Subdiffusion in a nonconvex polygon

Kim Ngan Le and William McLean
The University of New South Wales

Bishnu Lamichhane
University of Newcastle

Monash Workshop on Numerical PDEs, February 2016

Outline

Time-fractional diffusion

Poisson equation on a nonconvex polygon

Error bounds for fractional diffusion

Numerical examples

Smoothing property of diffusion equations

Time-fractional diffusion

Let $0 < \alpha < 1$ and seek $u = u(x, t)$ satisfying

$$\partial_t u - \partial_t^{1-\alpha} K \nabla^2 u = 0 \quad \text{for } x \in \Omega \text{ and } t > 0,$$

together with the initial condition $u(x, 0) = u_0(x)$ and homogeneous Dirichlet boundary conditions,

$$u(x, t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0.$$

Riemann–Liouville fractional derivative in time,

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

Recover classical (Brownian) diffusion in limit $\alpha \to 1$.

Spatial discretisation by finite elements

Assume that Ω is a 2D polygon. Triangulate Ω and let $V_h \subseteq H_0^1(\Omega)$ denote the corresponding space of continuous, piecewise-linear finite element functions that vanish on $\partial\Omega$.

Variational solution $u : [0, \infty) \to H_0^1(\Omega)$ satisfies

$$\langle \partial_t u, v \rangle + a(\partial_t^{1-\alpha} u, v) = 0 \quad \text{for all } v \in H_0^1(\Omega),$$

with $u(0) = u_0$, where

$$a(u, v) = K \int_\Omega \nabla u \cdot \nabla v \, dx.$$

Finite element solution $u_h : [0, \infty) \to V_h$ satisfies

$$\langle \partial_t u_h, \chi \rangle + a(\partial_t^{1-\alpha} u_h, \chi) = 0 \quad \text{for all } \chi \in V_h,$$

with $u_h(0) = u_{0h} \approx u_0$.

Method of lines

Let

$$\begin{aligned} N &= \dim V_h = \text{number of degrees of freedom}, \\ \mathbf{U}(t) &= \text{vector of nodal values of } u_h(t), \\ \mathbf{M} &= \text{mass matrix}, \\ \mathbf{S} &= \text{stiffness matrix}. \end{aligned}$$

Obtain a system of integrodifferential equations in $\mathbb{R}^N$:

$$\mathbf{M}\partial_t \mathbf{U} + \mathbf{S}\partial_t^{1-\alpha}\mathbf{U} = \mathbf{0}.$$

Reduces to usual method of lines for the heat equation in the limiting case when $\alpha \to 1$.

Convex case

Notation: $Av = -K\nabla^2 v : H_0^1(\Omega) \to H^{-1}(\Omega)$, and $P_h : L_2(\Omega) \to V_h$ denotes the orthoprojector.

Theorem (McLean & Thomée, 2010)

Let $u_{0h} = P_h u_0$. If $u_0 \in L_2(\Omega)$, then

$$\|u_h(t) - u(t)\| \le C t^{-\alpha} h^2 \|u_0\|, \quad \text{for } t > 0.$$

If $u_0 \in D(A) = H^2(\Omega) \cap H_0^1(\Omega)$, then

$$\|u_h(t) - u(t)\| \le C h^2 \|Au_0\|, \quad \text{for } t \ge 0.$$

Classical case $\alpha = 1$ proved by Bramble, Schatz, Thomée & Wahlbin (SINUM, 1977).

Error analysis relies on H^2-regularity of the Poisson problem,

$$-K\nabla^2 u = f(x) \quad \text{for } x \in \Omega, \quad \text{with } u(x) = 0 \text{ for } x \in \partial\Omega.$$

If Ω is convex and $f \in L_2(\Omega)$, then the (variational) solution u belongs to $H^2(\Omega)$, and

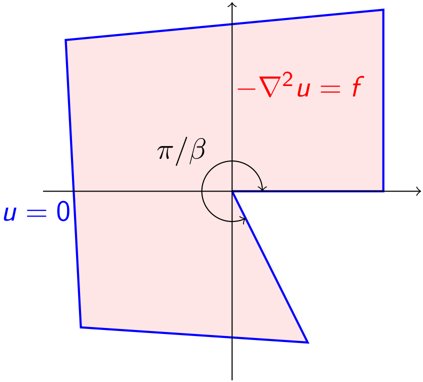
$$\|u\|_2 \leq C\|f\|.$$

Here, we use the abbreviation $\|v\|_m = \|v\|_{H^m(\Omega)}$.

But H^2-regularity breaks down if Ω is a polygon with a re-entrant corner.

Poisson equation on a nonconvex polygon

Suppose only one re-entrant corner at the origin with angle π/β for $1/2 < \beta < 1$.



Polar coordinates

Separating variables, we find that the functions

$$u_n^{\pm} = r^{\pm n\beta} \sin(n\beta\theta), \quad n \in \{1, 2, 3, \ldots\},$$

satisfy

$$\nabla^2 u_n^{\pm} = 0 \quad \text{for } 0 < r < \infty \text{ and } 0 < \theta < \pi/\beta,$$

with

$$u_n^{\pm} = 0 \quad \text{for } 0 < r < \infty \text{ and } \theta = 0 \text{ or } \pi/\beta.$$

Let $\eta = \eta(r)$ be a C^∞ cutoff function equal to 1 for small r. Then,

$$\eta u_n^+ \in H_0^1(\Omega) \quad \text{but} \quad \eta u_n^- \notin H_0^1(\Omega) \quad \text{for all } n \geq 1.$$

Also,

$$\eta u_n^+ \in H^2(\Omega) \text{ for all } n \geq 2 \quad \text{but} \quad \eta u_1^+ \notin H^2(\Omega).$$

Singular behaviour

Recall $A = -K\nabla^2$ and put

$$\mathcal{R} = \{\, Av : v \in H_0^1(\Omega) \cap H^2(\Omega)\,\},$$
$$\mathcal{N} = \{\, v \in L_2(\Omega) : Av = 0 \text{ in } \Omega,\ v = 0 \text{ on } \partial\Omega\,\}.$$

Lemma

$L_2(\Omega) = \mathcal{R} \oplus \mathcal{N}$ *and* $\dim \mathcal{N} = 1$.

Theorem

There exists $q \in \mathcal{N}$ *(depending only on* Ω *and* η*) such that if* $f \in L_2(\Omega)$ *then the variational solution* $u \in H_0^1(\Omega)$ *of the Poisson problem,*

$$-K\nabla^2 u = f(x) \quad \text{for } x \in \Omega, \quad \text{with } u(x) = 0 \text{ for } x \in \partial\Omega,$$

satisfies

$$\left\| u - \langle q, f\rangle \eta u_1^+ \right\|_2 \le C\|f\|.$$

Local mesh refinement

Consider a family of shape-regular triangulations $\mathcal{T}_h$. For each element $\triangle \in \mathcal{T}_h$, let

$$\begin{aligned} h_\triangle &= \text{diameter of } \triangle, \\ r_\triangle &= \text{distance from 0 to } \triangle, \\ h &= \max_{\triangle \in \mathcal{T}_h} h_\triangle. \end{aligned}$$

For some $\gamma \geq 1$, assume

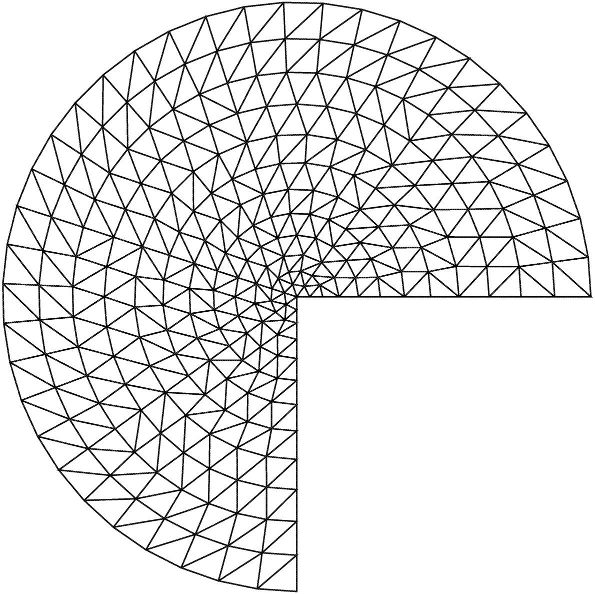
$$c h r_\triangle^{1-1/\gamma} \leq h_\triangle \leq C h r_\triangle^{1-1/\gamma} \quad \text{whenever } h^\gamma \leq r_\triangle \leq 1,$$

and

$$c h^\gamma \leq h_\triangle \leq C h^\gamma \quad \text{whenever } r_\triangle < h^\gamma.$$

Elements increase in size from h^γ near 0 to h when $r_\triangle \geq c > 0$.

"Generalised polygon" with $\gamma = 3/2$



Approximation property

Given $v \in C(\overline{\Omega})$ let $\Pi_h v \in V_h$ denote the nodal interpolant to v.

Theorem

If $f \in L_2(\Omega)$, then the solution of the Poisson problem

$$-K\nabla^2 u = f(x) \quad \text{for } x \in \Omega, \quad \text{with } u(x) = 0 \text{ for } x \in \partial\Omega,$$

satisfies

$$\|u - \Pi_h u\| \le C h\epsilon(h,\gamma)\|f\| \quad \text{and} \quad \|u - \Pi_h u\|_{H_0^1(\Omega)} \le C\epsilon(h,\gamma)\|f\|,$$

where

$$\epsilon(h,\gamma) = \begin{cases} h^{\gamma\beta}/\sqrt{\gamma^{-1} - \beta}, & 1 \le \gamma < 1/\beta, \\ h\sqrt{\log(1 + h^{-1})}, & \gamma = 1/\beta, \\ h/\sqrt{\beta - \gamma^{-1}}, & \gamma > 1/\beta. \end{cases}$$

Finite element error for the Poisson problem

Corollary

$$\|u_h - u\| \leq C\epsilon(h,\gamma)^2\|f\| \quad and \quad \|u_h - u\|_1 \leq C\epsilon(h,\gamma)\|f\|.$$

Proof.

Error bound in $H_0^1(\Omega)$ follows from quasi-optimality,

$$\|u_h - u\|_1 \leq C \min_{v \in V_h} \|v - u\|_1.$$

Error bound in $L_2(\Omega)$ follows by usual duality argument (Nitsche trick). □

So for a quasi-uniform mesh ($\gamma = 1$) we have

$$\|u_h - u\| \leq C h^{2\beta}\|f\| \quad \text{and} \quad \|u_h - u\|_1 \leq C h^{\beta}\|f\|.$$

Error bounds for fractional diffusion

Let $P_h : L_2(\Omega) \to V_h$ denote the orthoprojector and $R_h : H_0^1(\Omega) \to V_h$ the Ritz projector.

Theorem

For general initial data $u_0 \in L_2(\Omega)$ *and all* $t > 0$,

$$\|u_h(t) - u(t)\| \leq \|u_{0h} - P_h u_0\| + Ct^{-\alpha}\epsilon(h,\gamma)^2\|u_0\|$$

and

$$\|u_h(t) - u(t)\|_1 \leq Ct^{-\alpha}\|u_{0h} - P_h u_0\| + C(t^{-\alpha} + t^{-2\alpha})\epsilon(h,\gamma)\|u_0\|.$$

For "smoother" initial data such that $A^{1+\delta}u_0 \in L_2(\Omega)$ *and for* $0 \leq t \leq T$,

$$\|u_h(t) - u(t)\| \leq \|u_{h0} - R_h u_0\| + C\delta^{-1}\epsilon(h,\gamma)^2\|A^{1+\delta}u_0\|.$$

Integral representation of $u(t)$

The proof relies on the Laplace transform,

$$\hat{u}(z) = \int_0^\infty e^{-zt} u(t)\, dt.$$

Since

$$\partial_t u + \partial_t^{1-\alpha} A u = 0$$

we have

$$z\hat{u}(z) - u_0 + z^{1-\alpha} A\hat{u} = 0$$

and so

$$(z^\alpha I + A)\hat{u}(z) = z^{\alpha-1} u_0.$$

Inversion formula: for a suitable contour Γ in the complex plane,

$$u(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} \hat{u}(z)\, dz, \quad t > 0.$$

Integral representation of $u_h(t)$

Similarly,

$$\partial_t u_h + \partial_t^{1-\alpha} A_h u = 0$$

where $A_h : V_h \to V_h$ is defined by

$$\langle A_h v, w \rangle = a(v, w) \quad \text{for } v,\ w \in V_h.$$

Thus,

$$(z^\alpha I + A_h)\hat{u}_h(z) = z^{\alpha-1} u_{0h}$$

and

$$u_h(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} \hat{u}_h(z)\, dz, \quad t > 0,$$

leading to a representation of the error,

$$u_h(t) - u(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} z^{\alpha-1} \left[(z^\alpha I + A_h)^{-1} u_{0h} - (z^\alpha I + A)^{-1} u_0 \right] dz.$$

Numerical examples

We choose Ω to be the domain

$$0 < r < 1 \quad \text{and} \quad 0 < \theta < \pi/\beta \quad \text{for } \beta = 3/2.$$

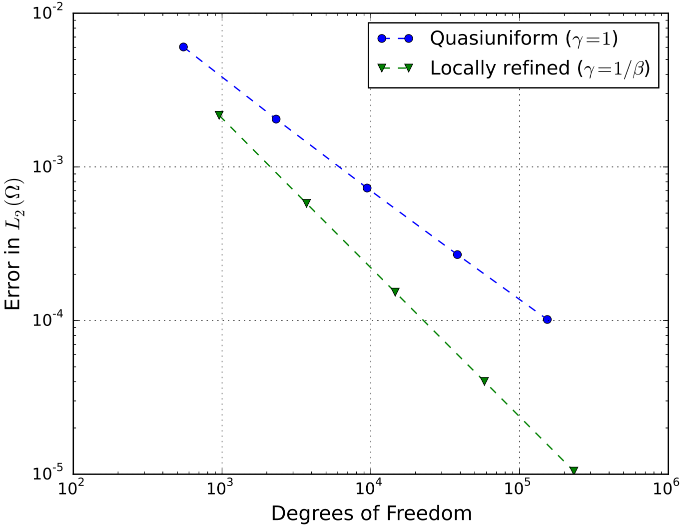
In the first example we solve an (inhomogeneous) fractional diffusion equation with exact solution

$$u = \left(1 + \frac{t^\alpha}{\Gamma(\alpha+1)}\right) r^\beta (1-r) \sin(\beta\theta),$$

with $\alpha = 1/2$.

Time discretisation uses a quadrature approximation to the Laplace inversion formula.

Errors $\|u_h(t) - u(t)\|$ at $t = 1$.



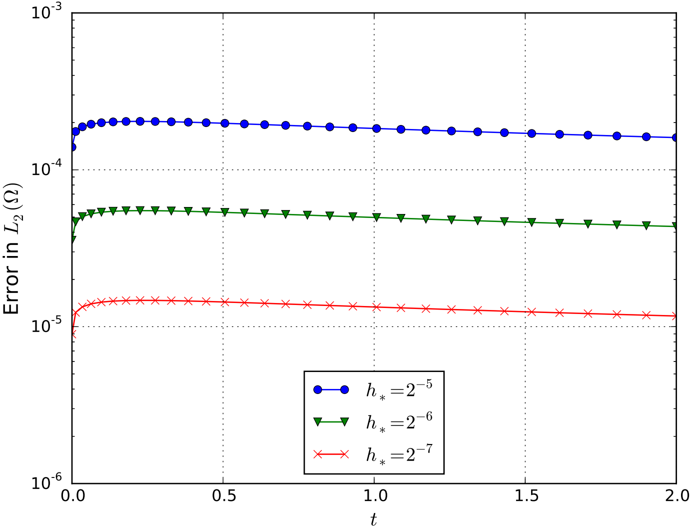
In the second example we impose mixed boundary conditions and choose the initial data to be the first eigenfunction of $A = -K\nabla^2$,

$$u_0 = J_{\beta/2}(\omega r)\sin(\tfrac{1}{2}\beta\theta),$$

where ω is the smallest positive zero of $J_{\beta/2}$. For triangulations $\mathcal{T}_h$ with $\gamma = 2/\beta = 3$ we observe the following convergence rates at $t = 1$.

		$\alpha = 1/4$		$\alpha = 3/4$	
h_*	N	error	rate	error	rate
2^{-4}	1957	1.465e-03		1.452e-03	
2^{-5}	7593	3.673e-04	1.996	3.640e-04	1.997
2^{-6}	29771	9.471e-05	1.955	9.380e-05	1.956
2^{-7}	117039	2.420e-05	1.969	2.391e-05	1.972
2^{-8}	466089	6.059e-06	1.998	5.931e-06	2.011

Error $\|u_h(t) - u(t)\|$ as a function of t, for $\alpha = 1/2$



Smoothing property of diffusion equations

Let ϕ_1, ϕ_2, ϕ_3, ... denote the orthonormal Let (ϕ_n, λ_n) denote the nth eigenpair of $A = -K\nabla^2$ in Ω:

$$A\phi_n = \lambda_n \phi_n \quad \text{in } \Omega, \quad \text{with } \phi_n = 0 \text{ on } \partial\Omega.$$

Thus, $\phi_n \in H_0^1(\Omega)$ with

$$a(\phi_n, \phi_m) = \lambda_n \delta_{mn} \quad \text{and} \quad \langle \phi_n, \phi_m \rangle = \delta_{mn}.$$

Expand the solution of the fractional diffusion equation in a generalised Fourier series

$$u(t) = \sum_{n=1}^{\infty} u_n(t)\phi_n.$$

Modes $u_n(t)$ are damped as $n \to \infty$, for any fixed $t > 0$.

Mittag–Leffler function

Each mode satisfies a fractional relaxation equation,

$$\partial_t u_n + \lambda_n \partial_t^{1-\alpha} u_n = 0, \quad \text{with } u_n(0) = \langle u(0), \phi_n \rangle.$$

Using the identity

$$\partial_t^\beta \frac{t^\alpha}{\Gamma(\alpha+1)} = \frac{t^{\alpha-\beta}}{\Gamma(\alpha-\beta+1)}$$

we find $u_n(t) = u_n(0) E_\alpha(-\lambda_n t^\alpha)$ where

$$E_\alpha(z) = \sum_{p=0}^{\infty} \frac{z^p}{\Gamma(1+p\alpha)}.$$

Series representation

Thus,

$$u(t) = \sum_{n=1}^{\infty} u_n(0) E_\alpha(-\lambda_n t^\alpha)\phi_n.$$

Note that

$$E_\alpha(-\lambda_n t^\alpha) \to E_1(-\lambda_n t) = e^{-\lambda_n t} \quad \text{as } \alpha \to 1,$$

giving the usual representation for the solution of the heat equation.