

# Reliable numerical schemes for a linear diffusion equation on a nonsmooth domain

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## Abstract

The solution of a linear reaction diffusion equation on a non-convex polygon is proved to be globally regular in a suitable weighted Sobolev space. This result is used to design an optimally convergent Fourier-Finite Element Method (FEM) where the mesh size is suitably refined. Furthermore, the coupled Non-Standard Finite Difference Method (NSFDM)-FEM is presented as a reliable scheme that replicates the essential properties of the exact solution.

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## 1 Introduction

We consider the linear reaction diffusion equation

$$\frac{\partial u}{\partial t} - \Delta u + \lambda u = f \text{ in } \Omega \times (0, +\infty), \quad \lambda \geq 0, \quad u(x, 0) = g(x) \text{ and } u = 0 \text{ on } \partial\Omega \times (0, +\infty), \quad (1)$$

where  $\Omega \subset \mathbb{R}^2$  is a polygonal domain with boundary  $\partial\Omega \equiv \Gamma$ . The origin of the plane, viewed as the center of polar co-ordinates  $(r, \theta)$ , is assumed to be the only non-convex vertex of the polygon with angle  $\omega$  such that one of the two sides adjacent to the origin is on the abscissa axis [1]. We will make use of the function  $S = \psi r^{\frac{\pi}{\omega}} \sin \frac{\pi}{\omega} \theta$ ,  $\psi \equiv \psi(r)$  being a smooth cut-off function that is equal to 1 near 0 i.e. for  $r \leq 1/4$ . We assume that  $f \in L^2((0, +\infty), L^2(\Omega))$  and  $g \in L^2((0, +\infty), H_0^1(\Omega))$  (see [2] for the function spaces). Given a Hilbert space  $X$ , we will more generally use the Sobolev space  $H^s((0, +\infty), X)$ . The notation  $\tilde{H}^s((0, +\infty), X)$  stands for the space of functions  $v \in H^s((0, +\infty), X)$  such that the extension  $\tilde{v}$  by 0 outside  $(0, +\infty)$  belongs to  $H^s((-\infty, +\infty), X)$ . In practice,  $X$  will be the Sobolev space  $H^m(\Omega)$  or  $H_0^m(\Omega)$ .

Problem (1) has been widely studied in the literature. Here, the emphasis is on numerical schemes that replicate the dynamics of (1). In this regard, problem (1) has two specific features. Firstly, due to the presence of a non-convex corner on  $\Omega$ , the solution does not have the classical regularity  $u \in L^2((0, +\infty), H^2(\Omega))$  and this negatively affects the rate of convergence of the classical FEM. We overcome this difficulty by giving the global regularity of  $u$  in a weighted Sobolev space (Sect 2) and by designing optimally convergent finite element-based methods with suitably refined space mesh (Sects 3-4). Secondly, in the space independent case, the first equation in (1) with  $f = 0$  reduces to the decay equation. Following the methodology in [3] and [4], we propose for (1) a new scheme, i.e. a coupled non-standard finite difference method (NSFDM)-FEM, which is reliable as it replicates the properties of the exact solution in the above-mentioned limit case (Sect 5). Numerical experiments that confirm the theory are given in Sect 6. The theoretical part of this work was announced in [5].

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## 2 Global regularity

We assume without loss of generality that  $g = 0$  in what follows. It is proved in [6] that the unique solution  $u \in L^2((0, +\infty), H_0^1(\Omega)) \cap \tilde{H}^1((0, +\infty), L^2(\Omega))$  admits a decomposition into regular and singular parts. Our constructive treatment of (1) is based on the following result in [5]:

**Theorem 1.** *The solution has the global regularity  $u \in L^2((0, +\infty), H^{2,\beta}(\Omega))$  such that*

$$\|u\|_{L^2((0, +\infty), H^{2,\beta}(\Omega))} \leq C \|f\|_{L^2((0, +\infty), L^2(\Omega))}$$

where the weighted Sobolev space  $H^{2,\beta}(\Omega) := \{v \in H^1(\Omega); r^\beta D^\alpha v \in L^2(\Omega), |\alpha| = 2\} \subset C^0(\bar{\Omega})$ , with  $1 > \beta > 1 - \frac{\pi}{\omega}$ , is defined in [1]. Here and below,  $C$  stands for various constants that are independent of the involved arguments and parameters (e.g. Fourier, step sizes, etc.)

## 3 Semi-discrete FEM

Instead of the Singular Function Method [7], which is based on the singular decomposition in [6], we present here the Mesh Refinement Method (MRM). By the Laplace transform, (1) becomes

$$\Delta \hat{u} + p \hat{u} + \lambda \hat{u} = \hat{f} \quad \text{in } \Omega, \quad \hat{u} = 0 \quad \text{on } \partial\Omega. \quad (2)$$

Let  $(\tau_h)$  be a regular family of triangulations of  $\bar{\Omega}$  consisting of compatible triangles  $T$  of diameter  $h_T \leq h$  (see [8]). Consider the finite element space

$$V_h := \{v \in C^0(\bar{\Omega}); v|_{\partial\Omega} = 0, v|_T \in P_1, T \in \tau_h\} \subset H_0^1(\Omega)$$

where  $P_1$  is the space of polynomials of degree  $\leq 1$ . By Lax-Milgram Lemma, there exists  $\hat{u}_h \equiv \hat{u}_h(p) \in V_h$ , which is the unique solution of

$$\int_{\Omega} (\nabla \hat{u}_h \nabla \bar{v}_h + (p + \lambda) \hat{u}_h \bar{v}_h) dx = \int_{\Omega} \hat{f} \bar{v}_h dx, \quad \forall v_h \in V_h, \quad p = \xi + i\eta, \quad \xi \geq 0, \quad (3)$$

such that

$$\|\hat{u}_h\|_{H^1(\Omega, 1+\sqrt{|p|})}^2 := \|\nabla \hat{u}_h\|_{L^2(\Omega)}^2 + (1 + \sqrt{|p|})^2 \|\hat{u}_h\|_{L^2(\Omega)}^2 \leq C \|\hat{f}\|_{L^2(\Omega)}^2. \quad (4)$$

By the Céa Lemma and the interpolation theory based on the local regularization operator of Clément as well as on the Lagrange local interpolant  $\Pi_T \hat{u}$  defined in [8], we have

$$\|\hat{u} - \hat{u}_h\|_{H^1(\Omega, 1+\sqrt{|p|})}^2 \leq C \left\{ \sum_{T \in \tau_h} \|\nabla \hat{u} - \nabla \Pi_T \hat{u}\|_{L^2(T)}^2 + (1 + \sqrt{|p|}) h^2 \|\hat{u}\|_{H^1(\Omega)}^2 \right\}. \quad (5)$$

The following local error estimates can be proved:

$$\|\nabla \hat{u} - \nabla \Pi_T \hat{u}\|_{L^2(T)}^2 \leq C \begin{cases} h_T^2 (\inf_T r^{2\beta})^{-1} \sum_{|\alpha|=2} \int_T |r^\beta D^\alpha \hat{u}|^2 dx & \text{if } 0 \notin T \\ h_T^{2(1-\beta)} \|\hat{u}\|_{H^{2,\beta}(\Omega)}^2 & \text{if } 0 \in T. \end{cases} \quad (6)$$

Thus, the triangulations are subject to the following mesh refinement conditions:

$$h_T \leq Ch^{\frac{1}{1-\beta}} \quad \text{if } 0 \in T \quad \text{and} \quad h_T \leq Ch \inf_T r^\beta \quad \text{if } 0 \notin T. \quad (7)$$

In view of (4)-(7) and of the uniform estimates of  $\hat{u}$  (see [5]), we have

$$\|\hat{u} - \hat{u}_h\|_{H^1(\Omega, 1+\sqrt{|p|})}^2 \leq Ch^2 \left\{ \|\hat{u}\|_{H^{2,\beta}(\Omega)}^2 + (1 + \sqrt{|p|})^2 \|\hat{u}\|_{H^1(\Omega)}^2 \right\} \leq Ch^2 \|\hat{f}\|_{L^2(\Omega)}^2.$$

Furthermore, the Aubin-Nitsche duality argument yields  $\|\hat{u} - \hat{u}_h\|_{L^2(\Omega)}^2 \leq Ch^4 \|\hat{f}\|_{L^2(\Omega)}^2$ . Plancherel-Parseval theorem and the inverse Fourier transform imply the following result:

**Theorem 2.** *Assume that the triangulations are refined according to (7). Then the semi-discrete solution  $u_h(t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{it\eta} \hat{u}_h(i\eta) d\eta$  is such that*

$$\|u - u_h\|_{L^2((0, +\infty), L^2(\Omega))}^2 + h^2 \|u - u_h\|_{L^2((0, +\infty), H^{\frac{1}{2}}(\Omega)) \cap H^{\frac{1}{2}}((0, +\infty), L^2(\Omega))}^2 \leq Ch^4 \|f\|_{L^2((0, \infty), L^2(\Omega))}^2.$$

## 4 Fourier-FEM

To use the Fourier-FEM [9] as a fully discrete process, fix  $N \in \mathbb{N}$  and consider the following expansions in  $L^2((0, 2\pi), X)$ :

$$u(x, t) = \sum_{k \in \mathbb{Z}} e^{ikt} u_k(x), \quad f(x, t) = \sum_{k \in \mathbb{Z}} e^{ikt} f_k(x).$$

In the previous arguments, the Laplace transforms  $\hat{u}(p)$  and  $\hat{f}(p)$  are replaced by the Fourier coefficients  $u_k$  and  $f_k$ . Solve the discrete problem (3) for  $p = ik$  with  $|k| \leq N$  and  $k \in \mathbb{Z}$  to obtain the solution  $u_{k,h} \in V_h$ . The properties of Fourier series and of the truncated series  $u^N := \sum_{|k| \leq N} e^{ikt} u_k(x)$  ([10]) as well as the density of  $H^1((0, 2\pi), H^1(\Omega))$  in  $L^2((0, 2\pi), H^1(\Omega))$  yield the following result:

**Theorem 3.** *The discrete solution  $u_h^N := \sum_{|k| \leq N} e^{ikt} u_{k,h}(x)$  converges to  $u$  in  $L^2((0, 2\pi), H^1(\Omega))$  as  $N \rightarrow +\infty$  and  $h \rightarrow 0$ . There hold the error estimates*

$$\|u_h^N - u\|_{L^2((0, 2\pi), L^2(\Omega))} \leq C(h^2 + N^{-1}) \quad \text{and} \quad \|u_h^N - u\|_{L^2((0, 2\pi), H^1(\Omega))} \leq C(h + N^{-1}),$$

the second estimate being valid under the tangential regularity  $u \in H^1((0, 2\pi), H^1(\Omega))$ .

## 5 Coupled NSFDM-FEM

We now consider a new fully discrete process. To motivate it, we observe that when  $f = 0$  and  $\lambda > 0$ , the space independent equation of the first equation in (1) is the decay equation, which has the exact scheme [3, 4]

$$\frac{u^{k+1} - u^k}{(e^{\lambda \Delta t} - 1)/\lambda} + \lambda u^{k+1} = 0, \quad u^0 := g \quad (8)$$

where  $t_k := k\Delta t$ ,  $\Delta t$  being the time step size. We thus approximate (1) by the following (space) FEM and (time) non-standard finite difference method: with the initial guess  $u_h^0 := \Pi_h g \in V_h$  via the global interpolation operator  $\Pi_h$ , let  $(u_h^k)_{k \geq 1}$  be the sequence in the finite element space  $V_h$  defined recursively as unique solution of

$$\int_{\Omega} \left( \frac{u_h^{k+1} - u_h^k}{(e^{\lambda \Delta t} - 1)/\lambda} v_h + \nabla u_h^{k+1} \cdot \nabla v_h + \lambda u_h^{k+1} v_h \right) dx = \int_{\Omega} f v_h dx, \quad \forall v_h \in V_h. \quad (9)$$

**Theorem 4.** *Assume that  $g$  is smoother and  $u$  is tangentially smoother in the sense that  $g$  and  $u$  are in the spaces  $L^2((0, +\infty), H^2(\Omega))$  and  $H^2((0, +\infty), L^2(\Omega)) \cap H^1((0, +\infty), H^{2,\beta}(\Omega))$ , respectively. Then, there hold the error estimates*

$$\|u_h^k - u(t_k)\|_{L^2(\Omega)} \leq C(\Delta t + h^2) \quad \text{and} \quad \|u_h^k - u(t_k)\|_{H^1(\Omega)} \leq C(\sqrt{\Delta t} + h).$$

Furthermore, in the limit case when  $\Delta u = f = 0$  on a subset  $\Omega' \subset \Omega$ , the discrete solution replicates the monotonic properties of the solution of the decay equation.

*Proof.* In view of the asymptotic relation

$$(e^{\lambda \Delta t} - 1)/\lambda = \Delta t + O[(\Delta t)^2],$$

the estimates follow from [11], assuming that  $\Delta t$  is proportional to  $h^2$  for the error in the energy norm. Furthermore, its uniform convergence results imply point-wise convergence for  $x \in \Omega'$ .  $\square$

## 6 Numerical Experiments

We take  $\Omega$  to be an  $L$ -shaped domain with  $\omega = 3\pi/2$  being the interior angle at the origin. In (1) we take  $f$  such that

$$u(x, t) = te^{-t}\psi(r)r^{\frac{\pi}{\omega}}\sin\frac{\pi}{\omega}\theta.$$

The refinement parameter  $\beta$  is taken to be  $\beta = 1/3$  and  $h = 1/n$  with  $n = 10, 50, 100, 125$ . The domain  $\Omega$  is refined following the procedure of [12] summarized in [1]. This is shown in Fig 1 for  $n = 10$ . The errors in  $H^1$  and  $L^2$  norms of the NSFDM-FEM (9) are shown on Tables 1 and 2, which confirm the theoretical optimal order of convergence for the refined FEM as well as the poor convergence of the usual FEM. This is further confirmed by the slope of the curves in Figure 2, computed in logarithm scale. The computations were generated by Matlab R14 with the following parameters:  $\lambda = 3$ ,  $\Delta t = 0.5$ , time period  $t = 4$ .

Figure 1:

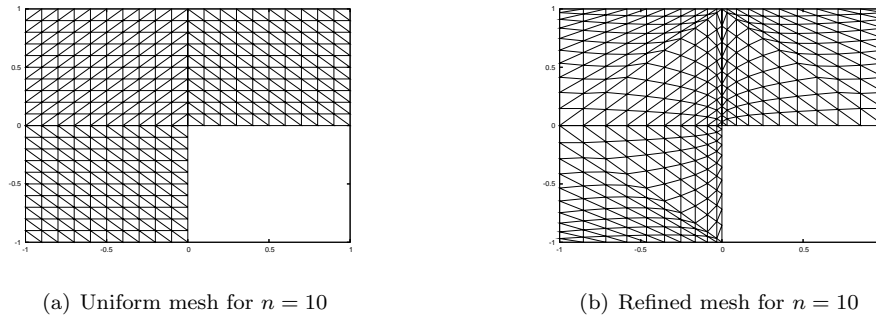


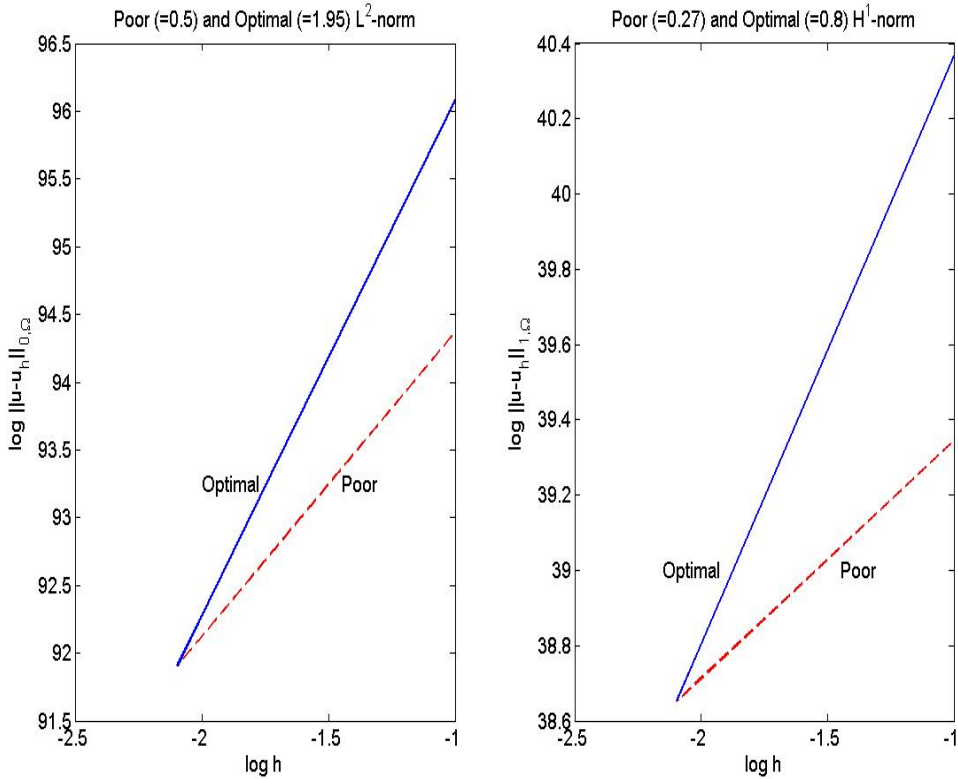
Table 1: Numerical error in the  $H^1$ -norm for both uniform and refined meshes.

$n$	Uniform Mesh	Refined Mesh
	$\ u - u_h\ _{1,\Omega}$	$\ u - u_h\ _{1,\Omega}$
10	3.0854E-3	2.9221E-3
50	1.2875E-3	5.8442E-4
100	9.0016E-4	2.9110E-4
125	8.1009E-4	2.3288E-4

Table 2: Numerical error in the  $L^2$ -norm for both regular and refined meshes.

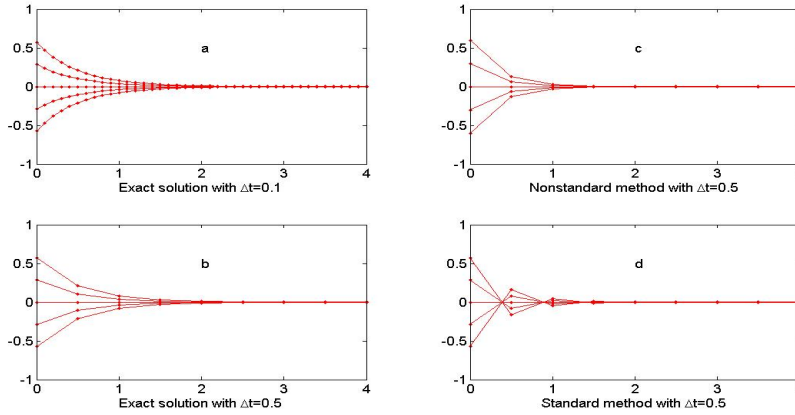
$n$	Uniform Mesh	Refined Mesh
	$\ u - u_h\ _{0,\Omega}$	$\ u - u_h\ _{0,\Omega}$
10	1.2469E-3	1.3411E-6
50	2.4939E-4	5.5372E-8
100	1.3027E-4	1.3860E-8
125	1.0457E-4	8.8717E-9

Figure 2:



To demonstrate the power of the NSFDM, we consider  $u(x, t) = \alpha e^{-\lambda t} \psi(r) r^{\frac{2}{3}} \sin \frac{2}{3} \theta$  that is a solution of (1) for the parameters  $\lambda = 3$  and  $\alpha = \pm 0.5$ . Fix  $x = (-0.0316, 0.05540)$  so that  $|x| \leq 1/4$ . Then  $u(t) \equiv u(x, t)$  as solution of the decay equation (8) is displayed against time on Figs 3a-b. For the same fixed  $x$ , Fig 3c and Fig 3d depict  $u_h^k \equiv u_h^k(x)$  obtained from the NSFDM-FEM (9) as well as from the classical difference method with  $\Delta t = 0.5$ . For the latter method, there is no restriction on the value of  $\Delta t$  since it is implicit [11]. The figures speak for themselves.

Figure 3:



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## References

- [1] P. Grisvard, *Elliptic Problems in Non-Smooth Domains*, Pitman, Boston, 1985.
- [2] J.L. Lions and E. Magenes, *Non-Homogeneous Boundary Value Problems and Applications Vol. I*, Springer-Verlag, New York, 1972.
- [3] R. Anguelov and J.M-S. Lubuma, Contributions to the mathematics of the Non-standard finite difference method and applications, *Num. Meth. Partial Differential Eq.*, **17**(2001), 518-543.
- [4] R.E. Mickens, *Nonstandard Finite Difference Models of Differential Equations*, World Scientific, Singapore, 1994.
- [5] P.W.M. Chin, J.M.-S Lubuma and K.C. Patidar, Regularity and discrete schemes for the heat equation on non-smooth domains. In: T.E. Simos and G. Maroulis(Ed), American Institute of Physics-AIP Conference Proceedings **963** (2007), 1170-1173.
- [6] P. Grisvard, *Singularities in Boundary Value Problems*, Springer-Verlag, Berlin, 1992.
- [7] J. M.-S. Lubuma and S. Nicaise, Méthode de fonctions singulières pour problèmes aux limites avec singularités d'arêtes. *C. R. Acad. Sci. Paris, Série I*, **319**, (1994), 1109-1114.
- [8] P.G. Ciarlet, *The Finite Element Method For Elliptic Problems*, North Holland, Amsterdam, 1978.
- [9] B. Heinrich, The Fourier-finite element method for Poisson's equation in axisymmetric domains with edges, *SIAM J. Numer. Anal.* **33**, (1996), 1885-1911.
- [10] C. Canuto, M.Y. Hussaini, A. Quarteroni and T.A. Zang, *Spectral Methods in Fluid Dynamics*, Springer-Verlag, Berlin, 1988.
- [11] V. Thomée, *Galerkin Finite Element Methods for Parabolic Problems*, Springer-Verlag Lecture Notes Math. 1054, 1984.
- [12] G. Raugel, Résolution numérique par une méthode d'éléments finis du problème de Dirichlet pour le Laplacien dans un polygone, *C. R. Acad. Sci. Paris*, **286**, (1978), 791-794.