Numerical Solution of a Fractional Diffusion Equation

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1. Fractional-order evolution equation

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3. Method 2

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Literature:

Sheen, Sloan, Thomée (1999)	$O(N^{-2})$
Sheen, Sloan, Thomée (2003)	$O(N^{-ct})$
Lopez-Fernandez, Palencia (2004)	$O(e^{-cN/\log N})$
McLean, Thomée (2004)	$O(e^{-c\sqrt{N}})$
Gavrilyuk, Makarov (2005)	$O(e^{-c\sqrt{N}})$
Lopez-Fernandez, Palencia, Schädle (2006)	$O(e^{-cN})$
McLean, Sloan, Thomée (2006)	$O(e^{-cN/\log N})$
Weidemann (2006)	$O(e^{-cN})$.

N	N^{-2}	$e^{-\sqrt{N}}$	$e^{-N/\log N}$	e^{-N}
5	4.00e-02	1.07e-01	4.47e-02	6.74e-03
10	1.00e-02	4.23e-02	1.30e-02	4.54e-05
20	2.50e-03	1.14e-02	1.26e-03	2.06e-09
30	1.11e-03	4.18e-03	1.48e-04	9.36e-14
40	6.25e-04	1.79e-03	1.95e-05	4.25e-18
60	2.78e-04	4.32e-04	4.32e-07	8.76e-27
80	1.56e-04	1.30e-04	1.18e-08	1.80e-35
100	1.00e-04	4.54e-05	3.71e-10	3.72e-44
150	4.44e-05	4.80e-06	9.97e-14	7.18e-66
200	2.50e-05	7.21e-07	4.04e-17	1.38e-87

Fractional-order Evolution Equation

For $-1 < \alpha < 1$ consider the initial value problem

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

For simplicity, assume $A = -\nabla^2$ densely defined in $L_2(\Omega)$ with

$$D(A) := \{\, u \in C^2(\Omega) : u = 0 \text{ on } \partial\Omega \,\}.$$

Cases:

$\alpha = 0$	classical heat equation.
$-1 < \alpha < 0$	fractional diffusion equation.
$0 < \alpha < 1$	fractional wave equation.

For $-1 < \alpha \le 0$, the IVP models the density of diffusing particles with mean-square displacement $\propto t^{1+\alpha}$. Case $\alpha < 0$ known as *anomalous sub-diffusion*.

If $0 < \alpha < 1$, we interpret $\partial_t^{-\alpha} v$ as a *Riemann-Liouville fractional integral*,

$$\partial_t^{-\alpha} v := \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} v(s)\, ds.$$

If $-1 < \alpha < 0$, then we instead have a fractional derivative,

$$\partial_t^{-\alpha} v := \partial_t(\partial_t^{-(1+\alpha)})v = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\alpha}}{\Gamma(1+\alpha)} v(s)\, ds.$$

Denoting the *Laplace transform* of $v(t)$ by

$$\hat{v}(z) = \mathcal{L}\{v(t)\} := \int_0^\infty e^{-zt} v(t)\, dt,$$

we find that

$$\mathcal{L}\{\partial_t^{-\alpha} v\} = z^{-\alpha} \hat{v}(z) \quad \text{for } -1 < \alpha < 1.$$

Laplace transformation of the IVP gives (formally)

$$z\hat{u} + z^{-\alpha} A\hat{u} = u_0 + \hat{f}(z).$$

Thus, define $g(z) := u_0 + \hat{f}(z)$ and consider the elliptic BVP for $w = \hat{u}$,

$$(z^{1+\alpha} + A)w = z^{\alpha} g(z).$$

Since spectrum$(A) \subseteq (0, \infty)$ we have a unique solution

$$w(z) = \hat{\mathcal{E}}(z)g(z) \quad \text{where} \quad \hat{\mathcal{E}}(z) := z^{\alpha}(z^{1+\alpha} + A)^{-1},$$

provided $z^{1+\alpha} \notin (-\infty, 0]$. In general, if A is a *sectorial operator*, so that

$$\left\|(z - A)^{-1}\right\| \le \frac{M}{1 + |z|} \quad \text{for} \quad |\arg z| < \varphi,$$

then

$$\|\hat{\mathcal{E}}(z)\| \le \frac{M|z|^{\alpha}}{1 + |z|^{1+\alpha}} \le \frac{M}{|z|} \quad \text{for} \quad |\arg z| \le \overline{\beta} < \min\left(\pi, \frac{\pi - \varphi}{1 + \alpha}\right).$$

We assume

$$0 < \varphi < (1-\alpha)\frac{\pi}{2} \quad \text{so that} \quad \frac{\pi}{2} < \overline{\beta} < \pi,$$

which ensures that the closed sector $\Sigma_{\overline{\beta}} := \{\, z : |\arg z| < \overline{\beta} \,\}$ crosses into the left half-plane.

Recall the Laplace inversion formula,

$$u(t) = \mathcal{L}^{-1}\{\widehat{u}(z)\} = \frac{1}{2\pi i}\int_{\Gamma_0} e^{zt}\widehat{u}(z)\,dz,$$

where $\Gamma_0 := \omega + i\mathbb{R}$, $\omega > 0$. Taking $f(t) \equiv 0$, and deforming Γ_0 to a suitable contour $\Gamma \subseteq \Sigma_{\overline{\beta}}$, yields a solution operator for the homogeneous problem:

$$\mathcal{E}(t)u_0 = \frac{1}{2\pi i}\int_{\Gamma} e^{zt}\widehat{\mathcal{E}}(z)u_0\,dz, \qquad t > 0.$$

Since $\mathcal{L}^{-1}\{\widehat{\mathcal{E}}(z)\widehat{f}(z)\} = (E * f)(t)$, in the general case we have the *Duhamel formula*

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

The resolvent estimate for A allows one to show that

$$\left\|A^\sigma \mathcal{E}^{(k)}(t)u_0\right\| \le CMt^{-\sigma(1+\alpha)-k}\|u_0\| \quad \text{for } t > 0,\ \sigma \ge 0,\ k \ge 0.$$

In particular, the IVP is *stable*:

$$\|u(t)\| \le CM\left(\|u_0\| + \int_0^t \|f(s)\|\,ds\right).$$

Thus, in a numerical method we may for convenience replace $f(t)$ by an approximation $f_\epsilon(t)$ provided $\int_0^t \|f_\epsilon(s) - f(s)\|\,ds$ is small.

Method 1

Assume $\frac{1}{2}\pi < \beta < \overline{\beta} < \pi$, $\omega \geq 0$ and $\widehat{f}(z)$ analytic in $\Sigma_\beta^\omega := \omega + \Sigma_\beta$. Define Γ to have the parametric representation

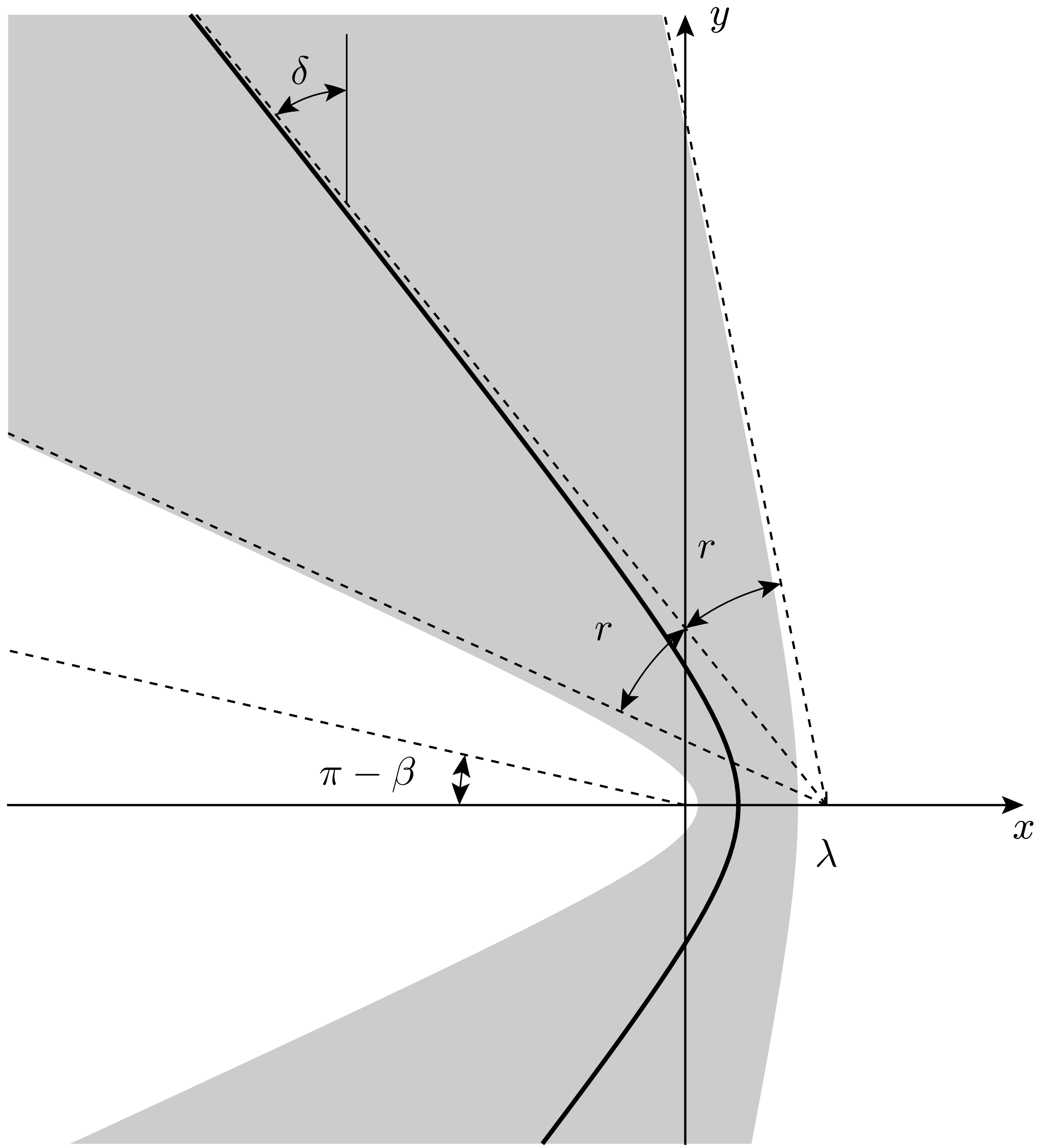
$$z(\xi) = \omega + \lambda\Big(1 - \sin(\delta - i\xi)\Big), \qquad -\infty < \xi < \infty,$$

for parameters λ and δ satisfying

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

Writing $z = x + iy$, we find that Γ is the left branch of the hyperbola with asymptotes $y = \pm(x - \omega - \lambda)\cot\delta$, so

$$\Gamma \subseteq \Sigma_\beta^\omega.$$



y
δ
r
r
π − β
x
λ

Recall that $w(z) = \widehat{u}(z) = \mathcal{E}(z)g(z)$ and

$$u(t) = \frac{1}{2\pi i}\int_\Gamma e^{zt}w(z)\,dz = \frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{z(\xi)t}w\Big(z(\xi)\Big)z'(\xi)\,d\xi.$$

Crucial observation:

$$|e^{z(\xi)t}| = e^{\omega t}e^{\lambda(1-\sin\delta\cosh\xi)t}$$

so for $t > 0$ the integrand exhibits a *double exponential decay* as $|\xi| \to \infty$.

For a suitable quadrature step $k > 0$ and let

$$\xi_j := jk, \quad z_j := z(\xi_j), \quad z'_j := z'(\xi_j).$$

In Method 1, we define the approximate solution

$$U_N(t) := \frac{k}{2\pi i}\sum_{j=-N}^{N} e^{z_j t}w(z_j)z'_j.$$

To compute $U_N(t)$ we must solve (approximately) the $2N+1$ elliptic problems

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

Note that these problems can be solved *in parallel*.

Can easily see that if u_0, $f(t)$ and the coefficients of A are real, then

$$U_N(t) = \frac{\lambda \cos\delta}{2\pi} w(z_0) + 2\,\mathrm{Re}\left(\frac{k}{2\pi i} \sum_{j=1}^{N} e^{z_j t} w(z_j) z_j'\right),$$

so we have to solve only $N+1$ (complex) elliptic problems.

Let

$$\ell(t) := \max\bigl(1, \log(1/t)\bigr) = \begin{cases} \log(1/t), & 0 < t < e^{-1}, \\ 1, & e^{-1} \le t < \infty, \end{cases}$$

and note that $\ell(t) \uparrow \infty$ as $t \downarrow 0$.

Lemma (Lopez-Fernandez, Palencia, Schädle, 2006) Assume that $v(\zeta)$ is analytic for $|\operatorname{Im}\zeta| \le r$ and satisfies

$$|v(\zeta)| \le V_\eta e^{-\gamma_\eta \cosh \xi} \quad \text{for } \zeta = \xi + i\eta \text{ and } |\eta| \le r,$$

with V_η and γ_η positive and increasing in η. If

$$b \cosh b = \frac{2\pi r N}{\gamma \sin \delta} \quad \text{and} \quad k = \frac{b}{N} \le \frac{2\pi r}{\log 2},$$

then

$$\left| k \sum_{j=-N}^{N} v(\xi_j) - \int_{-\infty}^{\infty} v(\xi)\, d\xi \right| \le C V_r \ell(\gamma_{-r}) e^{-2\pi N/b}$$

and

$$k \sum_{j=-N}^{N} |v(\xi_j)| \le C V_0 \ell(\gamma_0).$$

To apply this lemma to Method 1, let S_r denote the image in the z-plane of the strip $|\operatorname{Im}\zeta| \le r$ under the conformal mapping

$$z = \omega + \lambda\Big(1 - \sin(\delta - i\zeta)\Big).$$

We assume

$$0 < \delta - r < \delta + r < \beta - \tfrac{1}{2}\pi$$

so that

$$S_r \subseteq \Sigma_\beta^\omega.$$

Let

$$\|g\|_Z := \sup_{z \in Z} \|g(z)\| \quad \text{for } Z \subseteq \mathbb{C}.$$

Theorem Fix a compact interval $[t_0, T] \subseteq (0, \infty)$ and let $0 < \theta < 1$. If

$$b = \operatorname{arcosh}\left(\frac{T}{\theta t_0 \sin\delta}\right), \quad \lambda = \frac{2\pi r\theta N}{bT}, \quad k = \frac{b}{N} \le \frac{2\pi r}{\log 2},$$

then, for $t_0 \le t \le T$,

$$\|U_N(t) - u(t)\| \le C_{\delta,r} M e^{\omega t} \ell(c_r N) e^{-\mu N}\left(\|u_0\| + \|\hat{f}\|_{\Sigma_\beta^\omega}\right)$$

and

$$\frac{k}{2\pi}\sum_{j=-N}^{N}\left\|e^{z_j t} w(z_j) z_j'\right\| \le C_{\delta,r} M e^{\omega t} \ell(c_0 N) e^{2\pi r\theta N/b}\left(\|u_0\| + \|\hat{f}\|_{\Gamma}\right),$$

where

$$c_\eta = \frac{2\pi r\theta t_0}{bT}\sin(\delta - \eta), \qquad \mu = \frac{2\pi r}{b}(1 - \theta).$$

We may avoid the instability by choosing $\theta = O(1/N)$ at the expense of a slower convergence rate $O(e^{-cN/\log N})$.

Method 2

The approximation $U_N(t) \approx u(t)$ deteriorates as $t \downarrow 0$. We now describe a scheme that is accurate uniformly on $[0, T]$; cf. Gavrilyuk and Makarov, 2005.

Since $\widehat{\mathcal{E}}(z) = z^\alpha(z^{1+\alpha} + A)^{-1} \sim z^{-1}$ we introduce

$$\widehat{\mathcal{E}}^0(z) := \widehat{\mathcal{E}}(z) - z^{-1} = -z^{-1}A(z^{1+\alpha} + A)^{-1} \sim -z^{\alpha-2}A;$$

if $g(z) = u_0 + \widehat{f}(z)$ possesses some spatial regularity then $\|\widehat{\mathcal{E}}^0(z)g(z)\|$ decays more rapidly than $\|\widehat{\mathcal{E}}(z)g(z)\|$ as $|z| \to \infty$ with $z \in \Sigma_\beta^\omega$. In fact,

$$\|\widehat{\mathcal{E}}^0(z)v\| \le \frac{C_\sigma M\|A^\sigma v\|}{|z|\big(1 + |z|^{1+\alpha}\big)^\sigma}, \qquad 0 \le \sigma \le 1.$$

Let

$$F(t) := \int_0^t f(s)\,ds \quad \text{so that} \quad \mathcal{L}\{u_0 + F(t)\} = z^{-1}g(z)$$

and thus

$$\begin{aligned} u(t) &= \frac{1}{2\pi i}\int_\Gamma e^{zt}\Big(z^{-1} + \big(\widehat{\mathcal{E}}(z) - z^{-1}\big)\Big)g(z)\,dz \\ &= u_0 + F(t) + \frac{1}{2\pi i}\int_\Gamma e^{zt}\widehat{\mathcal{E}}^0(z)g(z)\,dz. \end{aligned}$$

In Method 2, we define

$$U_N^0(t) := u_0 + F(t) + \frac{k}{2\pi i}\sum_{j=-N}^{N} e^{z_j t}w^0(z_j)z_j',$$

where to compute $w^0(z) := \widehat{\mathcal{E}}^0(z)g(z) = w(z) - z^{-1}g(z)$ we must again solve the elliptic problem

$$(z^{1+\alpha} + A)w(z) = z^\alpha g(z).$$

For an analytic integrand with *single exponential decay* we have the following error bound.

Lemma Assume that $v(\zeta)$ is analytic for $|\operatorname{Im}\zeta| \le r$ and satisfies

$$|v(\zeta)| \le V e^{-\gamma|\xi|} \quad \text{for } \zeta = \xi + i\eta \text{ and } |\eta| \le r.$$

If

$$k = \sqrt{\frac{2\pi r}{\gamma N}} \le \frac{2\pi r}{\log 2}$$

then

$$\left| k \sum_{j=-N}^{N} v(\xi_j) - \int_{-\infty}^{\infty} v(\xi)\, d\xi \right| \le C_r V \gamma^{-1} e^{-\sqrt{2\pi r \gamma N}}.$$

Let

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

Theorem Fix an interval $[0,T]$, let $0 < \sigma \le 1$ and put $\gamma := (1+\alpha)\sigma$. If

$$\lambda = \frac{\gamma}{[1-\sin(\delta - r)]T}, \qquad k = \sqrt{\frac{2\pi r}{N}} \le \frac{2\pi r}{\log 2},$$

and

$$\sigma_0 + \nu(1+\alpha)^{-1} \ge \sigma, \qquad \sigma_0 \ge 0, \qquad \nu \ge 0,$$

then, for $0 \le t \le T$,

$$\|U_N^0(t) - u(t)\| \le C_{\delta,r,\sigma} M\gamma^{-1}T^{\gamma}e^{\omega t}e^{-\sqrt{2\pi r\gamma N}}\Big(\|A^{\sigma}u_0\| + \|A^{\sigma_0}\widehat{f}\|_{\nu,\Sigma_\beta^\omega}\Big).$$

Remark: for $A = -\nabla^2$ we want $\sigma_0 < \frac{1}{4}$ so that $\widehat{f} \in D(A^{\sigma_0})$ without requiring $f(t) \equiv 0$ on $\partial\Omega$ for all $t > 0$.

Method 3

What if $\widehat{f}(z)$ does not have an analytic continuation to Σ_β^ω, or is difficult to compute?

Recall the Duhamel formula:

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

where

$$w(z,t) := \widehat{\mathcal{E}}(z)g(z,t) \quad \text{and} \quad g(z,t) := e^{zt}u_0 + \int_0^t e^{z(t-s)}f(s)\,ds.$$

Since

$$\frac{1}{2\pi i}\int_\Gamma z^{-1}g(z,t)\,dz = \operatorname*{res}_{z=0}\frac{g(z,t)}{z} = g(0,t) = u_0 + F(t),$$

we have

$$u(t) = u_0 + F(t) + \frac{1}{2\pi i}\int_\Gamma \widetilde{w}(z,t)\,dz$$

where

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

In Method 3, we define

$$\widetilde{U}_N(t) := u_0 + F(t) + \frac{k}{2\pi i}\sum_{j=-N}^{N}\widetilde{w}(z_j,t)z_j',$$

where, to compute $\widetilde{w}(z,t)$, we solve the elliptic problem

$$(z^{1+\alpha} + A)w(z,t) = z^\alpha g(z,t).$$

Disadvantage: the RHS, and hence the solution, now depend on t.

Theorem Fix an interval $[0,T]$, let $0 < \sigma \leq 1$ and put $\gamma = (1+\alpha)\sigma$. If

$$\omega = 0, \qquad \lambda = \frac{\gamma}{[1-\sin(\delta - r)]T}, \qquad k = \sqrt{\frac{2\pi r}{\gamma N}} \leq \frac{2\pi r}{\log 2},$$

and

$$\sigma_0 + \nu(1+\alpha)^{-1} \geq \sigma, \qquad \sigma_0 \geq 0, \qquad \nu \geq 0,$$

then, for $0 \leq t \leq T$,

$$\|\widetilde{U}_N(t) - u(t)\| \leq C_{\delta,r,\sigma} M \gamma^{-1} T^{\gamma} e^{\omega t} e^{-\sqrt{2\pi r \gamma N}} \Big(\|A^{\sigma} u_0\| + \|A^{\sigma_0} f(0)\| + \int_0^t \|A^{\sigma_0} f'(s)\| \, ds \Big).$$

Numerical Examples

Consider first a scalar problem

$$\partial_t u + \partial_t^{-\alpha} u = f(t) \quad \text{for } t > 0, \quad \text{with } u(0) = 1.$$

Take $\alpha = -1/2$; the exact solution is then expressible in terms of the complementary error function. Choose $f(t) = e^{-t} \cos \pi t$, and note that

$$\hat{f}(z) = \frac{z+1}{(z+1)^2 + \pi^2} \quad \text{has poles at } z = -1 \pm i\pi.$$

We also put

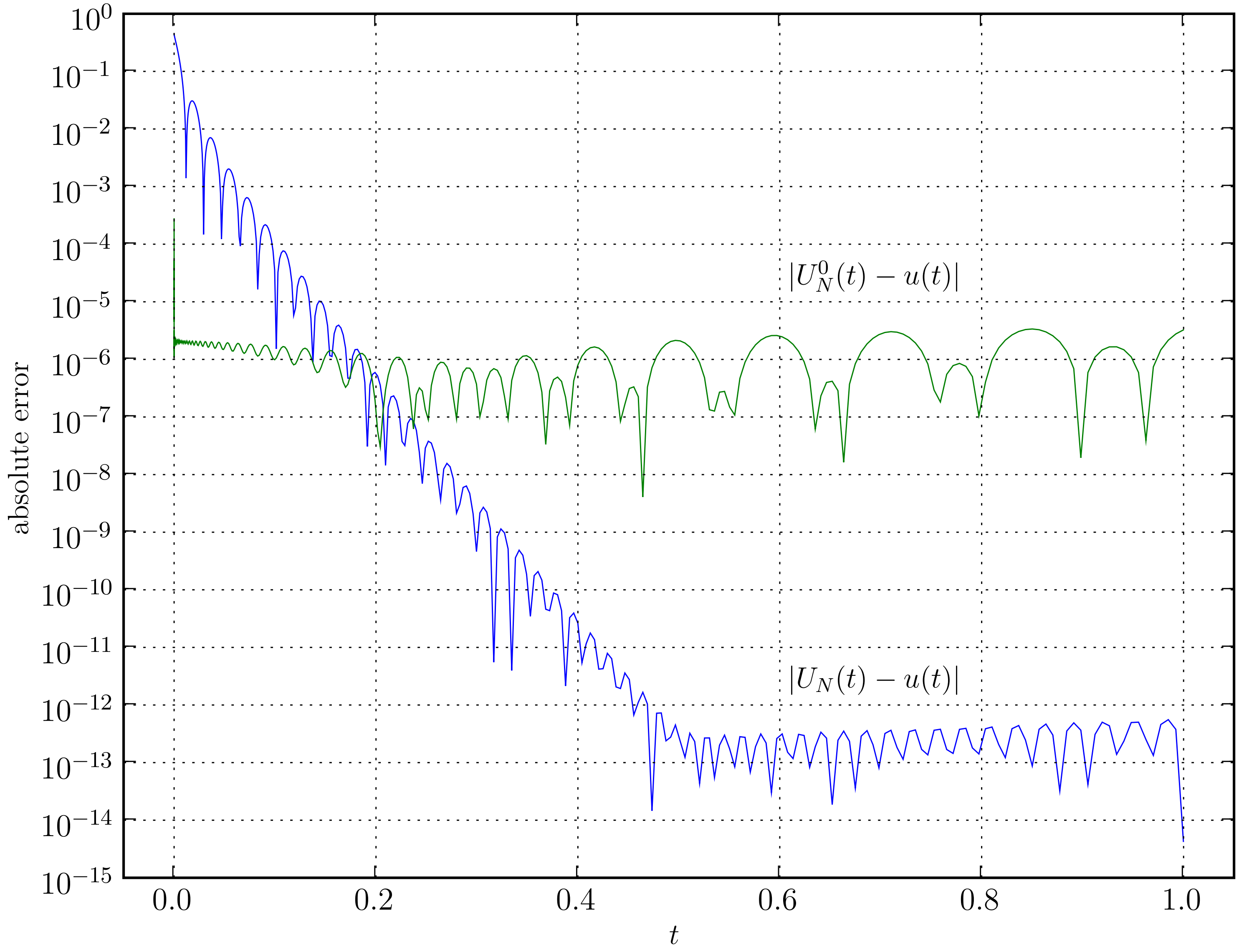
$$t_0 = 0.5, \quad T = 5.0, \quad \theta = 0.1, \quad \sigma = 1.0.$$

Results for Method 1 at $t = 2.0$.

	$\omega = 0.0,\ \delta = 0.1541$ $r = 0.1387$		$\omega = 2.0,\ \delta = 0.3812$ $r = 0.3431$	
N	error	$\ell(cN)e^{-\mu N}$	error	$\ell(cN)e^{-\mu N}$
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

Results for methods 2 and 3 at $t = 2.0$.

	$\omega = 1.0,\ \delta = 0.2835$ $r = 0.2551$		$\omega = 0.0,\ \delta = 0.7854$ $r = 0.7069$	
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



10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
absolute error
0.0
0.2
0.4
0.6
0.8
1.0
t
$|U_N^0(t) - u(t)|$
$|U_N(t) - u(t)|$

Now consider the 2D-problem with $\Omega = (0,4)^2$:

$$\partial_t u - \partial_t^{-1/2}\nabla^2 u = f(x,t) \quad \text{for } t > 0,$$
$$u(x,0) = \sin(\pi x_1/4)\sin(\pi x_2/4),$$

with $u(x,t) = 0$ for $x \in \partial\Omega$. Triangulate Ω by taking a uniform 100×100 grid and bisecting each square. Discretize in space via piecewise-linear finite elements, to obtain $U_{N,h}(t)$, $U^0_{N,h}(t)$ and $\widetilde{U}_{N,h}(t)$.

Let $f(x,t) = e^{-t/4}$. The Laplace transform $\hat{f}(x,z) = (z + \frac{1}{4})^{-1}$ has no singularities off the real axis, allowing us to take

$$\omega = 0.0, \quad \delta = 0.7854, \quad r = 0.7069.$$

Choose t_0, T, θ as before.

Note that $f(x,t)$ is not identically zero for $x \in \partial\Omega$.

Discrete ℓ_2 errors at $t = 2.0$.

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