Optimization in Nonlinear Models of Mass Transfer

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Abstract. Optimal control problem for convection–diffusion–reaction equation, in which reaction coefficient depends nonlinearly on substance's concentration, is considered. Numerical algorithms for solving nonlinear boundary value and optimal control problems are proposed for the equation under study. Separately, the results of the numerical experiments about nonlinear boundary value problems' solvability are presented. For this purpose the FreeFem++ solver is used. These studies allow to understand better the process of pollution's spread in the atmosphere and fight against its consequences. Particularly, they give an opportunity to reveal and eliminate the sources of pollution using the measured impurity's concentration in some available domain. Also the correctness of mathematical models of mass transfer and optimal control problems, which are considered in the paper, is justified.

Keywords: FreeFem++, nonlinear convection-diffusion-reaction equation, optimal control problem, multiplicative control problems, optimality system, numerical algorithm

1 Introduction. Boundary value problem

In a bounded domain $\Omega \subset \mathbb{R}^3$ with boundary Γ the following boundary value problem is considered

$$-\lambda\Delta\varphi + \mathbf{u}\cdot\nabla\varphi + k\varphi = f \text{ in } \Omega, \quad \varphi = 0 \text{ on } \Gamma. \tag{1}$$

Here function φ means polluting substance's concentration, $\mathbf{u}$ is a given vector of velocity, f is a volume density of external sources of substance, λ – constant diffusion coefficient, function $k = k(\varphi)$ is a reaction coefficient. This problem (1) will be called problem 1 below.

This study of optimal control problems for a model (1) is intended to develop efficient mechanisms to control chemical reactions' behavior. The decision to choose a velocity vector $\mathbf{u}$ as a control can signify the regularization of combustion process at

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the expense of fuel feed's intensity changing (see [1]). The efficiency criterion for such kind of control is the measured concentration of unburned fuel in a subdomain.

It should be mentioned that some inverse problems can be reduced to the optimal control ones as from the mathematical point of view optimal control problems are the problems of cost functionals' minimization on weak boundary problem's solutions. At the same time one or several functions can be changed in some certain convex closed sets. The mentioned functions are usually called controls, cause their changing is exactly the thing that influences on the minimum of the cost functional.

From the other side, one can thought that such functions are searched on the assumption of the minimum of corresponding cost functionals, which attaches these extremum problems the meaning of indentification problems of the functions and inverse problems. See [2–10] about similar methods and approaches.

Particularly, the optimal control problem, which is considered in this paper, can represent the indentification problem for a velocity and a direction of wind or a fuel, depending on the case and the situation.

With the help of this approach it's possible to reveal the hidden sources of pollution, which are located in the places, inaccessible for observation (under water, on the territory of the adjacent country). Then the data about the concentration of polluting substance in the domain, which is accessible for measurement, about the direction and the velocity of the wind or of the flow in the basin are used.

The results of numerical experiments, executed in FreeFEM++, are given for the solving of nonlinear boundary value problem. We should note a quick convergence of the simple iteration method while the initial approximation of the boundary value problem's solution was chosen not very successful. The computations are conducted for a number of reaction coefficients, which depend nonlinearly on the substance's concentration at different boundary conditions. The chosen geometry of the domain and the given velocity field simplify the understanding of numerical experiments' results.

The numerical algorithm for solving the optimal control problem is presented. This algorithm is based on using of optimality system, obtained for the extremum problem. Sufficient conditions of such algorithms' convergence were obtained in [20]. But these conditions have the meaning of either the smallness conditions for the initial data of a boundary value problem or demands greater values of the regularizer in an optimal control problem, which spoils the quality of the last one. That's why it's interesting to analyse the convergence of such algorithm depending on the initial approximation of the optimal control problem's solution. As in the case of the boundary value problem.

The reasoning of the correctess of the considered mathematical model implies the following. The global solvability of problem 1, when reaction coefficients belong to rather wide class of functions, is proved in [10–12]. In this paper it is shown that power coefficients from [13–15] are particular cases of the reaction coefficients considered in [10–12], with which nonlocal uniqueness of boundary value problem's solution takes place. The solvability of multiplicative control problem with common reaction coefficients is proved further. For a quadratic reaction coefficient optimality system is obtained, on the analysis of which sufficient conditions for local uniqueness of multiplicative control problems' solutions for particular cost functionals are received.

While studing problem 1 and optimal control problems Sobolev spaces will be used: $H^s(D)$, $\mathbf{H}^s(D) \equiv H^s(D)^3$, $s \in \mathbb{R}$ and $L^r(D)$, $1 \le r \le \infty$, where D is either a domain Ω or its boudary Γ. Scalar products in $L^2(\Omega)$, $H^1(\Omega)$ and $\mathbf{H}^1(\Omega)$ are denoted by $(\cdot,\cdot)$ and $(\cdot,\cdot)_1$, scalar products in $L^2(\Gamma)$ – by $(\cdot,\cdot)_\Gamma$, norm in $L^2(\Omega)$ – by $\|\cdot\|$, norm or semi-norm in $H^1(\Omega)$ – by $\|\cdot\|_1$ or $|\cdot|_1$.

It will be assumed that the domain Ω and its boundary Γ satisfy the following:

(i) Ω is a bounded domain in the space $\mathbb{R}^3$ with boundary $\Gamma \in C^{0,1}$.

Let $\mathcal{D}(\Omega)$ be the space of infinitely differentiable functions with finite support in Ω, $L^p_+(\Omega) = \{k \in L^p(\Omega) : k \ge 0\}$, $p \ge 3/2$. Also let $\mathbf{Z} = \{\mathbf{v} \in \mathbf{L}^4(\Omega) : \operatorname{div} \mathbf{v} = 0 \text{ in } \Omega\}$, $\mathbf{V} \equiv \mathbf{Z} \cap \mathbf{H}^1(\Omega)$.

From Poincare-Friedrichs inequality and from the continuity of the embedding operator $H^1(\Omega) \subset L^4(\Omega)$ this lemma follows:

Lemma 1. *If conditions (i) hold, then there are such positive constants C_0, δ, C_4 and γ, depending on Ω, that for any functions $\varphi, S \in H^1(\Omega)$, $k \in L^p_+(\Omega)$, where $p \ge 3/2$, $\mathbf{u} \in \mathbf{Z}$ these relations are correct:*

$$|(\nabla\varphi, \nabla S)| \le \|\varphi\|_1 \|S\|_1, \quad \|\varphi\|_{L^4(\Omega)} \le C_4 \|\varphi\|_1,$$

$$|(k\varphi, S)| \le C_0 \|k\|_{L^p(\Omega)} \|\varphi\|_1 \|S\|_1, \tag{2}$$

$$|(\mathbf{u}\cdot\nabla\varphi, S)| \le \gamma \|\mathbf{u}\|_{\mathbf{L}^4(\Omega)} \|\varphi\|_1 \|S\|_1 \le \gamma C_4 \|\mathbf{u}\|_1 \|\varphi\|_1 \|S\|_1,$$

$$(\mathbf{u}\cdot\nabla\varphi, \varphi) = 0 \ \forall \varphi \in H^1_0(\Omega), \tag{3}$$

and for any function $S \in H^1_0(\Omega)$ the inequality takes place

$$(\nabla S, \nabla S) \ge \delta \|S\|_1^2. \tag{4}$$

From lemma 1 follows that while conditions (i) are satisfied with the constant $\lambda_* = \delta\lambda$ when $k \in L^{3/2}_+(\Omega)$, then the coercitive inequality is met

$$\lambda(\nabla S, \nabla S) + (kS, S) \ge \lambda_* \|S\|_1^2 \ \forall S \in H^1_0(\Omega). \tag{5}$$

Let in addition to (i) the conditions hold:

(ii) $f \in L^2(\Omega)$, $\mathbf{u} \in \mathbf{Z}$.

(iii) $k \in L^p_+(\Omega)$, $p \ge 3/2$, wherein function $k = k(\varphi)$ is Lipschitz continuous of φ, i.e. if $\|\varphi_1\|_1 \le c$ and $\|\varphi_2\|_1 \le c$, then

$$\|k(\varphi_1) - k(\varphi_2)\|_{L^p(\Omega)} \le L\|\varphi_1 - \varphi_2\|_{L^4(\Omega)} \ \ \forall \varphi_1, \varphi_2 \in H^1_0(\Omega).$$

Let's multiply the equation in (1) by $S \in H^1_0(\Omega)$ and integrate over Ω. The following will be got

$$\lambda(\nabla\varphi, \nabla S) + (k(\varphi)\varphi, S) + (\mathbf{u}\cdot\nabla\varphi, S) = (f, S) \ \forall S \in H^1_0(\Omega). \tag{6}$$

As a result, the weak formulation of problem 1 is obtained. It consists in finding function $\varphi \in H^1_0(\Omega)$ from (6).

Definition 1. A function $\varphi \in H^1_0(\Omega)$ which satisfies (6) will be called a weak solution of problem 1.

The following theorem takes place [12].

Theorem 1. *If conditions (i)–(iii) hold, then a weak solution $\varphi \in H_0^1(\Omega)$ of problem 1 exists and the estimate takes place:*

$$\|\varphi\|_1 \leq M_\varphi = (1/\lambda_*)\|f\|. \tag{7}$$

If, besides, this condition is met

$$C_0 L\|f\| \leq \lambda_*^2, \tag{8}$$

then the problem 1's weak solution is unique.

From [12–14] it ensues that the power dependence is interesting as an example of particular cases of function $k = k(\varphi)$, $k = \varphi^2$ and $k(\varphi) = \varphi^2|\varphi|$, for instance. As the case of quadratic reaction coefficient was analysed in detail in [12]. In particular, it was shown that a function $k = \varphi^2$ satisfies conditions (iii) and for this function there is nonlocal uniqueness of problem 1's weak solution, so let's consider the function $k = \varphi^2|\varphi|$.

For $k = \varphi^2|\varphi|$ the equality is true:

$$k(\varphi_1) - k(\varphi_2) = \varphi_1^2(|\varphi_1| - |\varphi_2|) + (\varphi_1 - \varphi_2)(\varphi_1 + \varphi_2)|\varphi_2| \text{ a.e. in } \Omega$$

and also an estimate takes place:

$$\left(\int_\Omega (\varphi_1 - \varphi_2)^{3/2}\varphi_1^3\, d\Omega\right)^{2/3} \leq \|\varphi_1 - \varphi_2\|_{L^3(\Omega)}\|\varphi_1\|^2_{L^6(\Omega)}.$$

In such case function $k = \varphi^2|\varphi|$ satisfies the condition (iii).

When $k = \varphi^2|\varphi|$ nonlocal uniqueness of problem 1's solution takes place. Actually, let $k = \varphi^2|\varphi|$ and $\varphi_1, \varphi_2 \in H^1(\Omega)$ be two solutions of problem 1. Then their difference $\varphi = \varphi_1 - \varphi_2 \in H_0^1(\Omega)$ satisfies the ratio

$$\lambda(\nabla\varphi, \nabla h) + (\varphi_1^3|\varphi_1| - \varphi_2^3|\varphi_2|, h) + (\mathbf{u} \cdot \nabla\varphi, h) = 0 \ \forall h \in H_0^1(\Omega). \tag{9}$$

It's clear that

$$(\varphi_1^3|\varphi_1| - \varphi_2^3|\varphi_2|)(\varphi_1 - \varphi_2) = \varphi_1^4|\varphi_1| - \varphi_2^3|\varphi_2|\varphi_1 - \varphi_1^3|\varphi_1|\varphi_2 + \varphi_2^4|\varphi_2| \text{ a.e. in } \Omega$$

and on the strength of Young's inequality

$$\varphi_2^4\varphi_1 \leq (4/5)\varphi_2^5 + (1/5)\varphi_1^5, \ \ \varphi_1^4\varphi_2 \leq (4/5)\varphi_1^5 + (1/5)\varphi_2^5 \text{ a.e. in } \Omega.$$

In such case $(\varphi_1^3|\varphi_1| - \varphi_2^3|\varphi_2|, \varphi) \geq 0$ a.e. in Ω. Assuming $h = \varphi$ in (9), on the strength of lemma 1 it can be concluded that $\varphi = 0$ or $\varphi_1 = \varphi_2$ in Ω.

From aforesaid and [12] follows

Theorem 2. *Let conditions (i), (ii) hold. Then when $k = \varphi^2$ and $k = \varphi^2|\varphi|$, there is a unique weak solution $\varphi \in H_0^1(\Omega)$ of problem 1 and the estimate (7) is met.*

Let's separately consider the reaction coefficient $k(\varphi)$, which generalizes the forth power, but is not a function of φ in a common sense. Let $k(\varphi)$ be an operator acting form $\mathcal{T}$ to $L^p_+(\Omega)$, where $p \geq 3/2$ and satisfying the following conditions:

(1) for all $w_1, w_2 \in B_r = \{w \in \mathcal{T} : \|w\|_{1,\Omega} \leq r\}$ the following estimate holds:

$$\|k(w_1) - k(w_2)\|_{L^p(\Omega)} \leq L\|w_1 - w_2\|_{L^6(\Omega)},$$

where L is a constant, depending on r, but not depending on w_1, w_2;

(2) $k(\varphi)\varphi$ satisfies monotony condition

$$(k(\varphi_1)\varphi_1 - k(\varphi_2)\varphi_2, \varphi_1 - \varphi_2) \geq 0 \ \ \forall \varphi_1, \varphi_2 \in H_0^1(\Omega).$$

Let's consider a simple example of the operator $k(\varphi)$, satisfying the conditions (1), (2) and generalizing numerical functions: $k(\varphi) = \varphi^4$ in subdomain $Q \subset \Omega$ and $k(\varphi) = k_0$ in $\Omega \setminus \overline{Q}$, where $k_0 \in L_+^{3/2}(\Omega)$.

This example takes into account the influence on the chemical reaction's velocity not only of substance's concentration, but also of inhomogeneity of chemical reaction's behavior in the considered domain. Conditions (1), (2) are also met for the reaction coefficient $k(\varphi) = \alpha(x)\varphi^4$, where $\alpha(\mathbf{x}) \in L_+^\infty(\Omega)$.

It should be noted that the reaction coefficient $k(\varphi) = \varphi^4$ gives the convection-diffusion-equation the maximum possible nonlinearity of 5th power for the solution $\varphi \in H^1(\Omega)$. For such strong nonlinearity the theory of problem 1's solvability proving, which was stated above , is unacceptable in view of the fact that the boundary value problem's operator is not compact. The solvability of problem 1 at $k(\varphi)$, satisfying the conditions (1), (2) follows from the results of [16].

The following theorem holds

Theorem 3. *Let conditions (i), (1), (2) hold. Then there is a unique weak solution* $\varphi \in H_0^1(\Omega)$ *of problem 1 and the estimate (7) is met.*

2 Statement of optimal control problem and its solvability

Let's formulate an optimal control problem for problem 1. For this purpose the whole set of initial data will be devided into two groups: the group of fixed functions, in which function f is included, and the group of controlling functions, in which $\mathbf{u}$ will be included, assuming that it can be changed in some subset K.

Let's introduce an operator $F : H_0^1(\Omega) \times K \to H^{-1}(\Omega)$ by formula

$$\langle F(\varphi, \mathbf{u}), S\rangle = \lambda(\nabla\varphi, \nabla S) + (\mathbf{u} \cdot \nabla\varphi, S) + (k(\varphi)\varphi, S) - (f, S).$$

Then (6) can be rewritten in the following form:

$$F(\varphi, \mathbf{u}) = 0. \tag{10}$$

Let's suppose that these conditions hold

(j) $K \subset \mathbf{V}$ is a nonempty convex closed set;

(jj) $\mu_i \geq 0, i = 1, 2$ and K is a bounded set $\mu_l > 0, l = 0, 1$ and the functional I is bounded below.

Treating (10) as a conditional restriction on the state $\varphi \in H_0^1(\Omega)$ and on the control $\mathbf{u} \in K$, the problem of conditional minimization can be formulated as follows:

$$J(\varphi, k) \equiv \frac{\mu_0}{2} I(\varphi) + \frac{\mu_1}{2}\|\mathbf{u}\|_1^2 \to \inf, \ F(\varphi, \mathbf{u}) = 0, \ (\varphi, \mathbf{u}) \in H_0^1(\Omega) \times K. \tag{11}$$

The following cost functionals can be used in the capacity of the possible ones:

$$I_1(\varphi) = \|\varphi - \varphi_d\|_Q^2 = \int_\Omega |\varphi - \varphi_d|^2 d\mathbf{x}, \quad I_2(\varphi) = \|\varphi - \varphi_d\|_{1,Q}^2.$$

Here $\varphi_d \in L^2(Q)$ is a given function in some subdomain - $Q \subset \Omega$. The set of possible pairs for the problem (11) is denoted by $Z_{ad} = \{(\varphi, \mathbf{u}) \in H_0^1(\Omega) \times K : F(\varphi, \mathbf{u}){=}0, J(\varphi, \mathbf{u}){<}\infty\}$.

Theorem 3. *Let conditions (i)–(iii) and (j), (jj) hold. Then there is at least one solution of the optimal control problem (11).*

Proof. Let $(\varphi_m, \mathbf{u}_m)$ be a minimizing sequence, for which the following is true:

$$\lim_{m\to\infty} J(\varphi_m, \mathbf{u}_m) = \inf_{(\varphi_m, \mathbf{u}_m) \in Z_{ad}} J(\varphi_m, \mathbf{u}_m) \equiv J^*.$$

That and the conditions of theorem for the functional J from (11) imply the estimate $\|\mathbf{u}_m\|_1 \le c_1$. From theorem 1 follows directly that $\|\varphi_m\|_1{\le}c_2$, where constant c_2 doesn't depend on m.

Then the weak limits $\varphi^* \in H_0^1(\Omega)$ and $\mathbf{u}^* \in \mathbf{V}$ of some subsequences of sequences $\{\varphi_m\}$ and $\{\mathbf{u}_m\}$ exist. Corresponding sequences will be also denoted by $\{\varphi_m\}$ and $\{\mathbf{u}_m\}$. With this in mind it can be considered that

$$\varphi_m \to \varphi^* \in H^1(\Omega) \text{ weakly in } H^1(\Omega) \text{ ang strongly in } L^4(\Omega), \tag{12}$$

$$\mathbf{u}_m \to \mathbf{u}^* \in \mathbf{H}^1(\Omega) \text{ weakly in } \mathbf{H}^1(\Omega) \text{ and strongly in } \mathbf{L}^4(\Omega). \tag{13}$$

Let's show that $F(\varphi^*, \mathbf{u}^*) = 0$, i.e.

$$\lambda(\nabla\varphi^*, \nabla S) + (k(\varphi^*)\varphi^*, S) + (\mathbf{u}^* \cdot \nabla\varphi^*, S) = (f, S) \ \ \forall S \in H_0^1(\Omega). \tag{14}$$

And it should be taken into account that φ_m and $\mathbf{u}_m$ satisfy the relations

$$\lambda(\nabla\varphi_m, \nabla S) + (k(\varphi_m)\varphi_m, S) + (\mathbf{u}_m \cdot \nabla\varphi_m, S) = (f, S) \ \ \forall S \in H_0^1(\Omega). \tag{15}$$

Let's pass to the limit in (15) at $m \to \infty$. All linear summands in (15) turn into corresponding ones in (14). For the nonlinear summand $(k(\varphi_m)\varphi_m, S)$ the inequality takes place

$$|(k(\varphi_m)\varphi_m, S) - (k(\varphi^*)\varphi^*, S)| \le |(k(\varphi_m)(\varphi_m - \varphi^*), S)| + |(k(\varphi_m) - k(\varphi^*), \varphi^* S)|.$$

On the strength of lemma 1 and condition (iii) for the function $k = k(\varphi)$ it is obtained that

$$|(k(\varphi_m) - k(\varphi^*), \varphi^* S)| \le L\|\varphi_m - \varphi^*\|_{L^4(\Omega)}\|\varphi^*\|_{L^4(\Omega)}\|S\|_{L^4(\Omega)} \to 0 \text{ at } m \to \infty.$$

To apply the property (12) for the summand $|(k(\varphi_m)(\varphi_m - \varphi^*), S)|$, embedding density by norm $\|\cdot\|_1$ will be used. Let $\{S_n\} \in \mathcal{D}(\Omega)$ be such a sequence of functions that $\|S_n - S\|_1 \to 0$ at $n \to \infty$.

This inequality holds:

$$|(k(\varphi_m)(\varphi_m - \varphi^*), S_n)| \le$$

$$\|k(\varphi_m)\|_{L^{3/2}(\Omega)}\|S_n\|_{L^{12}(\Omega)}\|\varphi_m-\varphi^*\|_{L^4(\Omega)}\to 0 \text{ at } m\to\infty.$$

As far as

$$||(k(\varphi_m)(\varphi_m-\varphi^*),S_n)|-|(k(\varphi_m)(\varphi_m-\varphi^*),S)||\le|(k(\varphi_m)(\varphi_m-\varphi^*),S_n-S)|\le$$

$$\le\|k(\varphi_m)\|_{L^{3/2}(\Omega)}\|\varphi_m-\varphi^*\|_{L^6(\Omega)}\|S_n-S\|_{L^6(\Omega)}\to 0 \text{ at } n\to\infty,\ m=1,2,...$$

Then

$$\lim_{m\to\infty}(k(\varphi_m)\varphi_m,S)=(k^*(\varphi^*)\varphi^*,S).$$

For the nonlinear summand $(\mathbf{u}_m\cdot\nabla\varphi_m,S)$ this relation is satisfied

$$(\mathbf{u}_m\cdot\nabla\varphi_m,S)-(\mathbf{u}^*\cdot\nabla\varphi^*,S)=$$

$$=(\mathbf{u}^*\cdot\nabla(\varphi_m-\varphi^*),S)+((\mathbf{u}_m-\mathbf{u}^*)\cdot\nabla\varphi_m,S)\ \forall S\in H_0^1(\Omega). \tag{16}$$

On the strength of (12) a weak convergence takes place: $\nabla\varphi_m\to\nabla\varphi^*$ in $\mathbf{L}^2(\Omega)$, according to which

$$(\mathbf{u}^*\cdot\nabla(\varphi_m-\varphi^*),S)=(\nabla(\varphi_m-\varphi^*),\mathbf{u}^*S)\to 0 \text{ at } m\to\infty\ \forall S\in H_0^1(\Omega),$$

and from (13) follows that

$$|((\mathbf{u}_m-\mathbf{u}^*)\cdot\nabla\varphi_m,S)|\le\|\nabla\varphi_m\|_{\mathbf{L}^2(\Omega)}\|\mathbf{u}_m-\mathbf{u}\|_{\mathbf{L}^4(\Omega)}\|S\|_{L^4(\Omega)}\to 0 \text{ as } m\to\infty\ \forall S\in H_0^1(\Omega).$$

Then, taking (16) into account, it is obtained

$$\lim_{m\to\infty}(\mathbf{u}_m\cdot\nabla\varphi_m,S)=(\mathbf{u}^*\cdot\nabla\varphi^*,S).$$

As the functional J is weakly semicontinuous below on $H_0^1(\Omega)\times\mathbf{V}$, then from aforesaid follows that

$$J^*=\lim_{m\to\infty}J(\varphi_m,\mathbf{u}_m)=\underline{\lim}_{m\to\infty}J(\varphi_m,\mathbf{u}_m)\ge J(\varphi^*,\mathbf{u}^*)\ge J^*.\ \blacksquare$$

3 Optimality systems

Further the case of $k(\varphi)=\varphi^2|\varphi|$ will be considered and the principle of Lagrange multipliers for the problem (11) will be justified.

Let's introduce a Lagrange multiplier $(\lambda_0,\theta)\in\mathbb{R}\times H_0^1(\Omega)$ and a Lagrangian L : $H_0^1(\Omega)\times\mathbf{V}\times\mathbb{R}\times H_0^1(\Omega)\to\mathbb{R}$ by formula

$$\mathcal{L}(\varphi,\mathbf{u},\lambda_0,\theta)=\lambda_0J(\varphi,\mathbf{u})+\langle\theta,F(\varphi,\mathbf{u})\rangle\equiv\lambda_0J(\varphi,\mathbf{u})+\langle F(\varphi,\mathbf{u}),\theta\rangle. \tag{17}$$

A common analysis shows that Frechet derivative of the operator F with respect to φ in (10) for $k=\varphi^2|\varphi|$ in the point $(\hat\varphi,\hat{\mathbf{u}})\in H_0^1(\Omega)\times\mathbf{V}$ is a linear continuous operator $F'_\varphi(\hat\varphi,\hat{\mathbf{u}}):H_0^1(\Omega)\to H^{-1}(\Omega)$, which assigns to each element $\tau\in H_0^1(\Omega)$ an element $\hat l\in H^{-1}(\Omega)$, where

$$\langle\hat l,S\rangle=\lambda(\nabla\tau,\nabla S)+4(\hat\varphi^2|\varphi|\tau,S)+(\mathbf{u}\cdot\nabla\tau,S).$$

From lemma 1 follows that the operator $F'_\varphi(\hat{\varphi}, \hat{\mathbf{u}})$ is an isomorphism. Then according to [18, 19] the theorem takes place:

Theorem 5. *While conditions (i), (ii) and (j), (jj) hold, let* $(\hat{\varphi}, \hat{\mathbf{u}}) \in H_0^1(\Omega) \times \mathbf{V}$ *be an element, on which the local minimum is achieved in the problem (11) if* $k = \varphi^2|\varphi|$. *Then there is a unique nonzero Lagrange multiplier* $(1, \theta)$, *where* $\theta \in H_0^1(\Omega)$, *such as Euler–Lagrange equation is satisfied*

$$\langle J'_\varphi(\hat{\varphi}, \hat{\mathbf{u}}), \tau\rangle + \langle F'_\varphi(\hat{\varphi}, \hat{\mathbf{u}})\tau, \theta\rangle = 0 \;\; \forall \tau \in H_0^1(\Omega), \tag{18}$$

and is equivalent to

$$\lambda(\nabla\tau, \nabla\theta) + 4(\hat{\varphi}^2|\varphi|\tau, \theta) + (\mathbf{u} \cdot \nabla\tau, \theta) = -\mu_0(\hat{\varphi} - \varphi_d, \tau)_Q \;\; \forall \tau \in H_0^1(\Omega), \tag{19}$$

and also the minimum principle is true:

$$\langle \mathcal{L}'_{\mathbf{u}}(\hat{\varphi}, \hat{\mathbf{u}}, 1, \theta), \mathbf{u} - \hat{\mathbf{u}}\rangle \geq 0 \;\; \forall\, \mathbf{u} \in \mathbf{V},$$

which is equivalent to the inequality

$$\mu_1(\hat{\mathbf{u}}, \mathbf{u} - \hat{\mathbf{u}})_1 + ((\mathbf{u} - \hat{\mathbf{u}}) \cdot \nabla\hat{\varphi}, \theta) \geq 0 \; \forall \mathbf{u} \in \mathbf{V}. \tag{20}$$

The relation (19) together with the variational inequality (20) and the operational restriction (10), which is equivalent to the ratio (6), are the optimality system for the problem (11) when $k = \varphi^2|\varphi|$.

4 Computations

Two different nonlinear boundary value problems were solved in cases of reaction coeffecients $k(\varphi) = \varphi^2$ and $k(\varphi) = |\varphi|$. For both cases the exact solution $\varphi_e = 0.2(x^2 + y^2)$ was taken. Also, the same $\mathbf{u} = (0; 0)$, $\varphi_0 = 0.1(x + y), \lambda = 10$. The function f was simply calculated in each case by substituting the function φ in the equation by the exact solution. The domain is $[-1; 1] \times [0; 1]$. The relative error is obtained by formula $\frac{\|\varphi - \varphi_e\|^2}{\|\varphi_e\|^2}$.

FreeFem++ listing

```
border c1(t=-1,1){x = t; y = 0; label=1;};
border c2(t=0,1){x = 1; y = t;label=2; };
border c3(t=-1,1){x=t;y=1;label=3;};
border c4(t=0,1){x=-1;y=t;label=4;};
int n=3;
mesh Th = buildmesh(c1(20*n) + c2(10*n) + c3(-20*n) + c4(-10*n));
fespace Vh(Th,P2);
Vh u1, u2, phi, phi1, s, err0, phi0;
u1 = 0;
u2 = 0;
int lambda = 10;
```

```
Vh f=-lambda*0.8+(0.2*(x^2+y^2))^3;
Vh phiex = 0.2*(x^2+y^2);
phi0 = 0.1*(x+y);
plot(phi0, cmm="phi0", wait = true, value = 1, fill = 1);

problem equation1(phi1,s)=
int2d(Th)(lambda*(dx(phi1)*dx(s) + dy(phi1)*dy(s)))
+ int2d(Th)(phi0^2*phi1*s)
+ int2d(Th)((u1*dx(phi1) + u2*dy(phi1))*s)
- int2d(Th)(f*s)
+ on(1,phi1=0.2*x^2)
+ on(2,phi1=0.2+0.2*y^2)
+ on(3,phi1=0.2+0.2*x^2)
+ on(4,phi1=0.2+0.2*y^2);

real E0, E01, L2err0;
int i;
for (i=0;i<=20;i++){
equation1;
err0=phi1-phiex;
E0 = sqrt(int2d(Th)(err0^2));
E01 = sqrt(int2d(Th)(phiex^2));
L2err0 = E0/E01;
cout <<"L2err0 = "<<L2err0<<endl;
plot(phi1, cmm="phi", wait = true, value = 1, fill = 1);
plot(err0,  cmm="error", wait = true, value = 1, fill = 1);
phi0 = phi1;
}
```

4.1 Case 1

Let's first consider the case of $k(\varphi) = |\varphi|$. Then the initial equation's weak formulation will obtain the form

$$\lambda(\nabla\varphi, \nabla S) + (|\varphi|\varphi, S) + (\mathbf{u} \cdot \nabla\varphi, S) = (f, S) \; \forall S \in H_0^1(\Omega). \tag{21}$$

Then, taking into account that the exact solution is $\varphi = 0.2(x^2 + y^2)$ and $\mathbf{u} = (0; 0)$, the following $f = -0.8\lambda + (0.2(x^2 + y^2))^2$.

4.2 Case 2

Let's now consider the case of $k(\varphi) = \varphi^2$. Then the initial equation's weak formulation will obtain the form

$$\lambda(\nabla\varphi, \nabla S) + (\varphi^3, S) + (\mathbf{u} \cdot \nabla\varphi, S) = (f, S) \; \forall S \in H_0^1(\Omega). \tag{22}$$

Then, simillary, $f = -0.8\lambda + (0.2(x^2 + y^2))^3$.

Here we are presenting some computations for both cases. It should be mentioned that the relative error for the first case at the last step of the loop is $1.1914e-10$ and for the second one is $1.0646e-10$.

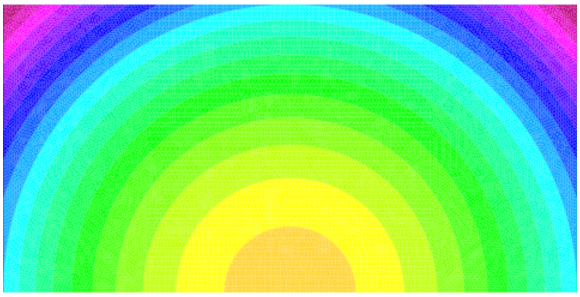

Fig. 1. Function φ_e, the values are ranged form -0.0210526 to 0.421053 (case 1)

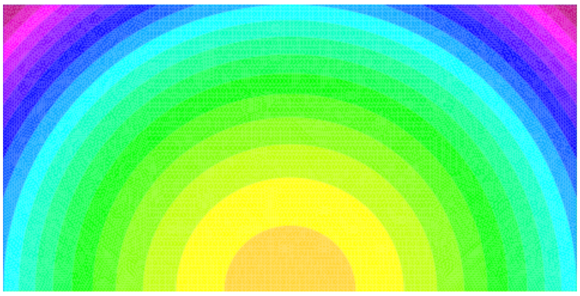

Fig. 2. The solution φ, the values are ranged form -0.0210526 to 0.421053 (case 1)

4.3 Additional algorithm

For the numerical research of extremum problems the algorithm from [20] will be used in future. Here are the recurrence relations, which stand for the algorithm for the case of the considered optimal control problem:

$$\varphi_{-1}=0,\ \ \theta_{-1}=0,\ \ \varphi_k,\ \theta_k\in H_0^1,\ \mathbf{u}_k\in K,\ k\geq 0,$$

$$\lambda(\nabla\tau,\nabla\theta_k)+4(\varphi_k^2|\varphi_k|\tau,\theta_k)+(\mathbf{u}_k\cdot\nabla\tau,\theta_{k-1})=-\mu_0(\varphi_k-\varphi_d,\tau)\ \ \forall\tau\in H_0^1, \tag{23}$$

$$\mu_1(\mathbf{u}_k,\mathbf{u}-\mathbf{u}_k)_1+((\mathbf{u}-\mathbf{u}_k)\cdot\nabla\varphi_{k-1},\theta_{k-1})\geq 0\ \forall\mathbf{u}\in K, \tag{24}$$

$$\lambda(\nabla\varphi_k,\nabla S)+(\mathbf{u}_k\cdot\nabla\varphi_k,S)+(\varphi_{k-1}^3|\varphi_k|,S)=(f,S)\ \ \forall S\in H_0^1. \tag{25}$$

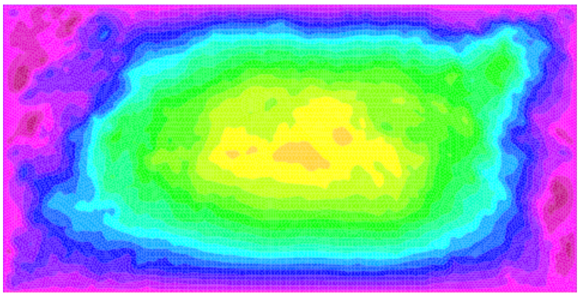

Fig. 3. The error of solution, the values are ranged form $-3.45449\,10^{-11}$ to $9.34075\,10^{-12}$ (case 1)

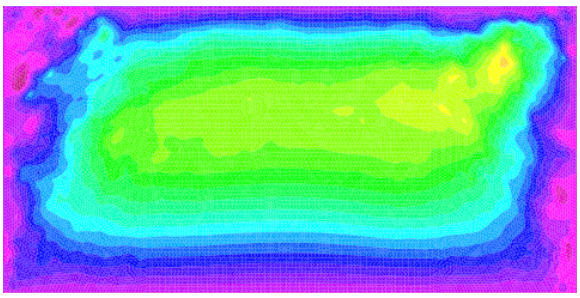

Fig. 4. The error of solution, the values are ranged form $-3.7904\,10^{-11}$ to $9.01527\,10^{-12}$ (case 2)

Under the condition $\mu_1 > 0$ and the fact that the set $K \subset \mathbf{V}$ is convex and closed, we can introduce the projection operator $P : \mathbf{V} \to K$. Then the variational inequality (24) is equivalent to the equation $\mathbf{u}_k = P(\varphi_{k-1}\theta_{k-1}/\mu_1)$, $k \geq 0$.

The result about this algorithm's convergence was obtained similarly to the [20].

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