Numerical Solution of a Fractional Diffusion Equation via Laplace Transformation

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Evolution Equation

Initial-value problem with parameter, $-1 < \alpha < 1$,

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

Laplace transform

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

Riemann–Liouville fractional integral or derivative

$$\partial_t^\nu u(t) := \mathcal{L}^{-1}\{z^\nu \hat{u}(z)\}, \quad -1 < \nu < 1.$$

Take $A = -\nabla^2$ in a bounded convex domain $\Omega \subseteq \mathbb{R}^d$ subject to homogeneous Dirichlet boundary conditions.

Thus, when $\alpha = 0$ we have the classical heat equation

$$\partial_t u - \nabla^2 u = f(t).$$

Laplace transformation gives

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

Formally, if we put

$$\hat{\mathcal{E}}(z) := z^{\alpha}(z^{1+\alpha} + A)^{-1},$$

then

$$\hat{u}(z) = \hat{\mathcal{E}}(z)\big(u_0 + \hat{f}(z)\big)$$

and

$$u(t) = \frac{1}{2\pi i}\int_{\Gamma_0} e^{zt}\hat{\mathcal{E}}(z)\big(u_0 + \hat{f}(z)\big)\,dz.$$

Resolvent estimate: given $0 < \phi < \pi$ we have $M = M(\phi) < \infty$ such that

$$\|(z - A)^{-1}\|_{L_2 \to L_2} \le \frac{M}{1 + |z|} \quad \text{for } |\arg(z)| \ge \phi.$$

Choose $M \ge 1$ and $\pi/2 < \beta < \pi$ such that

$$\|\hat{\mathcal{E}}(z)\|_{L_2 \to L_2} \le \frac{M|z|^\alpha}{1 + |z|^{1+|\alpha|}} \le \frac{M}{|z|} \quad \text{for } |\arg(z)| < \beta.$$

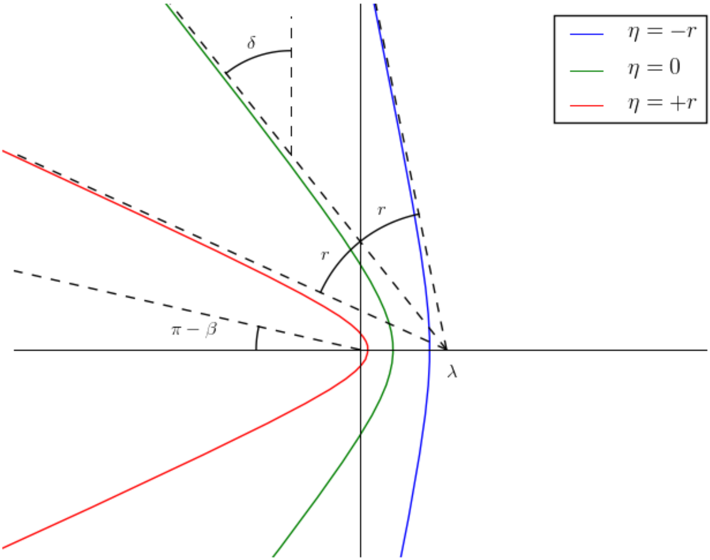
Follows that

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

satisfies

$$\|\mathcal{E}(t)v\| \le C\|v\| \quad \text{for } 0 \le t < \infty.$$

The contour Γ_η



Recapping:

$$\partial_t u + \partial_t^{-\alpha} A u = f(t),$$
$$\hat{u}(z) = \hat{\mathcal{E}}(z)\big(u_0 + \hat{f}(z)\big).$$

Formally, $u(t) = \mathcal{E}(t)u_0$ is the solution of the homogenous problem

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

For the *in*homogeneous problem, since

$$\mathcal{L}\{(\mathcal{E} * f)(t)\} = \hat{\mathcal{E}}(z)\hat{f}(z)$$

we obtain the Duhamel formula

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

Quadrature Method

Recalling

$$\mathcal{E}(t)v = \frac{1}{2\pi i}\int_{\Gamma_0} e^{zt}\hat{\mathcal{E}}(z)v\,dz$$

we have

$$\begin{aligned}\int_0^t \mathcal{E}(t-s)f(s)\,ds &= \int_0^t \left(\frac{1}{2\pi i}\int_{\Gamma_0} e^{z(t-s)}\hat{\mathcal{E}}(z)\,dz\right)f(s)\,ds \\ &= \frac{1}{2\pi i}\int_{\Gamma_0}\hat{\mathcal{E}}(z)\int_0^t e^{z(t-s)}f(s)\,ds\,dz\end{aligned}$$

so

$$u(t) = \frac{1}{2\pi i}\int_{\Gamma_0}\hat{\mathcal{E}}(z)g(z,t)\,dz$$

where

$$g(z,t) := e^{zt}u_0 + \int_0^t e^{z(t-s)}f(s)\,ds.$$

To achieve faster decay as $|z| \to \infty$, put

$$\hat{\mathcal{E}}^0(z) := \hat{\mathcal{E}}(z) - z^{-1} = -z^{-1-\alpha}\hat{\mathcal{E}}(z)A.$$

If $0 \le \sigma \le 1$ then we find

$$\|\hat{\mathcal{E}}^0(z)v\| \le \frac{C_\sigma M\|A^\sigma v\|}{|z|(1+|z|^{1+\alpha})^\sigma} \quad \text{for } |\arg(z)| < \beta,$$

so if $v \in D(A^\sigma)$ then

$$\|\hat{\mathcal{E}}^0(z)v\| = O(|z|^{-1-\gamma}) \quad \text{where } \gamma := (1+\alpha)\sigma.$$

Notice

$$\frac{1}{2\pi i}\int_{\Gamma_0}\Big(\hat{\mathcal{E}}(z)-\hat{\mathcal{E}}^0(z)\Big)g(z,t)\,dz = \frac{1}{2\pi i}\int_{\Gamma_0}\frac{g(z,t)}{z}\,dz$$
$$= \operatorname*{res}_{z=0}\frac{g(z,t)}{z}$$
$$= g(0,t) = u_0 + F(t)$$

where

$$F(t) = \int_0^t f(s)\,ds.$$

Integral representation

$$
\begin{aligned}
u(t) &= \frac{1}{2\pi i} \int_{\Gamma_0} \hat{\mathcal{E}}(z) g(z,t)\, dz \\
&= u_0 + F(t) + \frac{1}{2\pi i} \int_{\Gamma_0} \hat{\mathcal{E}}^0(z) g(z,t)\, dz,
\end{aligned}
$$

with

$$
\begin{aligned}
\hat{\mathcal{E}}^0(z) &= -z^{-1-\alpha} \hat{\mathcal{E}}(z) A = -z^{-1}(z^{1+\alpha} + A)^{-1} A, \\
g(z,t) &= e^{zt} u_0 + \int_0^t e^{z(t-s)} f(s)\, ds.
\end{aligned}
$$

With $\Gamma = \{\, z(\xi) : -\infty < \xi < \infty \,\}$ we take an equal-weight quadrature rule

$$\int_{\Gamma_0} v(z)\,dz = \int_{-\infty}^{\infty} v\bigl(z(\xi)\bigr) z'(\xi)\,d\xi \approx k \sum_{j=-N}^{N} v(z_j) z_j',$$

where

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

Achieve spectral-order accuracy if $v(z(\xi))z'(\xi)$ is bounded and analytic for $-r < \operatorname{Im}(\xi) < r$ with exponential decay as $|\operatorname{Re}(\xi)| \to \infty$.

Let

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

and

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

so that

$$u(t) = u_0 + F(t) + \frac{1}{2\pi i}\int_{\Gamma_0}\widetilde{w}(z,t)\,dz.$$

Approximate solution

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

Thus, for each quadrature point z_j we must solve an elliptic problem

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

Error Estimates

To measure spatial regularity, write

$$\|v\|_\sigma = \|A^\sigma v\| \quad \text{for} \quad v \in D(A^\sigma) = \dot{H}^{2\sigma}(\Omega).$$

Let β, r and δ be as before.
Choose $0 < \sigma \leq 1$ and $T > 0$, then put

$$\gamma := (1+\alpha)\sigma, \quad \kappa := 1 - \sin(\delta - r), \quad \lambda := \frac{\gamma}{\kappa T},$$

and define the contour Γ_0 by

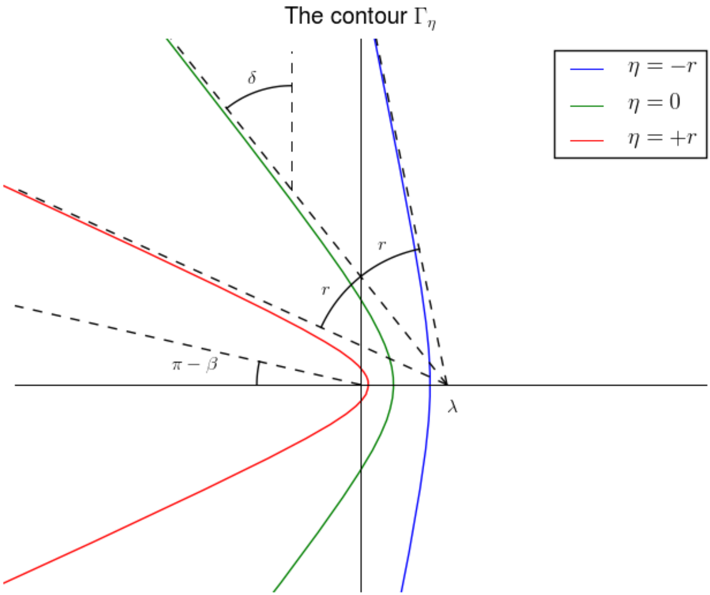
$$z(\xi) := \lambda\bigl(1 - \sin(\delta - i\xi)\bigr) \quad \text{for } -\infty < \xi < \infty.$$

Next, choose σ_0 satisfying

$$\sigma_0 + (1+\alpha)^{-1} \geq \sigma$$

and define the quadrature step-size

$$k := \sqrt{\frac{2\pi r}{\gamma N}}.$$



The contour Γ_η
$\eta = -r$
$\eta = 0$
$\eta = +r$
δ
r
r
$\pi - \beta$
λ

Theorem

With the assumptions above, if $k \leq 2\pi r / \log 2$ *then*

$$\|U_N(t) - u(t)\| \leq \frac{CMT^\gamma}{\gamma} e^{-\sqrt{2\pi r \gamma N}} \Big(\|u_0\|_\sigma + \|f(0)\|_{\sigma_0} + \int_0^t \|f'(s)\|_{\sigma_0} \, ds \Big) \quad \text{for } 0 \leq t \leq T,$$

where $C = C(\delta, r, \beta, \sigma, \sigma_0)$.

Remark: in practice we want $\sigma_0 < 1/4$ otherwise $f(0)$ and $f'(s)$ must vanish on $\partial\Omega$.

Spatial Discretization

Use continuous, piecewise-linear finite elements over a quasi-uniform triangulation of Ω, so $u_h : [0, T] \to V_h$ satisfies

$$\langle \partial_t u_h, v \rangle + \langle \partial_t^{-\alpha} \nabla u_h, \nabla v \rangle = \langle f(t), v \rangle$$

for all $v \in V_h$ and $0 \le t \le T$, with $u_h(0) = u_{0h} \approx u_0$ and $u_{0h} \in V_h$.
Can show

$$\|u_h(t) - u(t)\| \le \|u_{0h} - u_0\| + Ch^2 \left(\|u_0\|_{\dot{H}^2} + \int_0^t \|u'(s)\|_{\dot{H}^2} \, ds \right).$$

Fully-discrete solution: for $w_h(z_j,t) \in V_h$ given by

$$z_j^{1+\alpha}\langle w_h(z_j,t),\chi\rangle + \langle \nabla w_h(z_j,t), \nabla\chi\rangle = \langle g(z_j,t),\chi\rangle$$

for all $\chi \in V_h$, put

$$\widetilde{w}_h(z_j,t) := w_h(z_j,t) - z_j^{-1} g(z_j,t)$$

and then

$$U_{N,h}(t) := P_h\biggl(u_0 + F(t) + \frac{k}{2\pi i}\sum_{j=-N}^{N} \widetilde{w}_h(z_j,t) z_j'\biggr), \quad 0 \le t \le T.$$

(P_h is the L_2-projection onto V_h.)

Error bound

$$\begin{aligned}\|U_{N,h}(t) - u(t)\| &\leq \|U_{N,h}(t) - u_h(t)\| + \|u_h(t) - u(t)\| \\ &= O(e^{-c\sqrt{N}} + h^2)\end{aligned}$$

follows at once from results for $U_N(t)$ and $u_h(t)$.

Numerical Example

Let

$$A = -\nabla^2, \quad \Omega = (0,4) \times (0,4), \quad T = 5,$$

with

$$u_0(x) = \tfrac{1}{2}\sin(\tfrac{1}{4}\pi x_1)\sin(\tfrac{1}{4}\pi x_2) + \tfrac{3}{10}\sin(\tfrac{2}{4}\pi x_1)\sin(\tfrac{3}{4}\pi x_2)$$

and

$$f(t) = \begin{cases} t(2-t)^2, & 0 < t < 2, \\ 0, & 2 < t < \infty. \end{cases}$$

We remark that $\hat{f}(z) = O(e^{2|\operatorname{Re} z|}/|z|^3)$ as $|z| \to \infty$ with $z \in \Gamma_0$.

For the time discretization, we take

$$\delta = \frac{\pi}{4} \min\left(1, \frac{1-\alpha}{1+\alpha}\right)$$

with

$$r = 0.9\delta, \qquad \gamma = \min(1, 1+\alpha).$$

For the spatial discretiztaion, we take a uniform, 60×60 grid on Ω and bisect each square along its north-west to south-east diagonal.

Exact solution is not known, so we use a high-accuracy, reference solution computed with a large N and Richardson extrapolation in space.

Increase N keeping h fixed, until only the spatial error remains.

Errors in $U_{N,h}$ for $\alpha = -1/2$.

N	$t = 0.0$	$t = 1.0$	$t = 3.0$	$t = 5.0$
5	1.6655e-01	8.2316e-02	1.1979e-01	9.3548e-02
10	5.5016e-02	1.7858e-02	2.2820e-02	2.0539e-02
20	1.0004e-02	3.9879e-03	3.7614e-03	3.4283e-03
30	3.5077e-03	3.2388e-03	1.7528e-03	1.3733e-03
40	2.6674e-03	3.2388e-03	1.7296e-03	1.2651e-03
50	2.8163e-03	3.2388e-03	1.7296e-03	1.2651e-03
60	2.8741e-03	3.2388e-03	1.7296e-03	1.2651e-03
80	2.9043e-03	3.2388e-03	1.7296e-03	1.2651e-03

Errors in $U_{N,h}$ for $\alpha = 0$.

N	$t = 0.0$	$t = 1.0$	$t = 3.0$	$t = 5.0$
5	5.2112e-02	2.1288e-02	2.1385e-02	2.3927e-02
10	7.9343e-03	4.5562e-03	2.6404e-03	2.6243e-03
20	2.0079e-03	3.1085e-03	4.6697e-04	1.6832e-04
30	1.6319e-03	3.1085e-03	3.5982e-04	6.4468e-05
40	1.5893e-03	3.1085e-03	3.5100e-04	5.6079e-05
50	1.5829e-03	3.1085e-03	3.4990e-04	5.4931e-05
60	1.5814e-03	3.1085e-03	3.4971e-04	5.4739e-05
80	1.5810e-03	3.1085e-03	3.4966e-04	5.4694e-05

Errors in $U_{N,h}$ for $\alpha = +1/2$.

N	$t = 0.0$	$t = 1.0$	$t = 3.0$	$t = 5.0$
5	1.7901e-01	3.2777e-01	7.1592e-02	2.3052e-02
10	3.6276e-02	8.3494e-02	1.9718e-03	3.2560e-03
20	3.6340e-03	1.0699e-02	6.9519e-04	7.5804e-04
30	2.2102e-03	2.7341e-03	6.9519e-04	6.4513e-04
40	2.5698e-03	2.2754e-03	6.9519e-04	6.4710e-04
50	2.6234e-03	2.2754e-03	6.9519e-04	6.5022e-04
60	2.6310e-03	2.2754e-03	6.9519e-04	6.4920e-04
80	2.6336e-03	2.2754e-03	6.9519e-04	6.4935e-04