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Detection of dead cores for reaction-diffusion equations with a non-smooth nonlinearity

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A B S T R A C T

This paper studies a class of nonlinear elliptic PDEs, arising for stationary reaction-diffusion models. The non-smooth nonlinearity gives rise to dead cores, that is, subdomains where the solution of the PDE vanishes. The paper gives a solid foundation for the numerical solution of the problem, including proper extensions of known maximum–minimum principles, Céa lemma, and convergence estimation of the FEM for locally Hölder continuous operators. Based on these, we finally detect dead cores numerically in various typical situations.

1. Introduction

In this paper we study the following nonlinear partial differential equation (PDE), derived from a stationary reaction-diffusion problem:

$$\begin{cases} -\Delta u + k u^{\gamma} & = 0, \\ u|_{\partial\Omega} & = u_0 > 0, \end{cases} \tag{1}$$

where Ω is a bounded domain in $\mathbb{R}^d$, $0 < \gamma < 1$ and $k, u_0 > 0$ are given constants.

The reaction-diffusion model behind (1) can be summarized as follows, based on the paper [2]. Let us consider an irreversible steady-state reaction which takes place in a bounded planar domain $\Omega \subset \mathbb{R}^2$. Assume that the reagent used up in Ω is replaced through diffusion so that the steady-state can be reached. After eliminating the temperature, [2] writes the following problem for the concentration u of the reactant:

$$\begin{aligned} -\Delta u + \lambda f(u) = 0 \qquad & \text{in } \Omega, \\ u = 1 \qquad & \text{on } \partial\Omega, \end{aligned}$$

where the constant $\lambda > 0$ is the Thiele modulus [12], $f(u)$ is the ratio of the reaction rate at concentration u to the reaction rate at concentration unity for $u \geq 0$, which satisfies $f(0) = 0$ and $f(1) = 1$. In our case the function $f(u) = u^{\gamma}$ describes an isothermal reaction (the temperature of the system remains constant), where γ is called the order of the reaction. In our formulation (1) we do not consider unit concentration on the boundary but we will also study the relation of the three parameters γ, k, u_0.

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As described in [2], it may occur that the density u becomes 0 in a closed region Ω_0, called dead core, that is, here the solution of the nonlinear PDE vanishes. Since no reaction takes place here, the region Ω_0 is wasted. Such a dead core can be formed only if u_0 is small enough or k is large enough, that is the rate of the reaction stays high as the concentration decreases. Namely, in this case it might be impossible for the diffusion to draw some reactant fast enough from the external part of Ω so that it can reach the center of Ω_0. The boundary of the dead core, called free boundary, is not known in advance.

Dead cores have attracted a lot of more recent interest regarding their theoretical background, rules of evolution, and also interesting numerical experiments have been made in 1D, see, e.g., [5,4,10,11,13] on such issues.

In specific cases it is important to show whether such a dead core exists, and if so, then to know its location and geometric properties. This aim is important, e.g. in case of a chemical reaction if the reaction uses a catalyst. Since no reaction takes place in the dead core, this means that the region is wasted and the amount allocated to the dead core can be saved if we know the location of the region.

The goal of the present paper is to give a solid foundation for the numerical solution of problem (1). Thereby we obtain a way to define and characterize dead cores and free boundaries that provides reliable numerical results. Since $0 < \gamma < 1$, the function f is continuous but not differentiable at the origin. It is an important property which prevents us from a direct application of existing results to the numerical process. Instead, we must generalize various blocks of the solution process to the non-differentiable case. Namely, first we extend the well-known maximum and minimum principle for the nonlinear case motivated by our problem. Thus we can turn the problem to an operator equation from which the existence and uniqueness of the weak solution follows. Then we prove a Céa lemma related to the nonlinear Galerkin method and give its convergence estimation for locally Hölder continuous operators. Further, we derive regularity of the solution and prove fractional convergence of the finite element method. Finally, we detect dead cores and free boundaries in various typical situations with analytical and numerical calculations.

2. Maximum and minimum principle

We would like to prove that our original problem (1) has a unique solution and we would like to compute the numerical solution as well. In order to achieve these aims we need to rewrite our problem in the form of an operator equation. To allow this step we first have to reformulate our problem to the following form:

$$\begin{cases} -\Delta u + k|u|^{\gamma-1}u &= 0, \\ u|_{\partial\Omega} &= u_0, \end{cases} \tag{2}$$

where Ω is still a bounded domain, $0 < \gamma < 1$ and $k, u_0 > 0$ are constants. With this reformulation we extended the domain of definition, that is, now the formulas in the problem make sense for every function u, whereas in the original case only $u \geq 0$ was allowed. If we can prove that the solution of (2) satisfies $u \geq 0$, then it will imply that problems (1) and (2) are equivalent. In addition, we will prove the boundedness of the solution u.

2.1. The general maximum and minimum principle and its limitations

Maximum and minimum principles for general nonlinear boundary value problems were examined in [9]. Here we use its consequences for the maximum principle under Dirichlet boundary conditions for the problem

$$\begin{aligned} -\mathrm{div}\,(b(x,\nabla u)\nabla u) + q(x,u) &= f(x) \quad \text{in } \Omega, \\ u &= g(x) \quad \text{on } \partial\Omega, \end{aligned} \tag{3}$$

where Ω is a bounded domain in $\mathbb{R}^d$, under the following assumptions:

(A1) b: $\overline{\Omega} \times \mathbb{R}^d \to \mathbb{R}$, q: $\overline{\Omega} \times \mathbb{R} \to \mathbb{R}$ are continuously differentiable scalar functions in their domains. Further, $f \in L^2(\Omega)$ and $g = g^*|_{\partial\Omega}$ for some $g^* \in H^1(\Omega)$.

(A2) The function b satisfies

$$0 < \mu_0 \leq b(x,\eta) \leq \mu_1, \tag{4}$$

where μ_0, μ_1 are positive constants independent of (x,η), and the diadic product matrix $\eta \cdot \frac{\partial b(x,\eta)}{\partial \eta}$ is symmetric positive semidefinite and bounded.

(A3) Let $2 \leq p_1$ if $d = 2$, or $2 \leq p_1 \leq \frac{2d}{d-2}$ if $d > 2$. There exist constants $\alpha, \beta \geq 0$ such that for any $x \in \Omega$ and $\xi \in \mathbb{R}$

$$0 \leq \frac{\partial q(x,\xi)}{\partial \xi} \leq \alpha + \beta|\xi|^{p_1-2}, \tag{5}$$

Proposition 2.1. *Let assumptions (A1)–(A3) hold and let $u \in C^1(\Omega) \cap C(\overline{\Omega})$ be the weak solution of problem (3). If*

$$f(x) - q(x,0) \le 0, \; x \in \Omega \tag{6}$$

almost everywhere, then

$$\max_{\overline{\Omega}} u \le \max\{0, \max_{\partial\Omega} g\}. \tag{7}$$

If $g \ge 0$, then

$$\max_{\overline{\Omega}} u = \max_{\partial\Omega} g, \tag{8}$$

and if $g \le 0$, then we have the nonpositivity property

$$\max_{\overline{\Omega}} u \le 0. \tag{9}$$

Proof. Our problem (3) and the present proposition are special cases of problem (16) and Theorem 5 in the paper [9], respectively. □

We get the reformulated problem (2) from the general Dirichlet problem (3) if

- $b(x, \nabla u) \equiv 1$ and $q(x,u) = k|u|^{\gamma-1}u$,
- $f(x) \equiv 0$ and $g(x) \equiv u_0$.

In order to use the above Proposition 2.1, we have to consider whether (A1)-(A3) hold in this particular case.

(A1) b: $\overline{\Omega} \times \mathbb{R}^d \to \mathbb{R}$, $b(x,\eta) \equiv 1$ is continuously differentiable in its domain and q: $\overline{\Omega} \times \mathbb{R} \to \mathbb{R}$, $q(x,\xi) = k|\xi|^{\gamma-1}\xi$ is also continuously differentiable in its domain except when $\xi = 0$. Thus now q is not continuously differentiable in its whole domain as in the original case. Further $f \equiv 0 \in L^2(\Omega)$ and $g = g^*|_{\partial\Omega}$, where $g^* \in H^1(\Omega)$ stands for the function $g^* \equiv u_0$ since the constant function is trivially in $H^1(\Omega)$.
(A2) It holds for the function $b \equiv 1$ trivially.
(A3) Let $p_1 := \gamma + 1$. Since $\frac{\mathrm{d}}{\mathrm{d}\xi}\left(k|\xi|^{\gamma-1}\xi\right) = k\gamma|\xi|^{\gamma-1}$ $(\forall \xi \ne 0)$, thus assumption (5) is the following:

$$0 \le \gamma k|\xi|^{\gamma-1} \le \alpha + \beta|\xi|^{\gamma-1} \qquad (\xi \ne 0), \tag{10}$$

which holds trivially for $\alpha = 0$ and $\beta = \gamma k$, but only for $\xi \ne 0$. Moreover, here $1 < p_1 \le 2$.

Altogether, in this case the function q is not differentiable in 0, moreover, $p_1 \le 2$, thus (A1) and (A3) do not hold exactly. Hence we need to extend Proposition 2.1 to a more general form.

2.2. The extension of the maximum and minimum principle

Let us consider the problem

$$\begin{cases} -\Delta u + q(x,u) &= f(x), \\ u|_{\partial\Omega} &= g(x), \end{cases} \tag{11}$$

under the following assumptions:

$(\hat{\mathrm{A}}1)$ q: $\overline{\Omega} \times \mathbb{R} \to \mathbb{R}$, $q = q(x,\xi)$ is continuously differentiable in its domain except when $\xi = 0$. Further $f \in L^2(\Omega)$ and $g = g^*|_{\partial\Omega}$, where $g^* \in H^1(\Omega)$.
$(\hat{\mathrm{A}}3)$ Let $1 \le p_1$ if $d = 2$, or $1 \le p_1 \le \frac{2d}{d-2}$ if $d > 2$. There exist constants $\alpha, \beta \ge 0$ such that for any $x \in \Omega$ and $\xi \in \mathbb{R} \setminus \{0\}$

$$0 \le \frac{\partial q(x,\xi)}{\partial \xi} \le \alpha + \beta|\xi|^{p_1-2} \qquad (\xi \ne 0).$$

From the original assumptions (A2) trivially holds for problem (11), but assumptions (A1) and (A3) do not; this is why we had to introduce assumptions $(\hat{\mathrm{A}}1)$ and $(\hat{\mathrm{A}}3)$. Now we can prove the following result. For simplicity we only consider the case $q(x,0) = 0$ suited to our original problem.

Theorem 2.1. *Let assumptions (A2), ($\hat{A}1$) and ($\hat{A}3$) hold, and let $q(x,0)=0$. Further, let $u\in C^1(\Omega)\cap C(\overline{\Omega})$ be the weak solution of problem (11). If*

$$f(x)\le 0, \quad x\in\Omega \tag{12}$$

almost everywhere, then (7)-(9) hold.

Proof. The weak form of problem (11) is:

$$\int_\Omega (\nabla u\cdot\nabla v+q(x,u)v)\,\mathrm{d}x=\int_\Omega f v\mathrm{d}x \qquad \forall v\in H_0^1(\Omega) \tag{13}$$

where the integrals are finite due to the assumptions. Let $M:=\max\{0,\max\limits_{\partial\Omega} g\}$, and we introduce the piecewise C^1 function v:

$$v:=\max\{u-M,0\}. \tag{14}$$

Then we have $v\ge 0$ and $v|_{\partial\Omega}=0$, further, $u(x)=v(x)+M$ for any $x\in\Omega$, where $v(x)\ne 0$.

For this v, one can check on the one hand that the left-hand side of (13) satisfies

$$\int_\Omega (\nabla u\cdot\nabla v+q(x,u)v)\,\mathrm{d}x=\int_\Omega \left(|\nabla v|^2+q(x,u)v\right)\mathrm{d}x\ge 0.$$

Namely, since $u(x)=v(x)+M$ for any $x\in\Omega$ where $v(x)\ne 0$, thus $\nabla u\cdot\nabla v=\nabla v\cdot\nabla v$ both on the subdomains for the cases $v=0$ and $u=v+M$, i.e. on the whole Ω. Further, the function q increases monotonically in u because of assumption ($\hat{A}3$) and also it is equal to 0 at $u=0$. Thus, if $u<0$ then $q(x,u)\le 0$, but then $v=0$, whereas if $u>0$ then $q(x,u)\ge 0$ and $v\ge 0$. Altogether, we have $q(x,u)v\ge 0$ on the whole Ω, hence the integral is indeed nonnegative.

On the other hand, assumption $f\le 0$ implies that for our v the right-hand side of (13) satisfies $\int_\Omega f v\mathrm{d}x\le 0$. Therefore, altogether, we get

$$\int_\Omega \left(|\nabla v|^2+q(x,u)v\right)\mathrm{d}x=0.$$

Thus $|\nabla v|=0$, therefore v is constant which is nonnegative by definition, i.e.

$$v(x)\equiv c\ge 0 \qquad \text{on } \overline{\Omega}.$$

Because of the boundary condition $v|_{\partial\Omega}=0$ only $v\equiv 0$ is possible, i.e. (14) yields $u\le M$, i.e. we have proved (7). Finally, (8) and (9) are trivial consequences of (7). □

Similarly to the proposition above, the following minimum principle also holds:

Theorem 2.2. *Let assumptions (A2), ($\hat{A}1$) and ($\hat{A}3$) hold, and let $q(x,0)=0$. Further let $u\in C^1(\Omega)\cap C(\overline{\Omega})$ be the weak solution of problem (11). If*

$$f(x)\ge 0, \quad x\in\Omega \tag{15}$$

almost everywhere, then

$$\min_{\overline{\Omega}} u\ge \min\{0,\min_{\partial\Omega} g\}. \tag{16}$$

If $g\le 0$, then

$$\min_{\overline{\Omega}} u=\min_{\partial\Omega} g, \tag{17}$$

and if $g\ge 0$, then

$$\min_{\overline{\Omega}} u\ge 0. \tag{18}$$

Remark 2.1. The analogues of the above propositions hold in the same way for the case $u\in H^1(\Omega)$, without requiring $u\in C^1(\Omega)\cap C(\overline{\Omega})$. Then the maximum and minimum are replaced by $\operatorname{ess\,sup}$ and $\operatorname{ess\,inf}$, respectively, as in [9]. We will see that the solution $u\in H^1(\Omega)$ always exists.

Now we can exploit the achieved results to our reaction-diffusion problem. With the help of Propositions 2.1 and 2.2, we can derive the two-sided bounds $0 \le u \le u_0$ for the rewritten problem (2).

Theorem 2.3. *Let us consider problem* (2)*:*

$$\begin{cases} -\Delta u + k|u|^{\gamma-1}u & = 0, \\ u|_{\partial\Omega} & = u_0. \end{cases}$$

Then

$$0 \le u \le u_0\,.$$

Proof. We can use both the maximum and minimum principle from above, with $q(x,\xi) := k|\xi|^{\gamma-1}\xi$ because we have seen at the end of subsection 2.1 that ($\hat{A}1$) and ($\hat{A}3$) holds, and now $q(x,0) = 0$ and $f(x) = 0$. Thus Propositions 2.1 and 2.2 yield

$$\min\{0, \min_{\partial\Omega} g\} \le u \le \max\{0, \max_{\partial\Omega} g\}.$$

Furthermore in our case $g \equiv u_0 > 0$, thus

$$\begin{aligned} \min\{0, u_0\} &\le u \le \max\{0, u_0\}, \\ 0 &\le u \le u_0. \quad \square \end{aligned}$$

3. Operator properties

In what follows, it will be more practical to use the homogeneous boundary value problem, so it is worth reformulating the problem (2) to the following one:

$$\begin{cases} -\Delta z + k|z+u_0|^{\gamma-1}(z+u_0) & = 0, \\ z|_{\partial\Omega} & = 0, \end{cases} \tag{19}$$

here obviously $z = u - u_0$, i.e.

$$u = z + u_0.$$

This problem is equivalent to (2) and, because of Theorem 2.3, also to problem (1). If z^* is the solution of the homogeneous boundary value problem (19), then $u^* = z^* + u_0$ will be the solution of our original problem.

3.1. Weak formulation

Well-posedness in weak form can be derived using the theory of monotone potential operators [3]. First, using the given boundary constant u_0, we see that the nonlinearity $\hat{q}(\xi) := k|\xi + u_0|^{\gamma-1}(\xi + u_0)$ is continuous, increasing and with $p := \gamma + 1$, $c_2 = k$ and some $c_1 > 0$ we have

$$|\hat{q}(\xi)| \le c_1 + c_2|\xi|^{p-1} \qquad \xi \in \mathbb{R}. \tag{20}$$

The weak solution of the homogeneous problem (19) is a function $z \in H_0^1(\Omega)$ for which

$$\int_\Omega \Big(\nabla z \cdot \nabla v + k|z+u_0|^{\gamma-1}(z+u_0)v\Big) = 0 \qquad \forall v \in H_0^1(\Omega). \tag{21}$$

Now, based on [7, Prop. 2.1], using the above properties of the function $\hat{q}$ with growth condition (20), the well-posedness result holds:

Proposition 3.1. *Problem* (19) *has a unique weak solution.*

With the inner product $\langle u, v\rangle_{H_0^1} = \int_\Omega \nabla u \cdot \nabla v$, the weak form of (21) can be rewritten to the following nonlinear operator equations, where $F : H_0^1(\Omega) \to H_0^1(\Omega)$:

$$\langle F(z), v\rangle_{H_0^1} \equiv \int_\Omega \Big(\nabla z\cdot\nabla v + k|z+u_0|^{\gamma-1}(z+u_0)v\Big) = 0 \qquad \forall v\in H_0^1(\Omega), \tag{22}$$

$$\langle F(z), v\rangle_{H_0^1} = 0 \qquad \forall v\in H_0^1(\Omega),$$
$$\text{i.e.} \qquad F(z)=0. \tag{23}$$

Letting $\langle G(z), v\rangle_{H_0^1} := \int_\Omega (\hat{q}(x,z)v)$, $\forall v\in H_0^1(\Omega)$, the operator F satisfies $F = I + G$, where I is the identity operator. Based on [7, Prop. 5.1] we can derive the following facts. The operator G is Hölder continuous with the parameter γ, since $\hat{q}$ also has such properties. The identity I is trivially Lipschitz continuous. Thus I and G are also locally Hölder continuous, and we obtain the following:

Proposition 3.2. *The above operator F in (22) is locally Hölder continuous on $H_0^1(\Omega)$, i.e. for all $R>0$ there exists a constant $\hat{M}>0$ such that $\|F(u)-F(v)\| \le \hat{M}\|u-v\|^\gamma$ ($\forall u, v\in H_0^1(\Omega)$, where $\|u\|, \|v\|\le R$).*

3.2. Extension of the Galerkin method

Let us consider an operator equation

$$A(u) = b, \tag{24}$$

where H is a real Hilbert space and $b\in H$, and also $A: H\to H$ is a given nonlinear operator. Then the following facts are well-known. Let $H_n\subset H$ ($\forall n\in\mathbb{N}^+$) be subspaces for which $\forall u\in H$

$$dist(u, H_n) := \min\{||u-v_n|| : v_n\in H_n\} \to 0 \quad \text{as } n\to\infty, \tag{25}$$

and let us define the Galerkin solutions $u_n\in H_n$ with the following projected equation:

$$\langle A(u_n), v\rangle = \langle b, v\rangle \qquad \forall v\in H_n\ .$$

Then the residual vector $r_n = A(u_n) - b$ satisfies the Galerkin orthogonality $r_n \perp H_n$. Further, if A is uniformly monotone and Lipschitz continuous, then the nonlinear Céa lemma holds and, using (25), this implies the convergence of the Galerkin solution:

$$||u^* - u_n|| \to 0 \text{ as } n\to\infty.$$

In our case we cannot use the above in exactly the same way since the function $q(u) := |u|^{\gamma-1}u$ $(0<\gamma<1)$ is only Hölder continuous and not Lipschitz continuous, thus as we have seen, F is also only locally Hölder continuous. We have to examine how the above can be extended to the locally Hölder continuous case.

Let $A: H\to H$ be a nonlinear operator which is uniformly monotone and locally Hölder continuous: there exists a monotonically increasing function $\hat{M}: \mathbb{R}^+\to\mathbb{R}^+$ and constants $m>0$, $0<\gamma\le 1$ such that

$$\langle A(u)-A(v), u-v\rangle \ge m\|u-v\|^2 \text{ and} \tag{26}$$
$$\|A(u)-A(v)\| \le \hat{M}(R)\|u-v\|^\gamma \quad \forall u, v\in H,\ ||u||, ||v||\le R. \tag{27}$$

With the former notation, let $H_n\subset H$ be subspaces for which (25) holds.

We will need the following stability lemma:

Lemma 3.3. *Let H be a real Hilbert space and $A: H\to H$ a nonlinear operator satisfying (26). Consider the operator equation (24), and also let $\tilde{b} := b - A(0)$. Let $H_n\subset H$ be a given finite dimensional subspace and $u_n\in H_n$ be the Galerkin solution, and also $u^*\in H$ be the weak solution of the operator equation. Then*

$$\|u_n\| \le \frac{\|\tilde{b}\|}{m} \quad \textit{and} \quad \|u^*\| \le \frac{\|\tilde{b}\|}{m}.$$

Proof. Let us consider the operator $\tilde{A}$ defined by $\tilde{A}(u) := A(u) - A(0)$, then $\tilde{A}(u_n) = \tilde{b}$ and $\tilde{A}(0) = 0$. Further, $\langle\tilde{A}(u_n), v\rangle = \langle\tilde{b}, v\rangle$, $\forall v\in H_n$.
Then, based on (26) with $v=0$,

$$\langle A(u_n) - A(0), u_n - 0\rangle \ge m\|u_n - 0\|^2, \text{ i.e. } \langle\tilde{A}(u_n), u_n\rangle \ge m\|u_n\|^2.$$

From this

$$\|u_n\|^2 \le \frac{\langle \tilde{A}(u_n), u_n\rangle}{m} = \frac{\langle \tilde{b}, u_n\rangle}{m} \le \frac{|\langle \tilde{b}, u_n\rangle|}{m} \le \frac{\|\tilde{b}\| \cdot \|u_n\|}{m},$$

which implies

$$\|u_n\| \le \frac{\|\tilde{b}\|}{m}. \tag{28}$$

The same proof can be repeated for u^* instead of u_n. □

Theorem 3.1 *(Nonlinear Céa lemma for locally Hölder continuous operator). If assumptions (26)-(27) hold, then the Galerkin solutions $u_n \in H_n$ satisfy*

$$\|u^* - u_n\| \le \left(\frac{M}{m}\min\{\|u^* - v_n\| : v_n \in H_n\}\right)^{\frac{1}{2-\gamma}}, \text{ where } M := \hat{M}\left(\frac{\|b - A(0)\|}{m}\right).$$

Proof. With arbitrary $v_n \in H_n$

$$\begin{aligned} m\|u^* - u_n\|^2 &\le \langle A(u^*) - A(u_n), u^* - u_n\rangle = \langle A(u^*) - A(u_n), u^* - v_n\rangle \\ &\le \|A(u^*) - A(u_n)\|\|u^* - v_n\| \le M(R)\|u^* - u_n\|^\gamma \|u^* - v_n\|. \end{aligned}$$

We used here that the residual vector $r_n = A(u_n) - b$ satisfies the Galerkin orthogonality $r_n \perp H_n$, i.e. now $\langle A(u^*) - A(u_n), u_n - v_n\rangle = 0$. The above implies

$$\|u^* - u_n\|^{2-\gamma} \le \frac{M(R)}{m}\|u^* - v_n\|. \tag{29}$$

We also need to prove that $M(R) \le M$ for the given constant, i.e. it is independent of the R for which $R \ge \|u^*\|, \|u_n\|$. According to Lemma 3.3, we have indeed $\hat{M}(R) \le \hat{M}\left(\frac{\|b-A(0)\|}{m}\right) = M$. From this, taking min w.r.t. v_n and rearranging (29), we obtain our statement. □

Corollary 3.1. *Under condition (25) we have the convergence result*

$$\|u^* - u_n\| \le C \cdot (dist(u, H_n))^{\frac{1}{2-\gamma}} \to 0,$$

where $C > 0$ is independent of n.

4. Numerical approximation of the nonlinear PDE

In order to solve (2), we use the rewritten problem (19), that is, equation $-\Delta z + \tilde{q}(z) = 0$ with homogeneous boundary conditions. Then the solution of the original problem (2) is obtained by just adding the constant u_0, that is, $u = z + u_0$.

4.1. Construction of the finite element method (FEM)

In general, the FEM searches the numerical solution of problem (19) in a proper subspace $V_h \subset H_0^1(\Omega)$. We have seen that the weak form of the problem is (21). According to the Galerkin method, the elements of V_h are in the form $z_h = \sum_{i=1}^n c_i\phi_i$, hence the nonlinearity takes the form

$$\tilde{q}(z_h) = \tilde{q}(\sum_{i=1}^n c_i\phi_i) := k|\sum_{i=1}^n c_i\phi_i + u_0|^{\gamma-1}(\sum_{i=1}^n c_i\phi_i + u_0).$$

Substituting $v := \phi_j$ in (21), we obtain

$$\langle F(z_h), v\rangle_{H_0^1} = \langle F(\sum_{i=1}^n c_i\phi_i), \phi_j\rangle_{H_0^1} = \int_\Omega \left(\sum_{i=1}^n c_i \nabla\phi_i \cdot \nabla\phi_j + \tilde{q}(\sum_{i=1}^n c_i\phi_i)\phi_j\right),$$

and thus (21) becomes the following:

$$\sum_{i=1}^n \int_\Omega (\nabla\phi_i \cdot \nabla\phi_j)c_i + \int_\Omega \tilde{q}(\sum_{i=1}^n c_i\phi_i)\phi_j = 0,$$

which is a system of nonlinear equations for $c = (c_1, \dots, c_n)$.

In what follows, we use first degree Courant elements on a standard uniform triangular grid. Then $a_{ij} := \int_\Omega \nabla\phi_i \nabla\phi_j$ can be computed exactly, and we can use the simple numerical quadrature $\int_\Omega \tilde{q}(z)\phi_j \approx h^2\tilde{q}(c_j)$, where h is the mesh parameter for the grid and c_j is the coefficient of the basis function ϕ_j. Thus our system of nonlinear equations is the following:

$$0 = Ac + h^2\tilde{q}(c), \tag{30}$$

where $A := (a_{ij})$, $c = (c_i)$.

4.2. Fractional convergence of the FEM

Now we would like to estimate the order of convergence of the FEM. We can do this with the help of the nonlinear Céa Lemma 3.1 used for the convergence of the Galerkin method when $dist(u, H_n) \to 0$. Further, we first need to prove the following regularity property.

Proposition 4.1. *If the domain Ω is C^2-diffeomorphic to a convex domain, then the weak solution of (1) satisfies $u \in H^2(\Omega)$.*

Proof. Let us rearrange problem (1):

$$\begin{cases} -\Delta u &= -ku^\gamma, \\ u|_{\partial\Omega} &= \ \ u_0. \end{cases}$$

Based on Proposition 2.3 we know that the function u is bounded, namely, $0 \le u \le u_0$. Therefore the function u^γ and thus $f := -ku^\gamma$ are also bounded, hence also $f = -ku^\gamma \in L^2(\Omega)$. That is, u is the solution of the Poisson equation

$$\begin{cases} -\Delta u &= f, \\ u|_{\partial\Omega} &= u_0 \end{cases}$$

with a right-hand side $f \in L^2(\Omega)$. The Kadlec theorem [6] states that if Ω is C^2-diffeomorphic to a convex domain, then this solution satisfies $u \in H^2(\Omega)$. $\square$

Theorem 4.1. *We have*

$$|u - u_h|_{H^1} \le O(h^\beta), \qquad \textit{where} \quad \beta = \frac{1}{2-\gamma}.$$

Proof. Let us apply Proposition 3.1 to the homogenized problem (19) in the space $H = H_0^1(\Omega)$ under the norm $|u|_{H^1} = \left(\int_\Omega |\nabla u|^2\right)^{1/2}$, and for the subspace $H_n := V_h$:

$$|z - z_h|_{H^1} \le C \cdot \min\left\{|z - v_h|_{H^1} : \ v_h \in V_h\right\}^{\frac{1}{2-\gamma}}.$$

Let us consider the interpolation of z to the subspace V_h, denoted by $\Pi_h z \in V_h$, then

$$|z - z_h|_{H^1} \le C|z - \Pi_h z|_{H^1}^{\frac{1}{2-\gamma}}.$$

With the former Proposition 4.1 we have seen that $u \in H^2(\Omega)$, hence $z = u - u_0 \in H^2(\Omega)$. Since the triangulation is regular, we have the interpolation estimate $|z - \Pi_h z|_{H^1} \le ch|z|_{H^2}$, where $c > 0$ is independent of the triangulation and $|z|_{H^2} = \left(\int_\Omega |D^2 z|^2\right)^{1/2}$, see, e.g., [1]. Here

$$|z|_{H^2} = |u|_{H^2} \quad \text{and} \quad |z - z_h|_{H^1} = |u - u_h|_{H^1},$$

since $u = z + u_0$ and $u_h = z_h + u_0$ for the constant u_0. Thus, altogether,

$$|u - u_h|_{H^1} = |z - z_h|_{H^1} \le C|z - \Pi_h z|_{H^1}^{\frac{1}{2-\gamma}} \le \tilde{C}|z|_{H^2}^{\frac{1}{2-\gamma}} h^{\frac{1}{2-\gamma}} = \tilde{C}|u|_{H^2}^{\frac{1}{2-\gamma}} h^{\frac{1}{2-\gamma}},$$

hence our statement is proved. $\square$

4.3. Gradient method and power order convergence

We briefly quote the Sobolev gradient method on the operator level based on [7]. As shown there, the gradient method converges for Hölder continuous nonlinearity, which is non-differentiable with unbounded gradients and hence a Newton type method could not be applied. This is an extension of the standard Sobolev gradient method for nonlinear elliptic problems [8]. In fact, we will apply it in finite dimension under the FEM.

Let $z_0 \in H_0^1(\Omega)$ be an arbitrary initial guess and $y_n := F(z_n)$. The method defines a sequence

$$z_{n+1} = (1-\alpha_n)z_n - \alpha_n w_n$$

where the stepsize is $\alpha_n := \left(\frac{\gamma+1}{2M}\right)^{\frac{1}{\gamma}} \|F(z_n)\|^{\frac{1}{\gamma}-1}$ and w_n is the weak solution of the PDE $-\Delta w_n = \tilde{q}(z_n)$ with homogeneous boundary condition. Then we have

Proposition 4.2. [7, Thm. 5.1] *Let $\tilde{q}$ be Hölder continuous and increasing, further, let there exist $p \geq 1$ such that $|\tilde{q}(\xi)| \leq c_1 + c_2|\xi|^{p-1}$. Then there exists a constant $c > 0$ such that the errors $e_k := \|u_k - u^*\|_{H_0^1(\Omega)}$ satisfy $\min_{0\leq k\leq n} e_k \leq cn^{-\frac{\gamma}{\gamma+1}}$.*

5. Detection of the dead cores

5.1. An analytical result in 1D

We examine the following boundary value problem:

$$\begin{cases} -u'' + ku^\gamma &= 0, \\ u(0) = u(l) &= u_0 \end{cases}$$

on the interval $I = [0,l]$. We have seen that there exists a unique solution, thus let us suppose that the solution has the following form on a left subinterval: $u(x) = c(x_0 - x)^\delta$. Substituting this into the equations and with some calculation,

$$u(x) = c(\gamma,k)\cdot(x_0-x)^{\delta(\gamma)} = \left(\frac{2(1+\gamma)}{k(1-\gamma)^2}\right)^{\frac{1}{\gamma-1}} (x_0-x)^{\frac{2}{1-\gamma}},$$

$$x_0 = \left(\frac{u_0}{\left(\frac{2(1+\gamma)}{k(1-\gamma)^2}\right)^{\frac{1}{\gamma-1}}}\right)^{\frac{1-\gamma}{2}} = \left(\frac{u_0}{c(\gamma,k)}\right)^{\frac{1-\gamma}{2}}.$$

Due to symmetry, a dead core occurs if this function u reaches the level 0 before the center of the interval, which takes place if $x_0 < \frac{l}{2}$. Such a situation is illustrated in Fig. 1. In general, let $\Phi(\gamma,k,l) := c(\gamma,k)\cdot\left(\frac{l}{2}\right)^{\frac{2}{1-\gamma}}$. We obtain that a dead core occurs if u_0 is small enough, namely if

$$u_0 < \Phi(\gamma,k,l).$$

We note that the existence of dead cores in 1D has been studied under more complex nonlinearities with numerical experiments in [4,10,11].

5.2. Numerical experiments in 2D

In two dimensions there is no hope to have an analytical solution. We computed the numerical solution of problem (1) using MATLAB, defining various parameters γ, k and l. First we solved the homogenized system (30), then for our original problem we used the formula $u = z + u_0$.

5.2.1. Existence of the dead core

First we consider the domain $\Omega = [0,l]\times[0,l]$, partitioned with a uniform mesh with mesh parameter $h \approx 0.0071$. With fixed γ, k and l, the existence and size of the dead core depends on the magnitude of u_0, similarly to the one-dimensional case. This is illustrated for $\gamma = \frac{1}{2}$, $k = 30$ and $l = 2$. First, the solution of our problem for $u_0 = 2$ can be seen on Fig. 2: here the dead core exists and is a symmetric subdomain. Fig. 3 shows different cases of u_0 for the same values $\gamma = \frac{1}{2}$, $k = 30$ and $l = 2$. It can be seen that there occurs no dead core above a certain value, namely, above $u_0 \approx 5.85$.

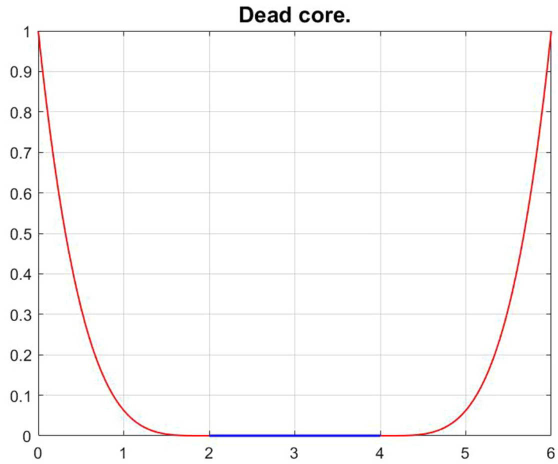

Fig. 1. Dead core: $\gamma = \frac{1}{2}$, $k = 3$, $l = 6$, $u(0) = u(6) = 1$.

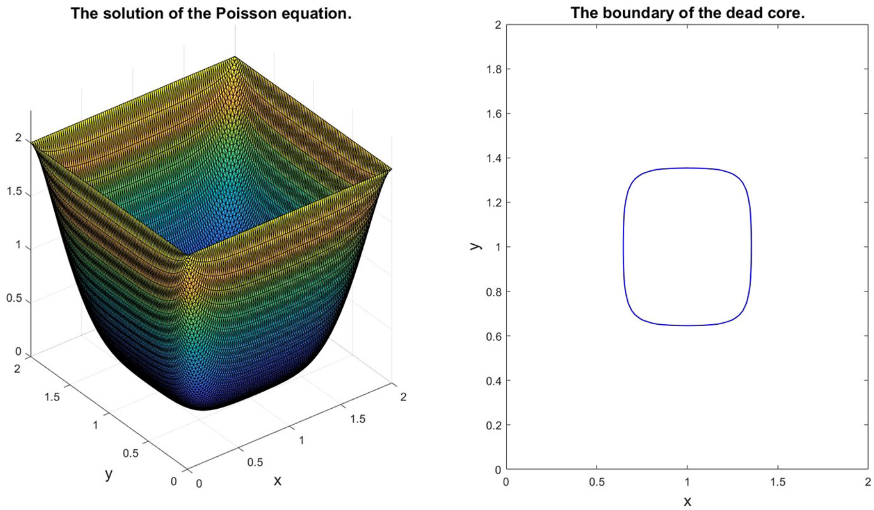

Fig. 2. The function u and the dead core: $\gamma = \frac{1}{2}$, $k = 30$, $u_0 = 2$, $l = 2$.

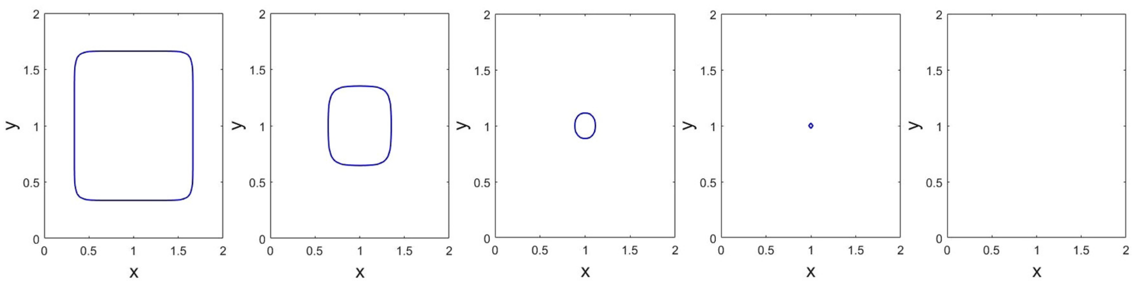

Fig. 3. The disappearance of the dead core: the value of u_0 is 0.25; 2; 5; 5.85 and 6 respectively.

5.2.2. The shape and location of the dead core

Now our goal is to study the geometric properties of the dead core in different typical situations. First, we define $u_0(x, y)$ as a nonconstant function on the boundary of the same unit square domain as before. We can indeed allow u_0 to be variable, assuming that it is a bounded function and that there exists $g^* \in H^2(\Omega)$ such that $g^*|_{\partial\Omega} \equiv u_0$. Then we can define $\hat{q}$ as $\hat{q}(x, \xi) := k|\xi + g^*(x)|^{\gamma-1}(\xi + g^*(x))$, which also satisfies (20) uniformly in x, and the regularity $u = z + g^* \in H^2(\Omega)$ also remains true. Secondly, we define more general non-rectangular shapes of the domain Ω, but then let u_0 be constant again.

In both cases we involve different values of u_0, γ and k. We can observe that the shape of the dead core changes compared to the case of square domain and constant u_0. We can find dead cores that are concave or have multicomponent

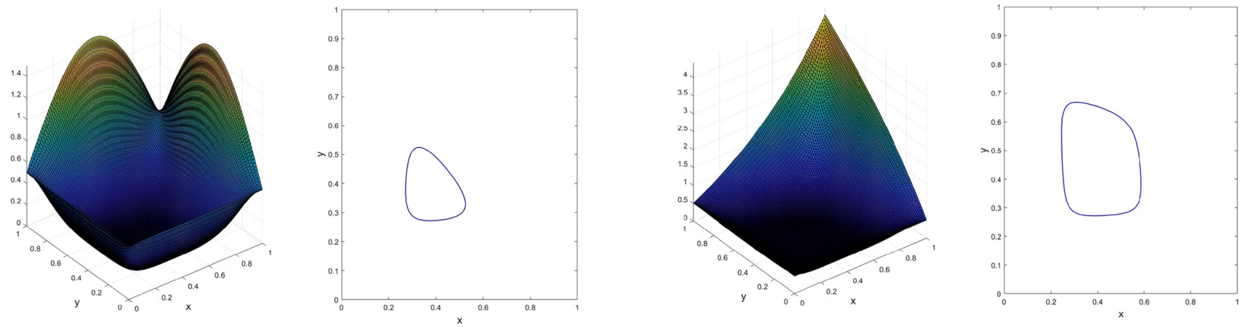

Fig. 4. $\gamma = \frac{1}{2}$, $k = 80$, $u_0(x, y) = \frac{1}{2} + \sin(\pi xy)$ and $u_0(x, y) = \frac{1}{2} + xye^x + xye^{1-y}$.

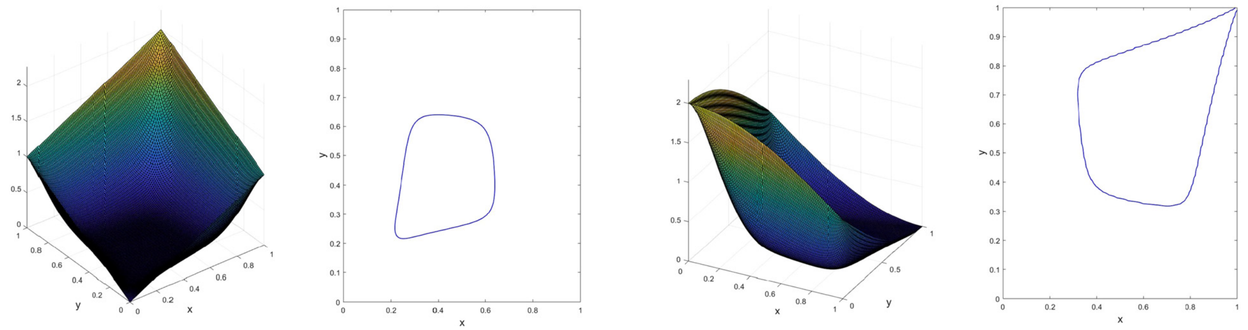

Fig. 5. $\gamma = \frac{1}{2}$, $k = 80$, $u_0(x, y) = x + y$ and $\gamma = \frac{1}{4}$, $k = 60$, $u_0(x, y) = 1 + \cos(\frac{\pi}{2}(x + y))$.

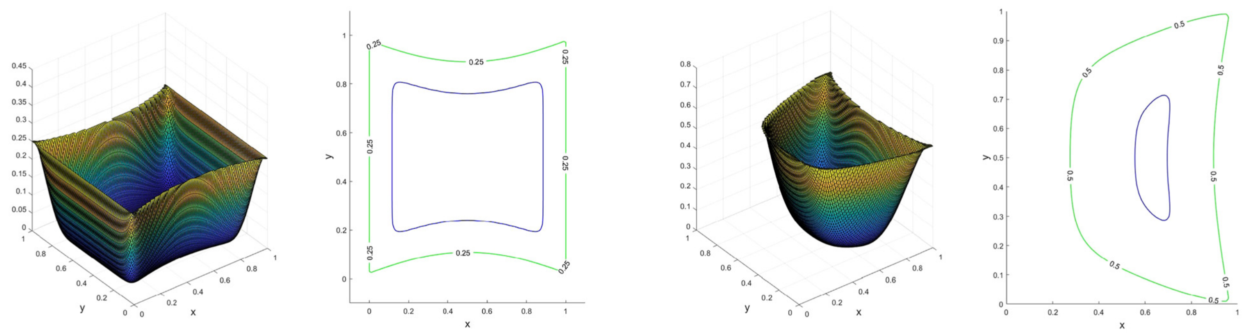

Fig. 6. $\gamma = \frac{1}{4}$, $k = 100$, $u_0 = 0.25$ and $\gamma = \frac{1}{4}$, $k = 60$, $u_0 = 0.5$.

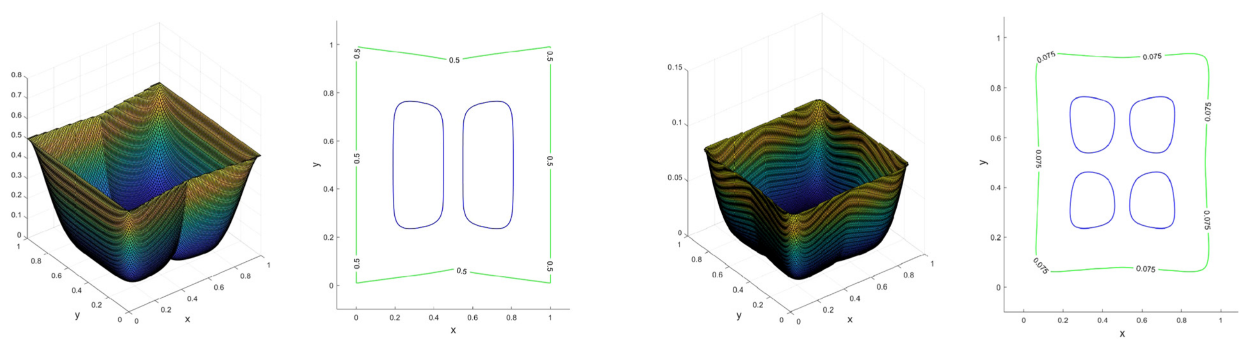

Fig. 7. $\gamma = \frac{1}{4}$, $k = 60$, $u_0 = 0.5$ and $\gamma = \frac{1}{2}$, $k = 80$, $u_0 = 0.075$.

forms. Figs. 4 and 5 show the function u and the shape of the dead core in a square with $l = 1$ and with various u_0, γ and k. Figs. 6 and 7 show dead cores on non-rectangular domains Ω when u_0 is constant.

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