = e^{-\bar{r}(1-\theta)N/b}$ and $e^{-\sqrt{\bar{r}\gamma N}}$ that occur in the preceding error bounds, we see that the larger the value of the angle r in Figure 1, the faster the convergence. Thus, in practice, one should choose r slightly smaller than $\delta = \frac{1}{2}(\beta - \frac{1}{2}\pi)$. Consider a problem in which the spectrum of A allows us to take $\overline{\beta}$ close to π, but $\widehat{f}(z)$ has poles at $z = p_l \in \Sigma_{\overline{\beta}}$ for $l = 1, 2, \dots, L$, forcing us to use a value of β close to $\frac{1}{2}\pi$ and hence a small value of r, or a large value of ω, resulting in serious exponential growth of the error bound. To improve the convergence rate, we may instead choose Γ passing to the left of the poles provided we incorporate the residues in the representation (2.7), so that

$$(3.11)\qquad u(t) = \sum_{l=1}^{L} u_l(t) + \frac{1}{2\pi i}\int_\Gamma e^{zt} w(z)\,dz,$$

where, if m_l denotes the multiplicity of the pole of $\widehat{f}(z)$ at $z = p_l$,

$$u_l(t) = \operatorname*{res}_{z=p_l} e^{zt} w(z) = \lim_{z\to p_l} \frac{1}{(m_l-1)!}\left(\frac{d}{dz}\right)^{m_l-1}\big((z-p_l)^{m_l} e^{zt} w(z)\big).$$

For a simple pole, i.e., for $m_l = 1$, we can compute $u_l(t) = e^{p_l t} v_l$ by solving the elliptic problem

$$(p_l^{1+\alpha} I + A)v_l = p_l^{\alpha} \operatorname*{res}_{z=p_l} \widehat{f}(z).$$

In Section 6, we present some numerical results where the integral in (3.11) is approximated as in Theorem 3.1.

We now turn to the error bound of our third method, which looks as for our second method, and is also valid uniformly down to $t = 0$. Since the method does not use $\widehat{f}(z)$ the error bound is now expressed directly in terms of u_0 and $f(t)$. Here we may use $\omega = 0$ and $\beta = \overline{\beta}$.

Theorem 3.3. *Let u be the solution of* (1.1)*. Let $0 < \sigma \le 1$, set $\gamma = (1+\alpha)\sigma$, and let $\Gamma \subset S_r \subset \Sigma_{\overline{\beta}}$ be defined by $\lambda = \gamma/(\kappa T)$, with $\kappa = 1 - \sin(\delta - r)$. Then, if $\sigma_0 + (1+\alpha)^{-1} \ge \sigma$, we have for the approximate solution $\widetilde{U}_N(t)$ from* (2.32)*, with $k = \sqrt{\bar r/(\gamma N)} \le \bar r/\log 2$ and $C = C_{\delta,r,\bar\beta,\sigma,\sigma_0}$,*

$$\|\widetilde{U}_N(t) - u(t)\| \le CM\gamma^{-1}T^{\gamma}e^{-\sqrt{\bar r\gamma N}}\Big(\|u_0\|_\sigma + \|f(0)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0}\,ds\Big), \quad \textit{for } 0 \le t \le T.$$

Proof. Recalling the definition (2.31) we show, for $z \in \Sigma_{\overline{\beta}}$,

$$\|\widetilde{w}(z,t)\| \le CM\,\frac{e^{\lambda\kappa t}}{|z|^{1+\gamma}}\Big(\|u_0\|_\sigma + \|f(0)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0}\,ds\Big). \tag{3.12}$$

For this purpose, we note that integration by parts gives

$$\begin{aligned}\widetilde{w}(z,t) &= \widehat{\mathcal{E}}^0(z)\Big(e^{zt}u_0 + \int_0^t e^{z(t-s)}f(s)\,ds\Big),\\ &= \widehat{\mathcal{E}}^0(z)\Big(e^{zt}u_0 + z^{-1}\Big(f(0)e^{zt} - f(t) + \int_0^t e^{z(t-s)}f'(s)\,ds\Big)\Big).\end{aligned}$$

Thus, using Lemma 3.3, we find, with $\gamma_0 = (1+\alpha)\sigma_0$,

$$\begin{aligned}\|\widetilde{w}(z,t)\| \le CMe^{\lambda\kappa t}\Big(&\frac{1}{|z|(1+|z|)^{\gamma}}\|u_0\|_\sigma\\ &+ \frac{1}{|z|(1+|z|)^{1+\gamma_0}}\Big(\|f(0)\|_{\sigma_0} + \|f(t)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0}\,ds\Big)\Big).\end{aligned}$$

Since $1 + \gamma_0 \ge \gamma$, and bounding $\|f(t)\|_{\sigma_0}$ in the obvious way, (3.12) follows. For

$$\widetilde{v}(\zeta,t) = \frac{1}{2\pi i}\,\widetilde{w}(\Phi(\zeta),t)\Phi'(\zeta),$$

we hence have, for $\zeta \in Y_r$,

$$\|\widetilde{v}(\zeta,t)\| \leq CM\, e^{\lambda\kappa t}\, \frac{|\Phi'(\zeta)|}{|\Phi(\zeta)|^{1+\gamma}} \Big(\|u_0\|_\sigma + \|f(0)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0}\, ds \Big).$$

We may now proceed as in the proof of Theorem 3.2. □

Since the factor $e^{-\lambda t \sin(\delta+\eta)\cosh \xi}$ of (3.9) is not present in the above estimate for $\|v(\zeta,t)\|$, the earlier argument for an $O(e^{-cN})$ error bound for t bounded away from zero does not apply. As mentioned in the introduction, the exponential factor is now needed to make the integral term in $g(z,t)$ in (2.30) appropriately convergent.

Similarly to (3.10) one shows easily the weak stability result

$$\|\widetilde{U}_N(t)\| \leq CM\sqrt{N} \bigg(\|u_0\| + \int_0^t \|f(s)\|\, ds \bigg), \quad \text{for } t \geq 0.$$

4. Spatial discretization by finite elements. In this section we prepare the analysis of our fully discrete methods by showing three error estimates for the spatially semidiscrete method (2.36) which are designed to be combined with the error bounds in Section 3 for our three time discretization methods. We begin with a nonsmooth data error estimate for the semidiscrete problem, which was shown in [**14**, Theorem 5.1] for $0 < \alpha < 1$. The argument for $-1 < \alpha \leq 0$ is the same, but for completeness and later reference we include the proof.

Theorem 4.1. *Let $u_h(t)$ and $u(t)$ be the solutions of* (2.36) *and* (2.35), *with $\widehat{f}$ analytic in Σ_β^ω, and let $u_{0h} = P_h u_0$. Then, with $C = C_{\beta,T}$,*

$$\|u_h(t) - u(t)\|_{L_2} \leq Ch^2\, t^{-1-\alpha} \big(\|u_0\|_{L_2} + \|\widehat{f}\|_{L_2,\Sigma_\beta^\omega} \big), \quad \textit{for } 0 < t \leq T.$$

Proof. With notation as above we have, taking $\Gamma = \partial\Sigma_\beta^\omega$,

$$u_h(t) - u(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt}\, z^\alpha\, G_h(z) g(z)\, dz, \tag{4.1}$$

where, with $A = -\Delta$ and $A_h = -\Delta_h$, cf. (2.4),

$$G_h(z) := z^{-\alpha}\big(\widehat{\mathcal{E}}_h(z)P_h - \widehat{\mathcal{E}}(z)\big) = (z^{1+\alpha}I + A_h)^{-1}P_h - (z^{1+\alpha}I + A)^{-1}.$$

We shall prove below that

$$\|G_h(z)v\|_{L_2} \le Ch^2\|v\|_{L_2}, \quad \text{for } z \in \Sigma_{\overline{\beta}}. \tag{4.2}$$

Assume this has been shown. Then, since $c_\beta|z-\omega| \le |z| \le |z-\omega| + \omega$ for $z \in \Sigma_\beta^\omega$, with $c_\beta = \sin\beta > 0$, we have, setting $z = \omega + se^{\pm i\beta} \in \Gamma$, that $|z|^\alpha \le Cs^\alpha$ when $\alpha < 0$ and $|z|^\alpha \le C(1+s^\alpha)$ when $\alpha \ge 0$. Hence, for $\alpha < 0$, since $e^{\omega t}$ is bounded for $t \le T$,

$$\|u_h(t) - u(t)\|_{L_2} \le Ch^2 \int_0^\infty s^\alpha e^{-cts}\,ds\,\|g\|_{L_2,\Gamma} \le Ch^2t^{-1-\alpha}\,\|g\|_{L_2,\Sigma_\beta^\omega},$$

and similarly, for $\alpha \ge 0$,

$$\|u_h(t) - u(t)\|_{L_2} \le Ch^2(t^{-1} + t^{-1-\alpha})\,\|g\|_{L_2,\Gamma} \le Ch^2t^{-1-\alpha}\,\|g\|_{L_2,\Sigma_\beta^\omega}.$$

Together these estimates show the result stated.

To show (4.2), we set $w = z^{1+\alpha}$, $\mathcal{R}(w) = (wI + A)^{-1}$ and $\mathcal{R}_h(w) = (wI + A_h)^{-1}$ and write

$$G_h(z) = \mathcal{R}_h(w)P_h - \mathcal{R}(w) = G_h^1(z) + G_h^2(z),$$

where

$$G_h^1(z) := (P_h - I)\mathcal{R}(w) \quad \text{and} \quad G_h^2(z) := \mathcal{R}_h(w)P_h - P_h\mathcal{R}(w).$$

We recall the elliptic regularity estimate

$$\|v\|_{H^2} \le C\|Av\|_{L_2}, \quad \text{if } v = 0 \text{ on } \partial\Omega. \tag{4.3}$$

Since $\|P_hv - v\|_{L_2} \le Ch^2\|v\|_{H^2}$ and since the operator $A\mathcal{R}(w)$ is uniformly bounded for $z \in \Sigma_{\overline{\beta}}$, we obtain

$$\|G_h^1(z)v\|_{L_2} \le Ch^2\|\mathcal{R}(w)v\|_{H^2} \le Ch^2\|A\mathcal{R}(w)v\|_{L_2} \le Ch^2\|v\|_{L_2}. \tag{4.4}$$

To bound $G_h^2(z)$, we use the Ritz projector $R_h : H_0^1(\Omega) \to V_h$, defined by

$$(\nabla R_h v, \nabla \chi) = (\nabla v, \nabla \chi), \quad \forall\, \chi \in V_h.$$

The identity $P_h A = A_h R_h$ implies

$$\begin{aligned} G_h^2(z) &= \mathcal{R}_h(w)\big(P_h(wI + A) - (wI + A_h)P_h\big)\mathcal{R}(w) \\ &= \mathcal{R}_h(w)A_h(R_h - P_h)\mathcal{R}(w) = \mathcal{R}_h(w)A_hP_h(R_h - I)\mathcal{R}(w). \end{aligned}$$

Since $\mathcal{R}_h(w)A_hP_h$ is uniformly bounded on $\Sigma_{\overline{\beta}}$, and using the well-known error estimate $\|R_h v - v\| \le Ch^2\|v\|_{H^2}$ together with (4.3), we obtain as in (4.4)

$$\|G_h^2(z)v\|_{L_2} \le Ch^2\|\mathcal{R}(w)v\|_{H^2} \le Ch^2\|v\|_{L_2}, \tag{4.5}$$

which completes the proof of (4.2), and thus of the theorem. □

We now show a smooth data estimate holding uniformly down to $t = 0$, intended for use with our second method. Recalling (2.28) and setting $\dot{H}^\sigma = \mathcal{B}^{\sigma/2}$ for $A = -\Delta$, with homogeneous Dirichlet boundary conditions, we use the notation

$$\|g\|_{\dot{H}^\sigma,\nu,Z} = \sup_{z\in Z}\big((1 + |z|)^\nu\|g(z)\|_{\dot{H}^\sigma}\big).$$

Theorem 4.2. *Let $u_h(t)$ and $u(t)$ be the solutions of* (2.36) *and* (2.35), *with $\widehat{f}$ analytic in Σ_β^ω, and with $u_{0h} = P_h u_0$. Then, if $0 < \sigma \le 1, \nu \ge 0$ and $(1 + \alpha)\sigma + \nu \ge 1 + \alpha$, we have, with $C = C_\beta$,*

$$\|u_h(t) - u(t)\|_{L_2} \le Ch^2e^{\omega t}\left(\|u_0\|_{\dot{H}^2} + \|\widehat{f}\|_{\dot{H}^{2\sigma},\nu,\Sigma_\beta^\omega}\right), \quad \textit{for } t \ge 0.$$

Proof. We shall again use (4.1), now with $\Gamma = \omega + \Gamma_t^0 \cup \Gamma_t^\infty$, where $\Gamma_t^0 = \{z : |z| = 1/t, |\arg z| \le \beta\}$ and $\Gamma_t^\infty = \{z :\ |\arg z| = \beta,\ |z| > 1/t\}$. First note that by (4.4) and (4.5), and since A commutes with $\mathcal{R}(w)$, we have, for $z \in \Sigma_\beta^\omega$,

$$\begin{aligned} \|G_h(z)v\|_{L_2} &\le Ch^2\|\mathcal{R}(w)Av\|_{L_2} \\ &\le \frac{Ch^2}{1 + |w|}\|Av\|_{L_2} \le \frac{Ch^2}{1 + |z|^{1+\alpha}}\,\|v\|_{\dot{H}^2}. \end{aligned} \tag{4.6}$$

Hence, in the case that $f(t) = 0$, we have

$$\|u_h(t) - u(t)\|_{L_2} \le Ch^2 e^{\omega t} \int_{\Gamma_t^0 \cup \Gamma_t^\infty} \frac{|e^{tz}|}{|z-\omega|}\,|dz|\,\|u_0\|_{\dot{H}^2},$$

and, since $|z| \ge c_\beta |z-\omega|$ on Σ_β^ω, the result stated follows in this case from

$$\int_{\Gamma_t^0} \frac{|e^{zt}|}{|z|}|dz| \le C \int_{-\beta}^{\beta} d\theta \le C \text{ and } \int_{\Gamma_t^\infty} \frac{|e^{zt}|}{|z|}|dz| \le C \int_{1/t}^{\infty} \frac{e^{-cst}}{s}\,ds \le C.$$

To treat the term in $\widehat{f}$, we interpolate between (4.6) and (4.2) to obtain

$$\|G_h(z)v\|_{L_2} \le \frac{Ch^2}{(1+|z|)^{(1+\alpha)\sigma+\nu}} \left((1+|z|)^\nu \|v\|_{\dot{H}^{2\sigma}}\right), \quad \text{for } z \in \Sigma_\beta^\omega,$$

cf. (3.7), and hence, since $(1+\alpha)\sigma + \nu \ge 1+\alpha$,

$$|z|^\alpha \|G_h(z)\widehat{f}(z)\|_{L_2} \le \frac{Ch^2}{|z|} \|\widehat{f}\|_{\dot{H}^{2\sigma},\nu,\Sigma_\beta^\omega}, \quad \text{for } z \in \Sigma_\beta^\omega.$$

In the same way as above this shows the result stated for $u_0 = 0$.

For the purpose of application to the analysis of our third time discretization method we next show a classical type smooth data estimate that does not use $\widehat{f}(z)$.

Theorem 4.3. *Let $u_h(t)$ and $u(t)$ be the solutions of* (2.36) *and* (2.35)*, respectively, with $u_{0h} = P_h u_0$. Then*

$$\|u_h(t) - u(t)\|_{L_2} \le Ch^2\Big(\|u_0\|_{\dot{H}^2} + \int_0^t \|u_t(s)\|_{\dot{H}^2}\,ds\Big), \quad \text{for } t > 0. \tag{4.7}$$

Proof. Writing $u_h - u = (u_h - R_h u) + (R_h u - u) =: \vartheta + \varrho$ we have, using again $\|R_h v - v\| \le Ch^2 \|v\|_{H^2}$,

$$\|\varrho(t)\|_{L_2} \le Ch^2 \|u(t)\|_{\dot{H}^2} \le Ch^2\Big(\|u_0\|_{\dot{H}^2} + \int_0^t \|u_t(s)\|_{\dot{H}^2}\,ds\Big).$$

Further, one easily finds

$$\partial_t \vartheta - \partial_t^{-\alpha} \Delta_h \vartheta = -P_h \varrho_t, \quad \text{for } t > 0,$$

and hence, using Duhamel's principle (2.9) and the stability of $\mathcal{E}_h(t)$,

$$\begin{aligned} \|\vartheta(t)\|_{L_2} &\le C\Big(\|\vartheta(0)\|_{L_2} + \int_0^t \|\varrho_t(s)\|_{L_2} ds\Big) \\ &\le Ch^2\Big(\|u_0\|_{\dot H^2} + \int_0^t \|u_t(s)\|_{\dot H^2}\, ds\Big). \qquad \square \end{aligned}$$

The integral on the right in (4.7) is finite under smoothness assumptions that do not require $f(t)$ to vanish on $\partial\Omega$ for $t > 0$. In fact, for $0 < \alpha < 1$, it follows from the regularity result [**11**, Theorem 2.4] (an improved version of [**13**, Theorem 5.6]) that, if $u_0 = 0$, then

$$\begin{aligned} \int_0^t \|u_t(s)\|_{\dot H^2}\, ds \le C\Big(& t^{(1+\alpha)\sigma-\alpha} \|f(0)\|_{\dot H^{2\sigma}} \\ & + \sum_{j=0}^{2} \int_0^t s^{j-\alpha} \|\partial_t^{j+1} f(s)\|_{L_2}\, ds\Big), \quad \text{if } \sigma > \alpha/(1+\alpha). \end{aligned}$$

The following alternative regularity result admits $-1 < \alpha \le 0$.

Lemma 4.1. *Let $-1 < \alpha < 1$ and $u_0 = 0$. Then, for $\sigma > \alpha/(1+\alpha)$,*

$$\int_0^t \|u_t(s)\|_{\dot H^2}\, ds \le Ct^{(1+\alpha)\sigma-\alpha}\Big(\|f(0)\|_{\dot H^{2\sigma}} + \int_0^t \|f_t(s)\|_{\dot H^{2\sigma}}\, ds\Big).$$

Proof. By Duhamel's principle (2.9) we have

$$u_t(t) = \frac{d}{dt}\int_0^t \mathcal{E}(\tau) f(t-\tau)\, d\tau = \mathcal{E}(t) f(0) + \int_0^t \mathcal{E}(\tau) f_t(t-\tau)\, d\tau,$$

and hence, with $A = -\Delta$,

$$Au_t(t) = A\mathcal{E}(t) f(0) + \int_0^t A\mathcal{E}(\tau) f_t(t-\tau)\, d\tau.$$

Using (2.10) (with σ replaced by $1-\sigma$ and u_0 by $A^\sigma u_0$) this shows

$$\|u_t(t)\|_{\dot H^2} \le Ct^{-(1+\alpha)(1-\sigma)}\|f(0)\|_{\dot H^{2\sigma}} + C\int_0^t \tau^{-(1+\alpha)(1-\sigma)}\|f_t(t-\tau)\|_{\dot H^{2\sigma}}\,d\tau.$$

Replacing t by s and integrating we obtain, since $(1+\alpha)(1-\sigma)<1$,

$$\int_0^t \|u_t(s)\|_{\dot H^2}\,ds \le Ct^{1-(1+\alpha)(1-\sigma)}\|f(0)\|_{\dot H^{2\sigma}} + C\int_0^t \tau^{-(1+\alpha)(1-\sigma)}\int_\tau^t \|f_t(s-\tau)\|_{\dot H^{2\sigma}}\,ds\,d\tau,$$

which is bounded as stated. □

We note that if $\alpha<0$ the inequality in Lemma 4.1 holds with $\sigma=0$. Further, if $0\le\alpha<1/3$, then $\alpha/(1+\alpha)<1/4$, and we may thus choose $\sigma<1/4$, so that boundary conditions on $f(t)$ will not be required.

5. Discretization in both time and space. In this section we analyze the error in the fully discrete methods obtained by applying our three time discretization methods to the spatially semidiscrete problem (2.36), or, equivalently, (2.37). The fully discrete solution $U_{N,h}(t)$ obtained by application of our first method (2.17) to (2.37), with $u_{0h}=P_hu_0$, is thus defined by

$$U_{N,h}(t) := \frac{k}{2\pi i}\sum_{j=-N}^{N} e^{z_jt}w_h(z_j)\,z_j', \quad w_h(z)=\widehat{\mathcal{E}}_h(z)P_hg(z). \tag{5.1}$$

To find $U_{N,h}(t)$ for a range of values of t it is now required to solve the $2N+1$ discrete elliptic problems, with $|j|\le N$,

$$z_j^{1+\alpha}\big(w_h(z_j),\chi\big)+\big(\nabla w_h(z_j),\nabla\chi\big)=z_j^\alpha\big(g(z_j),\chi\big),\quad \forall\,\chi\in V_h. \tag{5.2}$$

As before, these problems may be solved in parallel.

Since the triangle inequality gives

$$\|U_{N,h}(t)-u(t)\| \le \|U_{N,h}(t)-u_h(t)\|+\|u_h(t)-u(t)\|,$$

combining Theorem 3.1 (with A_h playing the role of A) and Theorem 4.1, we immediately obtain the following error bound for the fully discrete method.

Theorem 5.1. *Let $u(t)$ be the solution of* (2.35), *and, under the assumptions and with the notation of Theorem* 3.1, *let $U_{N,h}(t)$ be the approximate solution defined by* (5.1). *Then we have, for $t_0 \leq t \leq T$, with $C = C_{\delta,r,\beta,t_0,T}$,*

$$\|U_{N,h}(t) - u(t)\|_{L_2} \leq C(h^2 + \ell(\rho N)e^{-\mu N})\big(\|u_0\|_{L_2} + \|\widehat{f}\|_{L_2,\Sigma_\beta^\omega}\big).$$

Applying the modified time discretization method (2.26) to the spatially semidiscrete problem (2.36), again with $u_{0h} = P_h u_0$, we obtain a different fully discrete solution, namely, with $w_h^0(z_j) = w_h(z_j) - z_j^{-1} P_h g(z_j)$,

$$U_{N,h}^0(t) := P_h \mathcal{F}(t) + \frac{k}{2\pi i} \sum_{j=-N}^{N} e^{z_j t} w_h^0(z_j)\, z_j'. \tag{5.3}$$

Using Theorem 3.2 we now have the following estimate for the error in the discretization in time of the spatially semidiscrete problem (2.36). This estimate may then be combined with Theorem 4.2 to obtain a complete $O(h^2 + e^{-\sqrt{\bar{r}\gamma N}})$ error estimate for the fully discrete solution. This result will require a condition on the triangulations $\mathcal{T}_h$ underlying the finite element spaces V_h.

Theorem 5.2. *Let $u_h(t)$ be the solution of* (2.35), *and assume that the $\mathcal{T}_h$ are such that*

$$\|A_h^\sigma P_h v\|_{L_2} \leq C\|A^\sigma v\|_{L_2}, \quad \text{for } v \in D(A^\sigma), \quad \text{with } 0 < \sigma \leq 1. \tag{5.4}$$

Under the hypotheses of Theorem 3.2, let $U_{N,h}^0(t)$ be defined by (5.3). *Then, if $(1+\alpha)\sigma_0 + \nu \geq (1+\alpha)\sigma = \gamma$, we have, with $C = C_{\delta,r,\beta,\sigma,\sigma_0}$,*

$$\|U_{N,h}^0(t) - u_h(t)\|_{L_2} \leq C\gamma^{-1}T^\gamma e^{\omega t}\, e^{-\sqrt{\bar{r}\gamma N}}\big(\|u_0\|_{\dot{H}^{2\sigma}} + \|\widehat{f}\|_{\dot{H}^{2\sigma_0},\nu,\Sigma_\beta^\omega}\big), \quad \text{for } 0 \leq t \leq T, \tag{5.5}$$

We make some remarks concerning condition (5.4). We first note that in the case that the triangulations $\mathcal{T}_h$ form a quasiuniform family, then, as is easily seen, (5.4) holds with $\sigma = 1$.

We now recall from [**3**] that, in two space dimensions ($d = 2$), the L_2-projector P_h is stable in H_0^1 under weaker conditions on the $\mathcal{T}_h$ than quasiuniformity. More precisely, stability holds if $h_\tau/h_{\tau_0} \le C\delta^j$ for any τ, $\tau_0 \in \mathcal{T}_h$, where τ is "j triangles away from τ_0", under the assumption that $1 < \delta < \gamma^{-1/5} \approx 1.26$, where $\gamma = \sqrt{3} - \sqrt{2}$, thus allowing serious non-quasiuniformity. This result follows from Theorem 4 of [**3**], with $k = 1$, $p = 2$, $\alpha = \delta^2$ and $\beta = \alpha^2 = \delta^4$, since then $\alpha^{1/2}\beta\gamma = \delta^5\gamma < 1$. In this case, (5.4) holds with $\sigma = 1/2$. In fact,

$$\|A_h^{1/2} P_h v\|_{L_2}^2 = (A_h P_h v, P_h v) = \|\nabla P_h v\|_{L_2}^2 \le C\|\nabla v\|_{L_2}^2 = C\|A^{1/2} v\|_{L_2}^2.$$

By interpolation between this inequality and $\|P_h v\|_{L_2} \le \|v\|_{L_2}$, one finds that (5.4) holds for $0 \le \sigma \le 1/2$. In particular, since $H^s = \dot{H}^s = D(A^{s/2})$ for $0 \le s < 1/2$, this means that (5.5) applies if $\widehat{f}(z) \in H^{2\sigma_0}$ on Σ_β^ω, with $0 < \sigma_0 < 1/4$, thus not requiring $\widehat{f}(z) = 0$ on $\partial\Omega$, provided $\nu \ge (1+\alpha)(\frac{1}{2} - \sigma_0)$.

In one space dimension, the stability of P_h in H_0^1 holds for any $\tilde{\alpha} < 2$, which is a very weak condition on the partitions.

We now turn to the third method, applying (2.32) to (2.35), or taking

$$\widetilde{U}_{N,h}(t) := P_h \mathcal{F}(t) + \frac{k}{2\pi i} \sum_{j=-N}^{N} \widetilde{w}_h(z_j, t) z_j', \tag{5.6}$$

where $\widetilde{w}_h(z_j, t) = w_h(z_j, t) - z_j^{-1} P_h g(z_j, t)$, with $w_h(z_j, t)$ the solutions of the obvious modifications of the elliptic finite element equations (5.2). For this method, Theorem 3.3 gives the following bound.

Theorem 5.3. *Let $u_h(t)$ be the solution of* (2.35), *and under the assumptions of Theorem* 5.2, *let $\widetilde{U}_{N,h}(t)$ be defined by* (5.6). *Then, if $\sigma_0 + (1+\alpha)^{-1} \ge \sigma$, we have, with $C = C_{\delta,r,\bar{\beta},\sigma,\sigma_0}$,*

$$\|\widetilde{U}_{N,h}(t) - u_h(t)\|_{L_2} \le C\gamma^{-1} T^\gamma e^{-\sqrt{\bar{r}\gamma N}} \Big(\|u_0\|_{\dot{H}^{2\sigma}} + \|f(0)\|_{\dot{H}^{2\sigma_0}} + \int_0^t \|f_t(s)\|_{\dot{H}^{2\sigma_0}}\, ds \Big), \quad \text{for } 0 \le t \le T.$$

We note that, by the above, no boundary conditions on f or f_t are required if $\sigma_0 < 1/4$. If $\alpha \geq 0$, we may choose $\sigma = 1$, $\sigma_0 = 0$, and, for any $\alpha \in (-1, 1)$, we have $(1+\alpha)^{-1} > 1/2$, so that we may take $\sigma = 1/2$, $\sigma_0 = 0$. Combination of Theorem 5.3 with Theorem 4.3 then yields an $O(h^2 + e^{-\sqrt{\bar{r}\gamma N}})$ error estimate, uniformly down to $t = 0$, without artificial boundary conditions on f.

6. Numerical experiments.

6.1. *A scalar problem.* To see the effect of discretizing in time only, we consider a problem in which $\mathcal{B} = \mathbb{C}$, namely

$$\partial_t u + \partial_t^{-\alpha} a u = f(t), \quad \text{for } t > 0, \quad \text{with } u(0) = u_0, \tag{6.1}$$

for a scalar $a > 0$. The exact solution may be expressed in terms of the Mittag–Leffler function $E_\mu(x) = \sum_{k=0}^{\infty} x^k / \Gamma(1 + k\mu)$; in fact,

$$u(t) = E_{1+\alpha}(-at^{1+\alpha}) + \int_0^t E_{1+\alpha}(-as^{1+\alpha}) f(t-s)\, ds. \tag{6.2}$$

We take $\alpha = -1/2$, because in this case the Mittag–Leffler function can be expressed in terms of the complementary error function, $E_{1/2}(-x) = e^{x^2} \operatorname{cerf}(x)$, and is easily evaluated with the help of the function DERFCX from the specfun library [**2**]. The substitution $s = ty^2$ then yields the formula

$$u(t) = E_{1/2}(-a\sqrt{t}) + \int_0^1 E_{1/2}(-a\sqrt{t}\, y) f(t - ty^2) 2ty\, dy,$$

in which the integrand is a smooth function of y for any smooth $f(t)$, allowing accurate evaluation via Gauss–Legendre quadrature.

TABLE 1. Absolute error in $U_N(t)$ at $t = 2.0$ using two different contours.

	$\omega = 0.0,\ \delta = 0.1541$ $r = 0.1387$		$\omega = 2.0,\ \delta = 0.3812$ $r = 0.3431$	
N	error	$\ell(\rho N)e^{-\mu N}$	error	$\ell(\rho N)e^{-\mu N}$
10	4.50e-02	2.88e+00	1.95e-01	3.03e-01
20	2.01e-03	8.86e-01	5.73e-05	1.24e-02
30	2.68e-03	2.82e-01	9.18e-05	5.29e-04
40	4.49e-04	9.08e-02	2.21e-06	2.29e-05
60	3.92e-05	9.62e-03	1.07e-09	4.42e-08
80	1.79e-06	1.03e-03	1.01e-13	8.68e-11
100	6.76e-09	1.12e-04	1.38e-15	1.73e-13
120	8.81e-09	1.22e-05	8.59e-16	3.45e-16

We applied each of our three methods to problem (6.1) with $a = 1$, taking as the initial data and the inhomogeneous term

$$u_0 = 1 \quad \text{and} \quad f(t) = e^{-t}\cos \pi t.$$

Our choice of $f(t)$ makes the problem somewhat challenging because the Laplace transform $\widehat{f}(z) = (z+1)/((z+1)^2+\pi^2)$ has poles at $z = -1 \pm i\pi$, forcing $\beta < \pi/2 + \arctan((1+\omega)/\pi)$.

Table 1 shows the absolute values of the error at $t = 2.0$ for the approximation $U_N(t)$ defined in (2.17), where w is now the scalar function $w(z) = z^\alpha(z^{1+\alpha} + a)^{-1}g(z)$, with two choices of the set of parameters ω, δ and r. The integration contour was constructed as in Theorem 3.1 with $\theta = 0.1$ and $[t_0, T] = [0.5, 5.0]$. The table also shows the factor $\ell(\rho N)e^{-\mu N}$ that occurs in our theoretical error bound. For $N = 10$ the results are better with $\omega = 0$, but for larger N we observe faster convergence with $\omega = 2$, due to the larger allowable value of r.

Table 2 gives results for our other two methods. In this example, $U_N^0(t)$ is generally less accurate than $\widetilde{U}_N(t)$ because the integration contour for the latter is not constrained by the poles of $\widehat{f}(z)$, allowing a larger value for r. In other computations, we observed little difference between the accuracy of $U_N^0(t)$ and $\widetilde{U}_N(t)$ when using common values of ω, δ and r.

TABLE 2. Absolute error in $U_N^0(t)$ and $\widetilde{U}_N(t)$ at $t = 2.0$ using two different contours.

	$\omega = 1.0$, $\delta = 0.2835$ $r = 0.2551$		$\omega = 0.0$, $\delta = 0.7854$ $r = 0.7069$	
N	error in U_N^0	$\gamma^{-1}T^\gamma e^{\omega t} e^{-\sqrt{\bar{r}\gamma N}}$	error in $\widetilde{U}_N$	$\gamma^{-1}T^\gamma e^{-\sqrt{\bar{r}\gamma N}}$
10	1.14e-02	1.95e+00	1.06e-02	4.02e-02
20	5.08e-04	6.03e-01	1.25e-03	5.70e-03
40	3.65e-04	1.15e-01	6.01e-05	3.61e-04
60	1.42e-04	3.22e-02	5.71e-06	4.34e-05
80	1.22e-05	1.10e-02	7.93e-07	7.28e-06
100	2.90e-06	4.28e-03	1.36e-07	1.51e-06
120	2.19e-06	1.82e-03	2.86e-08	3.64e-07
160	6.97e-07	3.99e-04	1.71e-09	2.91e-08
200	9.32e-08	1.05e-04	1.48e-10	3.15e-09

Figure 2 shows how the errors $|U_N(t) - u(t)|$ and $|U_N^0(t) - u(t)|$ depend on t for the case $N = 100$. Note the logarithmic scale on the vertical axis and the range $0 \le t \le 1.0$ on the horizontal axis. We chose $[t_0, T] = [0.5, 5.0]$, with the values of ω, δ and r as in the left half of Table 2. As expected, for $t \ge t_0$ we observe that $U_N(t)$ is more accurate than $U_N^0(t)$, but as t decreases from $t_0 = 0.5$ the error in $U_N(t)$ grows steadily and becomes larger than the error in $U_N^0(t)$ at around $t = 0.2$. Observe also how $|U_N^0(t) - u(t)|$ changes abruptly near $t = 0$. Closer investigation revealed that this error drops from 2.75×10^{-4} at $t = 0$ to 2.31×10^{-6} at $t = 4 \times 10^{-6}$, perhaps because of the factor $e^{-\lambda t \sin(\delta+\eta)\cosh\xi}$ that occurs in (3.9) and whose influence is not captured by our error bound.

In Table 3 we present results using a contour that passes to the left of the poles of $\widehat{f}(z)$, using a modified version of $U_N(t)$ that incorporates the residues at $z = -1 \pm i\pi$, following the representation (3.11). In the left column we list the errors using the fixed value $\theta = 0.1$, and observe that these errors grow for $N \ge 60$. A perturbation analysis similar to the one discussed following Theorem 3.1 explains why the roundoff errors grow exponentially with N; for details, see [**9**]. In the right column, taking $\theta = 1/N$, the errors become much smaller for larger values of N, reaching the order of the machine precision when $N = 100$.

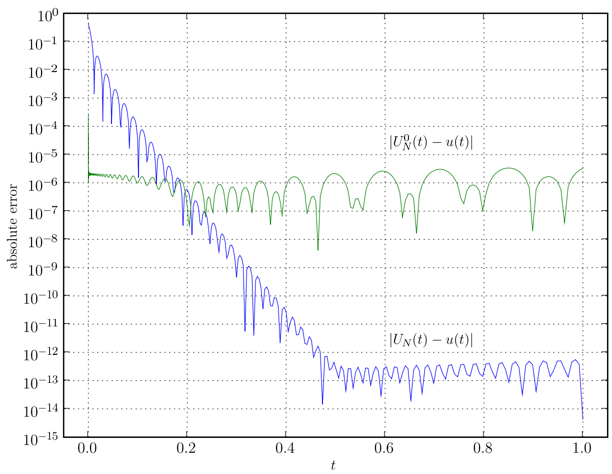

FIGURE 2. Absolute errors in $U_N(t)$ and $U_N^0(t)$ for $N = 100$.

TABLE 3. Absolute error in a modified version of $U_N(t)$ at $t = 2.0$ using two different choices of θ, for a contour passing to the left of the poles of $\widehat{f}(z)$.

	$\omega = 0.0$, $\delta = 0.7854$, $r = 0.7069$			
	$\theta = 0.1$		$\theta = 1/N$	
N	error	$\ell(\rho N)e^{-\mu N}$	error	$\ell(\rho N)e^{-\mu N}$
10	1.52e-04	4.28e-03	1.52e-04	4.28e-03
20	2.98e-06	3.11e-06	4.68e-06	8.59e-06
30	2.30e-07	2.37e-09	2.98e-08	2.67e-08
40	2.31e-08	1.85e-12	1.72e-09	1.06e-10
60	7.34e-10	1.16e-18	1.45e-12	2.67e-15
80	1.36e-09	7.52e-25	3.11e-15	1.01e-19
100	8.80e-09	4.92e-31	7.77e-16	5.10e-24
120	1.79e-07	3.25e-37	8.33e-16	3.19e-28
140	4.92e-06	2.16e-43	7.22e-16	2.36e-32
160	8.50e-04	1.45e-49	7.77e-16	2.02e-36

TABLE 4. Errors in $U_{N,h}(t)$, $U^0_{N,h}(t)$, $\widetilde{U}_{N,h}(t)$ at $t = 2.0$ for a 50×50 grid.

ω	1.0000	1.0000	0.0000
δ	0.2835	0.2835	0.7854
r	0.2551	0.2551	0.7069
N	method 1	method 2	method 3
20	1.2543e-02	6.2889e-03	4.1395e-03
30	6.1977e-03	6.1683e-03	4.6533e-04
40	2.4728e-04	2.7850e-03	2.6436e-04
60	5.0109e-04	3.2581e-04	4.6450e-04
80	4.8512e-04	4.6280e-04	4.8232e-04
120	4.8519e-04	4.9304e-04	4.8509e-04

6.2. *Two-dimensional problems.* We take $A = -\Delta$ on the square $\Omega = (0,4) \times (0,4)$ with homogenous Dirichlet boundary conditions. As in the scalar example, we choose $\alpha = -1/2$, $\theta = 0.1$, $[t_0, T] = [0.5, 5.0]$. To triangulate the spatial domain Ω, we first construct a uniform square grid and then bisect each square along its north-west to south-east diagonal. The regular structure of the mesh allows us to apply (5.4) with $\sigma = 1$, and, after incorporating a lumped-mass approximation, to handle the elliptic problems using a fast Poisson solver.

Table 4 shows results for a 50×50 grid when the initial data and the inhomogeneous term are of the form

$$u_0(x) = \phi_{11}(x) - \phi_{21}(x), \quad \text{where } \phi_{jk}(x) = \sin(j\pi x_1/4)\sin(k\pi x_2/4),$$
$$f(x,t) = e^{-t/2}\cos t\,\phi_{11}(x) + \frac{1}{2}e^{-t}\cos \pi t\,\phi_{21}(x);$$

notice that the ϕ_{jk} are eigenfunctions of the Laplacian. The exact solution is $u(x,t) = u_{11}(t)\phi_{11}(x) + u_{21}(t)\phi_{21}(x)$ where $u_{11}(t)$ and $u_{21}(t)$ have similar forms to the solution (6.2) of the scalar problem. Table 4 gives the discrete ℓ_2-error in the nodal values of $U_{N,h}(t)$, $U^0_{N,h}(t)$ and $\widetilde{U}_{N,h}(t)$ at $t = 2.0$, and also shows the contour parameters used. As in the scalar case, method 3 allows use of a more advantageous value of r because the poles of $\widehat{f}(\cdot, z)$ do not constrain the choice of Γ. The table shows that in this instance we achieve comparable accuracy to the semi-discrete solution $u_h(t)$ by taking N equal to about 40, 80 and 30 for methods 1, 2 and 3, respectively.

TABLE 5. Errors in $U_{N,h}(t)$, $U^0_{N,h}(t)$, $\widetilde{U}_{N,h}(t)$ at $t = 2.0$ for a 100×100 grid with $f(x,t) = e^{-t/4}$.

N	method 1	method 2	method 3
10	2.3995e-03	9.8575e-02	8.3087e-02
20	6.9963e-05	2.1067e-02	9.5705e-03
30	7.2634e-05	5.6638e-03	1.9222e-03
60	7.2623e-05	1.4630e-04	1.1144e-04
80	7.2623e-05	8.9950e-05	7.7738e-05
100	7.2623e-05	7.4365e-05	7.3500e-05

Finally, Table 5 shows the results obtained for a 100×100 grid using $u_0 = \phi_{11}$ and $f(x,t) = e^{-t/4}$, again taking the discrete ℓ_2-error at $t = 2.0$. For our reference solution, we used method 1 with $N = 120$, solving each elliptic problem with an accuracy of $O(h^4)$ by performing one step of Richardson extrapolation. Since $\widehat{f}(x,z) = 1/(z + \frac{1}{4})$ has no singularities off the real axis, we used for all three methods the values of ω, δ and r shown in the final column of Table 4. The accuracy of method 1 is striking: with $N = 20$ the error from the time discretization is already much smaller than the error from the spatial discretization, compared with $N = 80$ for methods 2 and 3. Of course, for t sufficiently close to zero method 1 would be less accurate than methods 2 and 3, as for the scalar case illustrated in Figure 2.

Note that the inhomogenous term $f(x,t) = e^{-t/4}$ does not vanish on $\partial\Omega$, so $\|f(\cdot,t)\|_{\dot{H}^{2\sigma_0}} < \infty$ if and only if $\sigma_0 < 1/4$. Nevertheless, with $\sigma_0 < 1/4$, our error bounds in Theorems 5.2 and 5.3 apply with $\sigma = 1$, taking $\nu \geq (1-\sigma_0)(1+\alpha) = \frac{1}{2}(1-\sigma_0)$ in Theorem 5.2.

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. W.J. Cody, *Algorithm* 715: *specfun–A portable Fortran package of special function routines and test drivers*, ACM Trans. Math. Software **19** (1993), 22–32 (http://www.netlib.org/specfun/).

3. M. Crouzeix and V. Thomée, *The stability in L_p and W^1_p of the L_2-projection onto finite element function spaces*, Math. Comp. **48** (1987), 521–532.

4. I.P. Gavrilyuk and V.L. Makarov, *Exponentially convergent algorithms for the operator exponential with applications to inhomogeneous problems in Banach spaces*, SIAM J. Numer. Anal. **43** (2005), 2144–2171.

5. R. Gorenflo, F. Mainardi, D. Moretti and P. Paradisi, *Time fractional diffusion: A discrete random walk approach*, Nonlinear Dynamics **29** (2002), 129–143.

6. B.I. Henry and S.L. Wearne, *Fractional reaction-diffusion*, Physica A **276** (2000), 448–455.

7. T.A.M. Langlands and B.I. Henry, *The accuracy and stability of an implicit solution method for the fractional diffusion equation*, J. Comp. Phys. **205** (2005), 719–736.

8. M. López-Fernandez and M. Palencia, *On the numerical inversion of the Laplace transform of certain holomorphic mappings*, Appl. Numer. Math. **51** (2004), 289–303.

9. M. López-Fernandez, C. Palencia and A. Schädle, *A spectral order method for inverting sectorial Laplace transforms*, SIAM J. Numer. Anal. **44** (2006), 1332–1350.

10. C. Lubich, I.H. Sloan, and V. Thomée, *Nonsmooth data error estimates for approximations of an evolution equation with a positive type memory term*, Math. Comp. **65** (1996), 1–17.

11. W. McLean and K. Mustapha, *A second-order accurate numerical method for a fractional wave equation*, Numer. Math. **105** (2007), 481–510.

12. W. McLean, I.H. Sloan, and V. Thomée, *Time discretization via Laplace transformation of an integrodifferential equation of parabolic type*, Numer. Math. **102** (2006), 497–522.

13. W. McLean and V. Thomée, *Numerical solution of an evolution equation with a positive type memory term*, J. Austral. Math. Soc. **35** (1993), 23–70.

14. ———, *Time discretization of an evolution equation via Laplace transforms*, IMA J. Numer. Anal. **24** (2004), 439–463.

15. 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.

16. R. Metzler and J. Klafter, *The random walk's guide to anomalous diffusion: A fractional dynamics approach*, Physics Reports **339** (2000), 1–77.

17. A. Pani and G. Fairweather, *An H^1-Galerkin mixed finite element method for an evolution equation with a positive type memory term*, SIAM J. Numer. Anal. **40** (2002) 1475–1490.

18. A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, Springer-Verlag, New York, 1983.

19. M.J. Sanz-Serna, *A numerical method for a partial integro-differential equation*, SIAM J. Numer. Anal. **25** (1988), 319–327.

20. A.H. Schatz and L.B. Wahlbin, *On the quasi-optimality in L_∞ of the H^1-projection into finite element spaces*, Math. Comp. **38** (1982), 1–22.

21. W.R. Schneider and W. Wyss, *Fractional diffusion and wave equations*, J. Math. Phys. **30** (1989), 134–144.

22. D. Sheen, I.H. Sloan and V. Thomée, *A parallel method for time-discretization of parabolic equations based on contour integral representation and quadrature*, Math. Comp. **69** (1999), 177–195.

23. ———, *A parallel method for time-discretization of parabolic equations based on Laplace transformation and quadrature*, IMA J. Numer. Anal. **23** (2003), 269–299.

24. B. Stewart, *Generation of analytic semigroups by strongly elliptic operators*, Trans. Amer. Math. Soc. **199** (1974), 141–161.

25. J.A.C. Weideman, *Optimizing Talbot's contours for the inversion of the Laplace transform*, SIAM J. Numer. Anal. **44** (2006), 2342–2362.

26. S.B. Yuste and L. Acedo, *An explicit finite difference method and a new von Neumann-type stability analysis for fractional diffusion equations*, SIAM J. Numer. Anal. **42** (2005), 1862–1874.

27. S.B. Yuste, L. Acedo and K. Lindenberg, *Reaction front in $A + B \to C$ reaction-subdiffusion process,* Physical Rev. E **69**, (2004).

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