

# Fictitious domain formulations of unilateral problems: analysis and algorithms

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Received: 7 May 2008 / Accepted: 13 January 2009 / Published online: 6 February 2009  
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**Abstract** The present article deals with fictitious domain methods for numerical realization of scalar variational inequalities with the Signorini type conditions on the boundary. Two variants are introduced and analyzed. A discretization is done by finite elements. It leads to a system of non-smooth, piecewise linear equations. This system is solved by the semismooth Newton method. Numerical experiments confirm the efficiency of this approach.

**Keywords** Unilateral problems · Fictitious domain methods · Semismooth Newton method

**Mathematics Subject Classification (2000)** 65F10 · 65N22

## 1 Introduction

Fictitious domain methods (FDM) belong to a class of methods for numerical realization of large scale linear algebraic systems arising from finite element discretizations of elliptic boundary value problems. Their idea is simple: the original problem defined in a domain  $\omega$  is replaced by a new one formulated in a larger domain  $\Omega \supset \omega$  with a simple shape (a box, e.g.). The new problem is chosen in such a way that its solution restricted to  $\omega$  coincides with the solution of the original problem. Since  $\Omega$  has a simple shape, one can use specific partitions for constructing finite element spaces. Here we confine ourselves to the so-called non-fitted meshes when the partition of  $\Omega$  does

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not respect the geometry of  $\omega$ . In this case uniform meshes represent a natural choice and the resulting stiffness matrix does not depend on  $\omega$ . In addition, it has a structure enabling us to use fast solvers. There are several ways how to define the problem in  $\Omega$  with the property mentioned above. One of them is the method of boundary Lagrange multipliers which has been used for solving Dirichlet boundary value problems [6–8] and Neumann problems [9]. This approach however suffers from a serious drawback: the solution is only from  $H^{3/2-\eta}(\Omega)$ ,  $\eta > 0$ , due to a generally non-zero jump of the normal derivative across  $\gamma$  (the boundary of  $\omega$ ). If non-fitted meshes are used, then this singularity appears inside of some elements of the used partition, namely those ones the interior of which is cut by  $\gamma$ . Consequently, the theoretical rate of convergence of approximate solutions in the  $H^1(\Omega)$ -norm can not exceed  $1/2$ . In addition, the biggest error is concentrated around  $\gamma$  which explains also a slower convergence in the  $H^1(\omega)$ -norm of solutions restricted to  $\omega$ . To improve the accuracy in  $\omega$ , the authors proposed in [10] a new variant of FDM. Instead of Lagrange multipliers on  $\gamma$  they used control variables defined on a close curve  $\Gamma$  in  $\Omega$  having a positive distance from  $\omega$  and enforcing the Dirichlet condition on  $\gamma$  to be satisfied. The solution is still singular in  $\Omega$  but the singularity is shifted from  $\gamma$  to  $\Gamma$  and as a result, convergence in  $\omega$  became faster. The aim of this article is twofold: first to introduce a fictitious domain formulation of unilateral boundary value problems and secondly, to propose its “smooth” variant in the spirit mentioned above. We focus on a simple scalar variational inequality with Signorini type conditions on  $\gamma$ , but a similar approach can be used for contact problems, e.g. Our fictitious domain formulation consists of an elliptic equation in  $\Omega$  completed by an equation on  $\gamma$  for the projection operator onto a convex set which represents the equivalent expression of the unilateral conditions prescribed there. Similarly to the Dirichlet problem we shall consider two cases, namely: (i) *boundary Lagrange multipliers on  $\gamma$* ; (ii) *control variables on  $\Gamma$* , where  $\Gamma$  is a close curve exterior to  $\omega$ . The reason for considering (ii) is the same as above, namely to smooth (at least partially) our fictitious domain solution in a vicinity of  $\omega$ . In both cases the auxiliary boundary variables enforce the satisfaction of the unilateral conditions. We prove the existence and uniqueness of the solution in (i). On the other hand, (ii) is more involved. The existence analysis is based on approximate controllability type results. We show that using square integrable controls on  $\Gamma$  we are able to satisfy the unilateral conditions either exactly provided that an appropriate small source term  $\delta$  is added on  $\gamma$  or with an arbitrary accuracy if this term is neglected. A typical finite element discretization gives a large system of linear equations completed with a small system of piecewise linear (i.e. non-smooth) equations which arise from a discretization of the unilateral conditions. The resulting algebraic problem is numerically solved by a semismooth Newton method [3, 4, 11]. Each linearized step leads to a non-symmetric, saddle-point type system which can be solved very efficiently by a projected Schur complement method [10]. The authors would like to emphasize that this article is focused *solely* on the continuous setting of this approach while its discretization is taken only as a tool for verifying its applicability.

The article is organized as follows: in Sect. 2 two variants of the fictitious domain formulation are introduced. Section 3 deals with the existence analysis for both variants, including the proof of an approximate controllability property which is needed in (ii). In Sect. 4, we describe a discretization of the problem. The special emphasize

is paid on the approximation of the non-smooth equation defining the unilateral conditions. Section 5 is devoted to algorithmic aspects of this method such as the semismooth Newton method, the active set strategy and main ideas of the projected Schur complement method. Finally, Section 6 presents numerical results of three model examples.

### 2 Setting of the problem

We shall consider the following unilateral problem in a bounded domain  $\omega \subset \mathbb{R}^2$  with the Lipschitz continuous boundary  $\gamma$ :

$$\left. \begin{aligned} &-\Delta u + u = f \quad \text{in } \omega, \\ &u \geq g, \quad \frac{\partial u}{\partial n_\gamma} \geq 0, \quad \frac{\partial u}{\partial n_\gamma}(u - g) = 0 \quad \text{on } \gamma, \end{aligned} \right\} \tag{2.1}$$

where  $f \in L^2_{loc}(\mathbb{R}^2)$ ,  $g \in H^{1/2}(\gamma)$  are given functions and  $\frac{\partial}{\partial n_\gamma}$  denotes the normal derivative of a function on  $\gamma$ .

The weak formulation of (2.1) reads as follows:

$$\left. \begin{aligned} &\text{Find } u \in K \text{ such that} \\ &(u, v - u)_{1,\omega} \geq (f, v - u)_{0,\omega} \quad \forall v \in K, \end{aligned} \right\} \tag{P}$$

where

$$K = \{v \in H^1(\omega) \mid v \geq g \text{ a.e. on } \gamma\}$$

is the closed convex set and  $(\cdot, \cdot)_{k,S}$  stands for the scalar product in  $H^k(S)$ ,  $k \geq 0$  integer ( $H^0(S) := L^2(S)$ ). It is well-known that (P) has a unique solution.

Denote

$$\begin{aligned} H^{1/2}(\gamma) &= \{\varphi \in L^2(\gamma) \mid \varphi = v \text{ on } \gamma, v \in H^1(\omega)\}, \\ H^{-1/2}(\gamma) &= (H^{1/2}(\gamma))' \quad (\text{dual of } H^{1/2}(\gamma)), \\ H_+^{-1/2}(\gamma) &= \text{cone of all non-negative elements of } H^{-1/2}(\gamma). \end{aligned}$$

An alternative (and equivalent) formulation of P is given by

$$\left. \begin{aligned} &\text{Find } u \in H^1(\omega) \text{ such that} \\ &(u, v)_{1,\omega} = (f, v)_{0,\omega} + \langle \frac{\partial u}{\partial n_\gamma}, v \rangle_\gamma \quad \forall v \in H^1(\omega), \\ &\frac{\partial u}{\partial n_\gamma} \in H_+^{-1/2}(\gamma), \\ &\langle \mu - \frac{\partial u}{\partial n_\gamma}, u - g \rangle_\gamma \geq 0 \quad \forall \mu \in H_+^{-1/2}(\gamma), \end{aligned} \right\} \tag{2.2}$$

where  $\langle \cdot, \cdot \rangle_\gamma$  is the duality pairing between  $H^{-1/2}(\gamma)$  and  $H^{1/2}(\gamma)$ .

**Assumption** Throughout this article we shall suppose that  $\frac{\partial u}{\partial n_\gamma} \in L^2_+(\gamma)$ . This assumption is satisfied provided that  $g \in H^{3/2}(\gamma)$  and  $\omega$  has a sufficiently smooth boundary or  $\omega$  is polygonal and convex since  $u \in H^2(\omega)$  [2]. In this case, the last inequality in (2.2) can be written as

$$\left(\mu - \frac{\partial u}{\partial n_\gamma}, u - g\right)_{0,\gamma} \geq 0 \quad \forall \mu \in L^2_+(\gamma). \tag{2.3}$$

Let  $P$  denote the projection of  $L^2(\gamma)$  onto  $L^2_+(\gamma)$ . Then

$$P\varphi = \max\{0, \varphi\} \quad \forall \varphi \in L^2(\gamma) \tag{2.4}$$

and (2.3) is equivalent to

$$\frac{\partial u}{\partial n_\gamma} = P\left(\frac{\partial u}{\partial n_\gamma} - \rho(u - g)\right), \tag{2.5}$$

where  $\rho > 0$  is arbitrary. Thus assuming  $\frac{\partial u}{\partial n_\gamma} \in L^2(\gamma)$ , problem  $\mathcal{P}$  can be expressed as the system of two equations:

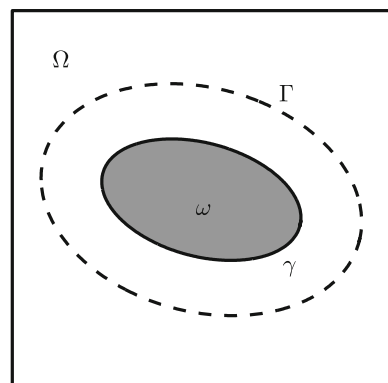
$$\left. \begin{aligned} (u, v)_{1,\omega} &= (f, v)_{0,\omega} + \left(\frac{\partial u}{\partial n_\gamma}, v\right)_{0,\gamma} \quad \forall v \in H^1(\omega), \\ \frac{\partial u}{\partial n_\gamma} &= P\left(\frac{\partial u}{\partial n_\gamma} - \rho(u - g)\right), \quad \rho > 0, \end{aligned} \right\} \tag{2.6}$$

which will be a starting point for our next considerations.

Next, we shall introduce two variants of a fictitious domain formulation. To this end we choose a bounded domain  $\Omega$  having a simple shape (a box, e.g.) such that  $\bar{\omega} \subset \Omega$  and construct a close curve  $\Gamma \subset \Omega$  surrounding  $\omega$ . We shall distinguish two cases depending on the mutual position of  $\gamma$  and  $\Gamma$ :

- (i)  $\gamma = \Gamma$ ; (ii)  $\text{dist}(\gamma, \Gamma) > 0$  (see Fig. 1).

**Fig. 1** Geometry of the problem



We define the following problem in  $\Omega$ :

$$\left. \begin{aligned} \text{Find } (\hat{u}, \lambda) \in H_0^1(\Omega) \times H^{-1/2}(\Gamma) \text{ such that} \\ (\hat{u}, v)_{1,\Omega} = (f, v)_{0,\Omega} + \langle \lambda, v \rangle_\Gamma \quad \forall v \in H_0^1(\Omega), \\ \frac{\partial}{\partial n_\gamma} \hat{u}(\omega) \in L^2(\gamma), \\ \frac{\partial}{\partial n_\gamma} \hat{u}(\omega) = P\left(\frac{\partial}{\partial n_\gamma} \hat{u}(\omega) - \rho(\hat{u}(\omega) - g)\right), \quad \rho > 0, \end{aligned} \right\} \quad (\hat{\mathcal{P}}(\Gamma))$$

where  $\hat{u}(\omega) := \hat{u}|_\omega$  and  $\langle \cdot, \cdot \rangle_\Gamma$  stands for the duality pairing between  $H^{-1/2}(\Gamma)$  and  $H^{1/2}(\Gamma)$ .

Problem  $\hat{\mathcal{P}}(\Gamma)$  will be called the *fictitious domain formulation* of the unilateral problem (2.1). If  $\Gamma = \gamma$ , we speak on the *nonsmooth* variant, otherwise  $\hat{\mathcal{P}}(\Gamma)$  is termed the *smooth* variant (the reason for this terminology will be clarified in Remark 3.2). The relation between  $\hat{\mathcal{P}}(\Gamma)$  and  $\mathcal{P}$  follows from the next Lemma.

**Lemma 2.1** *Let  $(\hat{u}, \lambda)$  be a solution of  $\hat{\mathcal{P}}(\Gamma)$ . Then  $\hat{u}(\omega)$  solves  $\mathcal{P}$ .*

*Proof* From the first equation in  $\hat{\mathcal{P}}(\Gamma)$  we obtain:

$$-\Delta \hat{u}(\omega) + \hat{u}(\omega) = f \quad \text{in } \omega.$$

The unilateral conditions on  $\gamma$  are hidden in the last equation in  $\hat{\mathcal{P}}(\Gamma)$ . □

*Remark 2.1* Any solution  $(\hat{u}, \lambda)$  of  $\hat{\mathcal{P}}(\Gamma)$  satisfies:

$$\left. \begin{aligned} -\Delta \hat{u} + \hat{u} &= f \quad \text{in } \Xi_1 \cup (\Omega \setminus \overline{\Xi_1}), \\ \left[ \frac{\partial \hat{u}}{\partial n_\Gamma} \right]_\Gamma &= \lambda \quad \text{on } \Gamma, \\ \hat{u} &= 0 \quad \text{on } \partial\Omega, \end{aligned} \right\}$$

where  $\Xi_1$  is the domain between  $\partial\Omega$  and  $\Gamma$ ,  $\left[ \frac{\partial}{\partial n_\Gamma} \right]_\Gamma$  stands for the jump of the normal derivative across  $\Gamma$ . In addition, the unilateral conditions for  $\hat{u}|_\omega$  are satisfied on  $\gamma$ .

*Remark 2.2* Instead of  $H_0^1(\Omega)$  appearing in  $\hat{\mathcal{P}}(\Gamma)$  other spaces can be used. In model examples presented in the last section we use  $H_{\text{per}}^1(\Omega)$ —the space of all periodic functions belonging to  $H^1(\Omega)$ . Just the fact that functions from  $H_{\text{per}}^1(\Omega)$  satisfy the periodic boundary conditions will play the crucial role in numerical realization.

Problem  $\hat{\mathcal{P}}(\Gamma)$  can be equivalently formulated as an optimal control problem. Indeed, let  $\hat{u}(\mu) \in H_0^1(\Omega)$  be the solution of the state equation

$$(\hat{u}(\mu), v)_{1,\Omega} = (f, v)_{0,\Omega} + \langle \mu, v \rangle_\Gamma \quad \forall v \in H_0^1(\Omega)$$

in which  $\mu \in H^{-1/2}(\Gamma)$  plays the role of a control variable and

$$\Psi(\mu) = \frac{1}{2} \left\| \frac{\partial}{\partial n_\gamma} (\hat{u}(\mu)|_\omega) - P\left(\frac{\partial}{\partial n_\gamma} (\hat{u}(\mu)|_\omega) - \rho(\hat{u}(\mu)|_\omega - g)\right) \right\|_{0,\gamma}^2 \quad (2.7)$$

be the cost functional for those  $\mu$  for which  $\frac{\partial}{\partial n_\gamma}(\hat{u}(\mu)|_\omega) \in L^2(\gamma)$ . Then  $(\hat{u}, \lambda)$  solves  $\hat{\mathcal{P}}(\Gamma)$  if and only if  $\Psi(\lambda) = 0$ .

### 3 Existence analysis

The aim of this section will be to analyze the solvability of the fictitious domain formulation  $\hat{\mathcal{P}}(\Gamma)$ . The situation is very easy when  $\Gamma = \gamma$  as follows from the next theorem.

**Theorem 3.1** *Let  $\Gamma = \gamma$  and suppose that the solution  $u$  of  $\mathcal{P}$  is such that  $\frac{\partial u}{\partial n_\gamma} \in L^2_+(\gamma)$ . Then  $(\hat{\mathcal{P}}(\gamma))$  has a unique solution.*

*Proof* Denote  $u(\Xi)$  the unique solution of the Dirichlet problem in  $\Xi = \Omega \setminus \bar{\omega}$ :

$$\left. \begin{aligned} -\Delta u(\Xi) + u(\Xi) &= f && \text{in } \Xi, \\ u(\Xi) &= 0 && \text{on } \partial\Omega, \\ u(\Xi) &= u && \text{on } \gamma \end{aligned} \right\} \tag{3.1}$$

and set

$$\hat{u} = \begin{cases} u & \text{in } \omega, \\ u(\Xi) & \text{in } \Xi. \end{cases}$$

Then  $(\hat{u}, [\frac{\partial \hat{u}}{\partial n_\gamma}]_\gamma)$  satisfies the first equation in  $(\hat{\mathcal{P}}(\gamma))$  as follows from Green’s formula. Since  $\hat{u}|_\omega$  solves  $\mathcal{P}$ , the non-smooth Eq. (2.5) on  $\gamma$  is automatically satisfied.  $\square$

If  $\text{dist}(\gamma, \Gamma) > 0$ , the problem is more involved and is closely related to a controllability type property. To see that let us define for any  $\lambda \in H^{-1/2}(\Gamma)$  the following problem in  $\Xi = \Omega \setminus \bar{\omega}$ :

$$\left. \begin{aligned} \text{Find } u(\lambda) &\in H^1(\Xi) \text{ such that} \\ (u(\lambda), v)_{1,\Xi} &= (f, v)_{0,\Xi} + \langle \lambda, v \rangle_\Gamma \quad \forall v \in H^1_0(\Xi), \\ u(\lambda) &= 0 \quad \text{on } \partial\Omega, \\ u(\lambda) &= u \quad \text{on } \gamma \end{aligned} \right\} \tag{\mathcal{P}(\lambda)}$$

(recall that  $u \in K$  solves  $\mathcal{P}$ ). If there was  $\bar{\lambda} \in H^{-1/2}(\Gamma)$  such that

$$\frac{\partial u(\bar{\lambda})}{\partial n_\gamma} + \frac{\partial u}{\partial n_\gamma} = 0 \quad \text{on } \gamma, \tag{3.2}$$

then the function

$$\hat{u} = \begin{cases} u & \text{in } \omega, \\ u(\bar{\lambda}) & \text{in } \Xi \end{cases}$$

would be a solution of  $\hat{\mathcal{P}}(\Gamma)$ .

Unfortunately, such  $\bar{\lambda}$  does not exist, in general. Only what we can prove is that (3.2) is satisfied with an arbitrary accuracy. To show that let us introduce the mapping  $\Phi : H^{-1/2}(\Gamma) \mapsto H^{-1/2}(\gamma)$  defined by

$$\Phi(\lambda) = \frac{\partial u(\lambda)}{\partial n_\gamma} \in H^{-1/2}(\gamma) \quad \forall \lambda \in H^{-1/2}(\Gamma), \tag{3.3}$$

where  $u(\lambda)$  solves  $(\mathcal{P}(\lambda))$  and denote  $\mathcal{V} := \Phi(H^{-1/2}(\Gamma)) \subseteq H^{-1/2}(\gamma)$ .

**Lemma 3.1** *The set  $\mathcal{V}$  is dense in  $H^{-1/2}(\gamma)$ .*

*Proof* Without loss of generality we may consider problem  $(\mathcal{P}(\lambda))$  with  $f \equiv 0$  and homogeneous Dirichlet data on  $\partial\Xi$ . Let  $u(\lambda) \in H_0^1(\Xi), \lambda \in H^{-1/2}(\Gamma)$ , be the solution of

$$(u(\lambda), v)_{1,\Xi} = \langle \lambda, v \rangle_\Gamma \quad \forall v \in H_0^1(\Xi). \tag{3.4}$$

Let  $w \in H^{1/2}(\gamma)$  be such that

$$\left\langle \frac{\partial u(\lambda)}{\partial n_\gamma}, w \right\rangle_\gamma = 0 \quad \forall \lambda \in H^{-1/2}(\Gamma). \tag{3.5}$$

We want to show that  $w = 0$ . For  $w$  satisfying (3.5) consider the Dirichlet problem:

$$\left. \begin{aligned} \text{Find } z \in H^1(\Xi) \text{ such that} \\ (z, v)_{1,\Xi} = 0 \quad \forall v \in H_0^1(\Xi), \\ z = 0 \quad \text{on } \partial\Omega, \\ z = w \quad \text{on } \gamma. \end{aligned} \right\} \tag{3.6}$$

Inserting  $v := u(\lambda) \in H_0^1(\Xi)$  into (3.6) we have:

$$(z, u(\lambda))_{1,\Xi} = 0 \quad \forall \lambda \in H^{-1/2}(\Gamma). \tag{3.7}$$

The symmetry of the scalar product, (3.4) and Green’s theorem yield:

$$\begin{aligned} 0 &= (u(\lambda), z)_{1,\Xi} = \langle \lambda, z \rangle_\Gamma + \left\langle \frac{\partial u(\lambda)}{\partial n_\gamma}, z \right\rangle_\gamma \\ &= \langle \lambda, z \rangle_\Gamma + \left\langle \frac{\partial u(\lambda)}{\partial n_\gamma}, w \right\rangle_\gamma = \langle \lambda, z \rangle_\Gamma \quad \forall \lambda \in H^{-1/2}(\Gamma) \end{aligned}$$

making use of (3.5)–(3.7). Therefore  $z = 0$  on  $\Gamma$  implying  $z \equiv 0$  in  $\Xi_1$  (recall that  $\Xi_1$  is a domain between  $\partial\Omega$  and  $\Gamma$ ). Then from the continuation theorem it immediately follows that  $z \equiv 0$  in  $\Xi$ . Thus  $w = 0$  on  $\gamma$ . □

On the basis of Lemma 3.1 we prove the following result.

**Theorem 3.2** Let  $\text{dist}(\gamma, \Gamma) > 0$  and suppose that the solution  $u$  of  $\mathcal{P}$  is such that  $\frac{\partial u}{\partial n_\gamma} \in L^2_+(\gamma)$ . Then for every  $\epsilon > 0$  there exist:  $\lambda_\epsilon \in H^{-1/2}(\Gamma)$ ,  $\hat{u}_\epsilon \in H^1_0(\Omega)$  and  $\delta_\epsilon \in H^{-1/2}(\gamma)$  satisfying:

$$\left. \begin{aligned} (\hat{u}_\epsilon, v)_{1,\Omega} &= (f, v)_{0,\Omega} + \langle \lambda_\epsilon, v \rangle_\Gamma + \langle \delta_\epsilon, v \rangle_\gamma \quad \forall v \in H^1_0(\Omega), \\ \frac{\partial}{\partial n_\gamma} \hat{u}_\epsilon(\omega) &\in L^2(\gamma), \\ \frac{\partial \hat{u}_\epsilon(\omega)}{\partial n_\gamma} &= P\left(\frac{\partial \hat{u}_\epsilon(\omega)}{\partial n_\gamma} - \rho(\hat{u}_\epsilon(\omega) - g)\right) \text{ on } \gamma, \quad \rho > 0, \\ \|\delta_\epsilon\|_{-1/2,\gamma} &\leq \epsilon, \end{aligned} \right\} \tag{3.8}$$

where  $\hat{u}_\epsilon(\omega) := \hat{u}_\epsilon|_\omega$ .

*Proof* Let  $\epsilon > 0$  be given. From Lemma 3.1 we know that there exists  $\lambda_\epsilon \in H^{-1/2}(\Gamma)$  such that

$$\left\| \frac{\partial u(\lambda_\epsilon)}{\partial n_\gamma} + \frac{\partial u}{\partial n_\gamma} \right\|_{-1/2,\gamma} \leq \epsilon,$$

where  $u(\lambda_\epsilon)$  solves  $(\mathcal{P}(\lambda_\epsilon))$ . Define a function  $\hat{u}_\epsilon \in H^1_0(\Omega)$  by

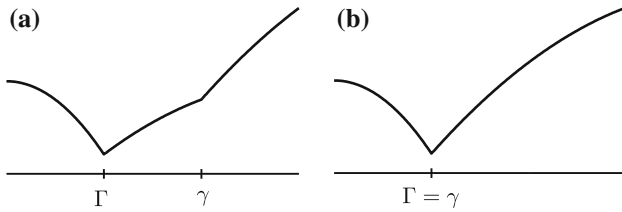
$$\hat{u}_\epsilon = \begin{cases} u & \text{in } \omega, \\ u(\lambda_\epsilon) & \text{in } \Xi \end{cases}$$

and set  $\delta_\epsilon := \frac{\partial u(\lambda_\epsilon)}{\partial n_\gamma} + \frac{\partial u}{\partial n_\gamma}$ . Then the triplet  $\{\hat{u}_\epsilon, \lambda_\epsilon, \delta_\epsilon\}$  solves (3.8) as follows from Green’s formula and the fact that  $\frac{\partial}{\partial n_\gamma} \hat{u}_\epsilon(\omega) = \frac{\partial u}{\partial n_\gamma}$  on  $\gamma$ . □

*Remark 3.1* The same analysis with the same result can be done when the space  $H^1_0(\Omega)$  is replaced by  $H^1_{\text{per}}(\Omega)$ . It is also readily seen that the space  $H^{-1/2}(\Gamma)$  can be replaced by  $L^2(\Gamma)$  and the density result of Lemma 3.1 holds true.

*Remark 3.2* Any solution  $\hat{u}_\epsilon$  of (3.8) is such that its restriction on  $\omega$  solves the original unilateral problem  $\mathcal{P}$ , i.e.  $\hat{u}_\epsilon(\omega)$  is defined in a unique way. As far as the global regularity of  $\hat{u}_\epsilon$  is concerned, the best what one can expect is that  $\hat{u}_\epsilon \in H^{3/2-\eta}(\Omega)$  for any  $\eta > 0$  in view of a generally non-zero jump of the normal derivative of  $\hat{u}_\epsilon$  across  $\Gamma$ . The same holds true for the solution  $\hat{u}$  of the non-smooth variant but there is an important difference. If  $\gamma \equiv \Gamma$ , the singularity of  $\hat{u}$  is located just on the boundary of the original domain  $\omega$  whereas is moved away from  $\omega$  if the smooth variant is used (see Fig. 2). The solution  $\hat{u}_\epsilon$  of (3.8) still has a singularity on  $\gamma$  due to the term  $\delta_\epsilon$ . But this term can be chosen in such a way that its norm is arbitrarily small. This is important from the computational point of view. If finite element spaces are constructed by using non-fitted meshes then the curves  $\Gamma$  and  $\gamma$  cut some elements of the respective partitions. This leads to a significant discretization error in a vicinity of  $\Gamma$ . Thus, if  $\gamma \equiv \Gamma$ , the error of the numerical solution is concentrated around  $\gamma$ , where





**Fig. 2** Singularity of the solution. **a** Smooth variant, **b** non-smooth variant

the unilateral conditions are prescribed. On the other hand, if  $\text{dist}(\gamma, \Gamma) > 0$  then the main singularity is moved away from  $\gamma$  and one can expect that the error on  $\gamma$  coming from  $\delta_\varepsilon$  could be “small”.

The formulation (3.8) can be hardly used for computations since  $\delta_\varepsilon$  is not known a-priori. Going back to the optimal control formulation of  $\hat{\mathcal{P}}(\Gamma)$  at the end of Sect. 2 one can prove that under appropriate regularity assumptions on the solutions to  $\mathcal{P}$  and  $(\mathcal{P}(\lambda))$  it holds:

$$\inf_{\mu \in L^2(\Gamma)} \Psi(\mu) = 0, \tag{3.9}$$

where  $\Psi$  is defined by (2.7) (if  $\gamma = \Gamma$  then inf can be replaced by min).

Indeed, we first show that the source terms  $\lambda_\varepsilon$  and  $\delta_\varepsilon$  in (3.8) can be taken more regular. To this end, let  $g \in H^{3/2}(\gamma)$  and the boundary  $\gamma$  be such that the solution  $u$  of  $\mathcal{P}$  belongs to  $H^2(\omega) \cap K$  implying  $u|_\gamma \in H^{3/2}(\gamma)$ ,  $\frac{\partial u}{\partial n_\gamma} \in H^{1/2}(\gamma)$ . Next we shall consider the auxiliary problem  $(\mathcal{P}(\lambda))$  with  $\lambda \in H^{1/2}(\Gamma)$ . We shall suppose that its solution  $u(\lambda) \in H^1(\Xi)$  is such that  $u(\lambda)|_{\Xi_2} \in H^2(\Xi_2)$ , where  $\Xi_2$  is the domain between  $\Gamma$  and  $\gamma$ . Consequently, the mapping  $\Psi$  defined by (3.3) can be considered as a mapping from  $L^2(\Gamma)$  into  $L^2(\gamma)$  preserving the density property:  $\Phi(L^2(\Gamma))$  is dense in  $L^2(\gamma)$ . From the definition of  $\delta_\varepsilon$  in the proof of Lemma 3.1 we see that in fact  $\delta_\varepsilon \in H^{1/2}(\gamma)$  and  $\|\delta_\varepsilon\|_{0,\gamma} \leq \varepsilon$ .

In what follows we shall suppose that (3.8) is satisfied by  $\{\hat{u}_\varepsilon, \lambda_\varepsilon, \delta_\varepsilon\} \in H_0^1(\Omega) \times L^2(\Gamma) \times L^2(\gamma)$  and  $\|\delta_\varepsilon\|_{0,\gamma} \leq \varepsilon$ . The solution  $\hat{u}_\varepsilon$  can be written as  $\hat{u}_\varepsilon = \hat{u}_\varepsilon^1 + \hat{u}_\varepsilon^2$ , where  $\hat{u}_\varepsilon^j \in H_0^1(\Omega)$ ,  $j = 1, 2$  solve:

$$\begin{aligned} (\hat{u}_\varepsilon^1, v)_{1,\Omega} &= (f, v)_{0,\Omega} + (\lambda_\varepsilon, v)_{0,\Gamma} \quad \forall v \in H_0^1(\Omega), \\ (\hat{u}_\varepsilon^2, v)_{1,\Omega} &= (\delta_\varepsilon, v)_{0,\gamma} \quad \forall v \in H_0^1(\Omega). \end{aligned}$$

Inserting the decomposition of  $\hat{u}_\varepsilon$  into the second equality in (3.8) and denoting  $\hat{u}_\varepsilon^j(\omega) := \hat{u}_\varepsilon^j|_\omega$  we obtain

$$\begin{aligned}
 & \left\| \frac{\partial \hat{u}_\varepsilon^1(\omega)}{\partial n_\gamma} - P\left(\frac{\partial \hat{u}_\varepsilon^1(\omega)}{\partial n_\gamma} - \rho(\hat{u}_\varepsilon^1(\omega) - g)\right) \right\|_{0,\gamma} & (3.10) \\
 & \leq \left\| \frac{\partial \hat{u}_\varepsilon^2(\omega)}{\partial n_\gamma} \right\|_{0,\gamma} + \left\| P\left(\frac{\partial \hat{u}_\varepsilon^1(\omega)}{\partial n_\gamma} + \frac{\partial \hat{u}_\varepsilon^2(\omega)}{\partial n_\gamma} - \rho(\hat{u}_\varepsilon^1(\omega) + \hat{u}_\varepsilon^2(\omega) - g)\right) \right. \\
 & \quad \left. - P\left(\frac{\partial \hat{u}_\varepsilon^1(\omega)}{\partial n_\gamma} - \rho(\hat{u}_\varepsilon^1(\omega) - g)\right) \right\|_{0,\gamma} \\
 & \leq 2 \left\| \frac{\partial \hat{u}_\varepsilon^2(\omega)}{\partial n_\gamma} \right\|_{0,\gamma} + \rho \|\hat{u}_\varepsilon^2(\omega)\|_{0,\gamma}
 \end{aligned}$$

provided that both  $\frac{\partial \hat{u}_\varepsilon^1(\omega)}{\partial n_\gamma}$  and  $\frac{\partial \hat{u}_\varepsilon^2(\omega)}{\partial n_\gamma}$  belong to  $L^2(\gamma)$ . Finally let us assume that  $\left\| \frac{\partial \hat{u}_\varepsilon^2(\omega)}{\partial n_\gamma} \right\|_{0,\gamma} \leq C \|\delta_\varepsilon\|_{0,\Gamma} \leq C\varepsilon$ . From this and (3.10) we arrive at (3.9).

### 4 Discretization

In this section we describe a finite element discretization of  $\hat{\mathcal{P}}(\Gamma)$ . We derive an algebraic problem while technical details will be postponed to the last section.

Let  $V_h \subset H_0^1(\Omega)$ ,  $\Lambda_H(\gamma) \subset L^2(\gamma)$ ,  $\Lambda_H(\Gamma) \subset L^2(\Gamma)$  be finite dimensional subspaces and  $\dim V_h = n$ ,  $\dim \Lambda_H(\gamma) = \dim \Lambda_H(\Gamma) = m$ . By a discretization of  $\hat{\mathcal{P}}(\Gamma)$  we mean the following problem:

$$\left. \begin{aligned}
 & \text{Find } (\hat{u}_h, \lambda_h) \in V_h \times \Lambda_H(\Gamma) \text{ such that} \\
 & (\hat{u}_h, v_h)_{1,\Omega} = (f, v_h)_{0,\Omega} + (\lambda_h, v_h)_{0,\Gamma} \quad \forall v_h \in V_h, \\
 & \delta_H \hat{u}_h = P(\delta_H \hat{u}_h - \rho(\tau_H \hat{u}_h - g_H)), \quad \rho > 0,
 \end{aligned} \right\} \quad (\hat{\mathcal{P}}(\Gamma)_h^H)$$

where  $\delta_H \hat{u}_h$ ,  $\tau_H \hat{u}_h$  and  $g_H$  are approximations of  $\frac{\partial \hat{u}_h|_\omega}{\partial n_\gamma}$ ,  $\hat{u}_h|_\gamma$  and  $g$ , respectively, in  $\Lambda_H(\gamma)$ .

It is easy to prove the existence of a solution of  $(\hat{\mathcal{P}}(\Gamma)_h^H)$  for a particular choice of finite element spaces and of the mappings  $\delta_H$  and  $\tau_H$  provided that  $\Gamma \equiv \gamma$  and  $\omega$  is polygonal. Indeed, let  $V_h$  be a space of piecewise linear functions over a triangulation  $\mathcal{T}_h$  of  $\bar{\Omega}$  which respects the geometry of  $\omega$ , i.e.  $\mathcal{T}_h|_\omega$  is a triangulation of  $\bar{\omega}$ , as well. Further, let  $\Lambda_H(\Gamma) = \Lambda_H(\gamma) := V_h|_\gamma$  be the space of restrictions on  $\gamma$  of all trial functions. Then the solution of  $(\hat{\mathcal{P}}(\Gamma)_h^H)$  can be obtained in a similar way as in the continuous case by sticking two finite element approximations of (2.1) and (3.1) in  $\omega$  and  $\Omega \setminus \bar{\omega}$ , respectively. The mappings  $\delta_H$  and  $\tau_H$  are defined by

$$(\delta_H \hat{u}_h, \tau_H \hat{u}_h) = (\lambda_h, w_{h|_\gamma}),$$

where  $(w_h, \lambda_h)$  is the unique solution to the mixed finite element approximation of (2.1) on  $V_h|_\omega \times \Lambda_H^+(\gamma)$  with  $\Lambda_H^+(\gamma)$  being the set of non-negative functions from  $\Lambda_H(\gamma)$ .

In what follows no assumptions on the mutual position of  $\Gamma$  and  $\gamma$  and used partitions will be imposed.

Let  $\{\varphi_j\}_{j=1}^n, \{\psi_i\}_{i=1}^m$  and  $\{\tilde{\psi}_i\}_{i=1}^m$  be basis functions of  $V_h, \Lambda_H(\gamma)$  and  $\Lambda_H(\Gamma)$ , respectively. In order to simplify our presentation, we suppose that  $\Lambda_H(\gamma)$  is the space of piecewise constant functions over a partition of  $\gamma$  enjoying the following two properties:

- (A1)  $\{\psi_i\}_{i=1}^m$  are orthonormal in the  $L^2(\gamma)$ -scalar product;
- (A2) the projection  $P\mu$  of  $\mu \in \Lambda_H(\gamma)$  is realized by projecting the coordinates of  $\mu$  with respect to  $\{\psi_i\}_{i=1}^m$  onto  $\mathbb{R}_+$ , i.e.,

$$\sigma = P(\mu) \iff \sigma_i = \max\{0, \mu_i\}, \quad i = 1, \dots, m,$$

where  $\mu = \sum_{i=1}^m \mu_i \psi_i, \sigma = \sum_{i=1}^m \sigma_i \psi_i$ .

We define:

$$g_H := \sum_{i=1}^m g_i \psi_i, \quad g_i = (\psi_i, g)_{0,\gamma}, \tag{4.1}$$

$$\tau_H \hat{u}_h := \sum_{i=1}^m \mu_i \psi_i, \quad \mu_i = (\psi_i, \hat{u}_h)_{0,\gamma}, \tag{4.2}$$

$$\delta_H \hat{u}_h := \sum_{i=1}^m \sigma_i \psi_i, \quad \sigma_i = (\psi_i, \delta_h \hat{u}_h)_{0,\gamma}, \tag{4.3}$$

i.e.  $g_H, \tau_H \hat{u}_h$  and  $\delta_H \hat{u}_h$  are the orthogonal projections of  $g, \hat{u}_h|_\gamma$  and  $\delta_h \hat{u}_h$  onto  $\Lambda_H(\gamma)$ , respectively. Here,  $\delta_h \hat{u}_h$  denotes an approximation of the normal derivative of  $\hat{u}_h$  on  $\gamma$  defined directly from the finite element solution  $\hat{u}_h$ .

We first describe how to define  $\delta_h \hat{u}_h$  when the smooth variant is used. The gradient  $\nabla \hat{u}_h$  is discontinuous on the interelement boundaries and the scalar product  $\nabla \hat{u}_h|_\gamma \cdot n_\gamma$  does not give a good approximation of the normal derivative. For this reason  $\nabla \hat{u}_h$  will be replaced by a suitable approximation from  $V_h \times V_h$ :

$$\tilde{\nabla} \hat{u}_h := \sum_{j=1}^n (\tilde{\nabla} \hat{u}_h)_j \varphi_j, \quad (\tilde{\nabla} \hat{u}_h)_j = \sum_{k \in \mathcal{K}} \alpha^{(k)} u_{j+k}, \tag{4.4}$$

where  $\alpha^{(k)} \in \mathbb{R}^2$  are appropriately chosen parameters and  $u_{j+k}$  denote the nodal values of  $\hat{u}_h$  at the nodes specified by the index set  $\mathcal{K}$ . A possible way how to choose  $\alpha^{(k)}$  is based on averaging of gradients. For some types of finite elements (linear, bilinear, e.g.) and for specific values of  $\alpha^{(k)}, k \in \mathcal{K}$ , it is known that  $\tilde{\nabla} \hat{u}_h$  approximates  $\nabla \hat{u}$  with a higher order of accuracy than  $\nabla \hat{u}_h$  itself; see [15]. Thus one can hope that the scalar product

$$\delta_h \hat{u}_h = \tilde{\nabla} \hat{u}_h|_\gamma \cdot n_\gamma$$

leads to a better approximation of the normal derivative. Numerical tests confirm this expectation even though the theoretical justification (to our knowledge) is not yet done.

Unfortunately, the previous construction can not be used for the non-smooth variant. In this case we introduce  $\delta_h \hat{u}_h$  as a piecewise linear function on (an approximation of)  $\gamma$  which is defined by the values  $\delta_h \hat{u}_h(x_k)$ , where  $x_k, k \in \mathcal{K}$ , are the intersections of  $\gamma$  with the finite element mesh on  $\bar{\Omega}$ . At each  $x_k, \delta_h \hat{u}_h(x_k)$  is given by the following second order differentiation formula:

$$\delta_h \hat{u}_h(x_k) = \frac{5\hat{u}_h(x_k - hn_\gamma) - 8\hat{u}_h(x_k - 2hn_\gamma) + 3\hat{u}_h(x_k - 3hn_\gamma)}{2h}, \quad k \in \mathcal{K}.$$

Inserting (4.1), (4.2) and (4.3) into the second equation in  $\hat{\mathcal{P}}(\Gamma)_h^H$  and using (A2), we obtain

$$(\psi_i, \delta_h \hat{u}_h)_{0,\gamma} = \max\{0, (\psi_i, \delta_h \hat{u}_h)_{0,\gamma} - \rho((\psi_i, \hat{u}_h)_{0,\gamma} - g_i)\}, \quad i = 1, \dots, m. \tag{4.5}$$

Since  $\hat{u}_h = \sum_{j=1}^n u_j \varphi_j$ , (4.5) can be written as

$$C_{\gamma,i} \vec{u} = \max\{0, C_{\gamma,i} \vec{u} - \rho(B_{\gamma,i} \vec{u} - g_i)\}, \quad i = 1, \dots, m,$$

where  $\vec{u} = (u_1, \dots, u_n)^\top$ ,  $C_{\gamma,i}$  and  $B_{\gamma,i}$  is the  $i$ th row of  $C_\gamma \in \mathbb{R}^{m \times n}$  and  $B_\gamma \in \mathbb{R}^{m \times n}$  with the entries

$$c_{\gamma,ij} = (\psi_i, \delta_h \hat{u}_h)_{0,\gamma}, \quad b_{\gamma,ij} = (\psi_i, \varphi_j)_{0,\gamma}, \quad i = 1, \dots, m, \quad j = 1, \dots, n,$$

respectively.

Finally, we arrive at the following algebraic representation of  $\hat{\mathcal{P}}(\Gamma)_h^H$ :

$$\left. \begin{aligned} & \text{Find } (\vec{u}, \vec{\lambda}) \in \mathbb{R}^n \times \mathbb{R}^m \text{ such that} \\ & A\vec{u} = \vec{f} + B_\Gamma^\top \vec{\lambda}, \\ & C_\gamma \vec{u} = \max\{0, C_\gamma \vec{u} - \rho(B_\gamma \vec{u} - g)\} \end{aligned} \right\} \tag{4.6}$$

Here the entries of  $\vec{\lambda} \in \mathbb{R}^m$  are the coordinates of  $\lambda_H \in \Lambda_H(\Gamma)$  with respect to  $\{\tilde{\psi}_i\}_{i=1}^m$ ,  $A \in \mathbb{R}^{n \times n}$  denotes the standard stiffness matrix,  $B_\Gamma \in \mathbb{R}^{m \times n}$  is defined analogously to  $B_\gamma$  replacing  $\gamma$  by  $\Gamma$ ,  $\vec{f} \in \mathbb{R}^n$  has components  $f_j = (f, \varphi_j)_{0,\Omega}$  and  $\vec{g} = (g_1, \dots, g_m)^\top$ . Let us note that the max-function in (4.6) is understood componentwisely.

### 5 Description of the algorithm

We will use the Newton-type method for numerical realization of (4.6). For this reason, we express our problem in the form of one equation. To simplify the presentation, the arrow over vectors will be omitted.

Let  $F : \mathbb{R}^{n+m} \mapsto \mathbb{R}^{n+m}$  be the function defined by

$$F(y) := \begin{pmatrix} Au - B_\Gamma^\top \lambda - f \\ G(u) \end{pmatrix}, \quad y := \begin{pmatrix} u \\ \lambda \end{pmatrix}, \tag{5.1}$$

where  $G(u) := C_\gamma u - \max\{0, C_\gamma u - \rho(B_\gamma u - g)\}$ . Then (4.6) can be written as

$$F(y) = 0. \tag{5.2}$$

This is a non-smooth equation due to the presence of the max-function. Fortunately,  $F$  is a  $PC^1$ -function and (5.2) can be solved by the following piecewise smooth Newton method [4]:

$$\left. \begin{array}{l} y^0 \in \mathbb{R}^{n+m} \text{ given, } k = 0; \\ \text{Find } d^k \in \mathbb{R}^{n+m} : F(y^k) + F^o(y^k)d^k = 0; \\ \text{set } y^{k+1} = y^k + d^k, k := k + 1, \\ \text{until stopping criterion.} \end{array} \right\} \tag{5.3}$$

Here  $F^o(y)$  plays the role of the Jacobian in the smooth Newton method. Taking into account the definition of the non-smooth term, it holds:

$$F^o(y) = \begin{pmatrix} A & -B_\Gamma^\top \\ G^o(u) & 0 \end{pmatrix},$$

where the  $i$ th row of  $G^o(u) \in \mathbb{R}^{m \times n}$  is given by

$$G_i^o(u) = C_{\gamma,i} - s(C_{\gamma,i}u - \rho(B_{\gamma,i}u - g_i)) (C_{\gamma,i} - \rho B_{\gamma,i}), \quad i = 1, \dots, m$$

with  $s : \mathbb{R} \mapsto \mathbb{R}$  defined by

$$s(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases}$$

Let us note that  $s$  is the so-called slanting function to the max-function [3, 11]. A more convenient setting of  $G^o$  uses an active set terminology.

Let  $\mathcal{M} := \{1, 2, \dots, m\}$ . We define the sets of *inactive* and *active* indices at  $y = (u^\top, \lambda^\top)^\top \in \mathbb{R}^{n+m}$  by

$$\begin{aligned} \mathcal{I}(u) &:= \{i \in \mathcal{M} : C_{\gamma,i}u - \rho(B_{\gamma,i}u - g_i) \leq 0\}, \\ \mathcal{A}(u) &:= \{i \in \mathcal{M} : C_{\gamma,i}u - \rho(B_{\gamma,i}u - g_i) > 0\}. \end{aligned}$$

It is readily seen that

$$G_i^o(u) = \begin{cases} C_{\gamma,i}, & i \in \mathcal{I}(u), \\ \rho B_{\gamma,i}, & i \in \mathcal{A}(u). \end{cases}$$

Let  $D(\mathcal{S})$  denote the diagonal matrix defined for  $\mathcal{S} \subseteq \mathcal{M}$  by

$$D(\mathcal{S}) = \text{diag}(s_1, \dots, s_m) \quad \text{with} \quad s_i = \begin{cases} 1, & i \in \mathcal{S}, \\ 0, & i \notin \mathcal{S}. \end{cases}$$

Using this notation, we obtain

$$G^o(u) = D(\mathcal{I}(u))C_\gamma + \rho D(\mathcal{A}(u))B_\gamma.$$

The Newton method (5.3) applied to (5.2) leads to the following active-set type algorithm, where  $u^0 \in \mathbb{R}^n$ ,  $\lambda^0 \in \mathbb{R}^m$  and  $\varepsilon_u > 0$  are given.

**Algorithm**  $ActiveSet[A, B_\gamma, C_\gamma, B_\Gamma, f, g, u^0, \lambda^0, \varepsilon_u] \rightarrow (u, \lambda)$

- (0) Set  $k := 0$  and choose  $\rho > 0$ .
- (1) Define the inactive and active sets:  $\mathcal{I}^k := \mathcal{I}(u^k)$ ,  $\mathcal{A}^k := \mathcal{A}(u^k)$ .
- (2) Solve:

$$\begin{pmatrix} A & -B_\Gamma^\top \\ D(\mathcal{I}^k)C_\gamma + \rho D(\mathcal{A}^k)B_\gamma & 0 \end{pmatrix} \begin{pmatrix} u^{k+1} \\ \lambda^{k+1} \end{pmatrix} = \begin{pmatrix} f \\ \rho D(\mathcal{A}^k)g \end{pmatrix}.$$

- (3) Set  $\text{err}^{(k)} := \|u^{k+1} - u^k\| / \|u^{k+1}\|$ . If  $\text{err}^{(k)} \leq \varepsilon_u$ , return  $u := u^{k+1}$ ,  $\lambda := \lambda^{k+1}$ .
- (4) Set  $k := k + 1$  and go to step (1).

We see that each iterative step (2) leads to a linear system arising from a finite element discretization of the fictitious domain formulation of a mixed Dirichlet–Neumann boundary value problem. It is also readily seen that  $\rho$  can be discarded from this system. Indeed, if the systems in step (2) were solved exactly then  $\rho$  would not play any role in the definitions of  $\mathcal{I}^k$  and  $\mathcal{A}^k$  for  $k \geq 1$  since always either  $C_{\gamma,i}u^k = 0$  or  $B_{\gamma,i}u^k - g_i = 0$ . Moreover, an appropriate choice of the initial iterate  $u^0$  (giving only the Dirichlet boundary condition on  $\gamma$ , e.g.) makes it possible to discard  $\rho$  completely from the algorithm.

The efficiency of the algorithm  $ActiveSet$  depends on how efficiently the following non-symmetric saddle-point like problems can be solved:

$$\begin{pmatrix} A & B_1^\top \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ h \end{pmatrix}. \tag{5.4}$$

As methods developed directly for such systems are rare, we recall main ideas of the *projected Schur complement method* presented in [10]. It combines the Schur complement reduction with the null-space method implemented by orthogonal projectors.

For  $B \in \mathbb{R}^{m \times n}$  we denote  $\mathbb{N}(B)$  the null-space and  $\mathbb{R}(B|\mathbb{V})$  the range-space of  $B$  on a subspace  $\mathbb{V} \subseteq \mathbb{R}^n$ . If  $\mathbb{V} = \mathbb{R}^n$ , we simply write  $\mathbb{R}(B) := \mathbb{R}(B|\mathbb{R}^n)$ . The system (5.4) has a unique solution iff [10]

$$\mathbb{N}(B_1^\top) = \{0\}, \tag{5.5}$$

$$\mathbb{N}(A) \cap \mathbb{N}(B_2) = \{0\}, \tag{5.6}$$

$$\mathbb{R}(A|\mathbb{N}(B_2)) \cap \mathbb{R}(B_1^\top) = \{0\}. \tag{5.7}$$

*Remark 5.1* We should prove that each system obtained in step (2) of the algorithm *ActiveSet* satisfies (5.5)–(5.7) being equivalent to the non-singularity of  $F^o(y)$ . It is readily seen that (5.5) is equivalent to the following condition:

$$(\mu_H, v_h)_{0,\Gamma} = 0 \quad \forall v_h \in V_h \Rightarrow \mu_H = 0 \text{ on } \Gamma. \tag{5.8}$$

To satisfy (5.8) it is sufficient to take the ratio  $H/h$  sufficiently large. Condition (5.6) is trivially satisfied whenever  $A$  is non-singular. If  $A$  is the stiffness matrix on the space  $V_h \subset H_{\text{per}}^1(\Omega)$  for the differential operator  $-\Delta u$  (i.e. without the absolute term) then  $\mathbb{N}(A) = \{(1, \dots, 1)^\top\}$  and (5.6) is satisfied for  $\mathcal{A}(u) \neq \emptyset$ . Unfortunately, (5.7) is not easy to verify in a general case. If  $\mathcal{A}(u) = \mathcal{M}$  and (5.8) holds then (5.7) is satisfied provided that  $\Gamma$  is a small perturbation of  $\gamma$  [10].

The block  $A$  in (5.4) corresponds to the stiffness matrix computed by the  $H^1(\Omega)$ -scalar product on  $V_h$  in our case, hence  $A$  is non-singular. On the other hand there are situations when  $A$  is singular (in numerical experiments we shall use  $V_h \subset H_{\text{per}}^1(\Omega)$  and the differential operator in (2.1) without the absolute term  $u$ , e.g.). For this reason we confine ourselves to this more complicated case. The modification for  $A$  regular is straightforward.

Suppose that  $A$  is singular with the defect  $l = \dim \mathbb{N}(A)$ ,  $l \geq 1$  and consider  $N_1 \in \mathbb{R}^{n \times l}$  and  $N_2 \in \mathbb{R}^{n \times l}$  whose columns span the null-space  $\mathbb{N}(A)$  and  $\mathbb{N}(A^\top)$ , respectively. Finally denote by  $A^\dagger$  a generalized inverse to  $A$ . In what follows we shall consider an arbitrary but fixed selections of  $A^\dagger$ ,  $N_1$  and  $N_2$ .

**Theorem 5.1** [10] *Let (5.5)–(5.7) hold. Then the second component  $\lambda$  of a solution to (5.4) is the first component of a solution to*

$$\begin{pmatrix} B_2 A^\dagger B_1^\top - B_2 N_1 & \\ -N_2^\top B_1^\top & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha \end{pmatrix} = \begin{pmatrix} B_2 A^\dagger f - h \\ -N_2^\top f \end{pmatrix}. \tag{5.9}$$

The first component  $u$  is given by the formulae

$$u = A^\dagger(f - B_1^\top \lambda) + N_1 \alpha.$$

The matrix in (5.9) is the (negative) *generalized Schur complement*. Let us note that (5.9) is formally the same saddle-point system as (5.4) but its size is considerably smaller. We shall solve (5.9) using two orthogonal projectors

$$P_1 := I - G_1^\top(G_1 G_1^\top)^{-1}G_1, \quad P_2 := I - G_2^\top(G_2 G_2^\top)^{-1}G_2,$$

on  $\mathbb{N}(G_1)$ ,  $\mathbb{N}(G_2)$ , where  $G_1 := -N_1^\top B_2^\top$ ,  $G_2 := -N_2^\top B_1^\top$ , respectively. In order to simplify the next presentation we denote  $S := B_2 A^\dagger B_1^\top$ ,  $d := B_2 A^\dagger f - h$  and  $e := -N_2^\top f$ .

**Theorem 5.2** [10] *Let (5.5)–(5.7) hold. Then  $\lambda$  is the first component of a solution to (5.9) iff  $\lambda = \lambda_{\mathbb{N}} + \lambda_{\mathbb{R}}$ , where  $\lambda_{\mathbb{N}} \in \mathbb{N}(G_2)$ ,  $\lambda_{\mathbb{R}} \in \mathbb{R}(G_2^\top)$  solve*

$$\lambda_{\mathbb{R}} = G_2^\top (G_2 G_2^\top)^{-1} e$$

and

$$P_1 S \lambda_{\mathbb{N}} = P_1 (d - S \lambda_{\mathbb{R}}). \quad (5.10)$$

The second component  $\alpha$  is given by

$$\alpha = (G_1 G_1^\top)^{-1} G_1 (d - S \lambda).$$

The last theorem enables us to find the solution to (5.9) by the separate computations of  $\lambda_{\mathbb{R}}$ ,  $\lambda_{\mathbb{N}}$  and  $\alpha$ . The heart of this strategy consists in solving the equation (5.10). We employ the projected BiCGSTAB method derived in [10] from its non-projected version [14].

In the  $k$ th step of the algorithm *ActiveSet*, the initial BiCGSTAB iterate uses the result from the previous Newton step, i.e.  $P_2 \lambda^k$ , and, in addition, an adaptive terminating tolerance  $\varepsilon_\lambda := \varepsilon_\lambda^{(k)}$  is chosen. The idea consists in respecting the precision  $\text{err}^{(k-1)}$  achieved in the previous Newton step. If the progress is not sufficiently large then the tolerance is reduced independently on  $\text{err}^{(k-1)}$  as follows:

$$\varepsilon_\lambda^{(k)} := \min\{\varepsilon_{\min} \times \text{err}^{(k-1)}, c_{\text{fact}} \times \varepsilon_\lambda^{(k-1)}\} \quad (5.11)$$

with  $0 < \varepsilon_{\min} < 1$ ,  $0 < c_{\text{fact}} < 1$ ,  $\text{err}^{(0)} = 2$  and  $\varepsilon_\lambda^{(0)} = \varepsilon_{\min}/c_{\text{fact}}$  (typically  $\varepsilon_{\min} = 10^{-2}$  and  $c_{\text{fact}} = 0.2$ ).

It should be noted that Theorem 5.2 generalizes ideas of the FETI domain decomposition method [5]. Another interpretation of this approach is the non-symmetric variant of the null-space method [1] applied to (5.9).

In the rest of this section, we will show how to accelerate both the Newton and BiCGSTAB iterations. As the fictitious domain  $\Omega$  has a simple geometry, it is easy to define a multilevel family of nested partitions and the corresponding spaces  $V_{h_j}$  with stepsizes  $h_j$ ,  $0 \leq j \leq J$ ,  $h_{j+1} < h_j$  ( $h_{j+1} = h_j/2$  e.g.). In order to accelerate iterations on the finest  $J$ th level, one can apply the hierarchical multigrid scheme called *nested iterations* [12], which is formulated below. Let us note that the index  $j$  refers to the  $j$ th level.

The computation starts on the coarsest level,  $j = 0$ , with the initial iterate  $(u^{0,(0)}, \lambda^{0,(0)})$  arbitrarily chosen ( $(0, 0)$  e.g.). The initial iterate on each subsequent level is determined as the prolonged result from the nearest lower level. The terminating tolerance  $\varepsilon_u = \varepsilon_u^{(j)}$  on the  $j$ th level is set proportionally to an expected discretization error that is  $\varepsilon_u^{(j)} := \nu h_j^p$  and  $\text{err}^{(0)} := \nu_1 h_j^p$  in (5.11), where  $p$  is an expected convergence rate (in the  $L^2(\omega)$ -norm) and  $0 < \nu < \nu_1$  are control parameters. The result obtained with such  $\varepsilon_u$  can be viewed as an inexact solution of the discretized problem (4.6) with the same convergence rate as the exact one.



**Algorithm**  $HMS[J, h_0, \dots, h_J, v, p]$

- (0) Set  $j := 0$  and choose  $u^{0,(0)}, \lambda^{0,(0)}$ .
- (1) If  $j > 0$  prolongate  $(u^{(j-1)}, \lambda^{(j-1)}) \rightarrow (u^{0,(j)}, \lambda^{0,(j)})$ .
- (2)  $ActiveSet[A^{(j)}, B_\gamma^{(j)}, C_\gamma^{(j)}, B_\Gamma^{(j)}, f^{(j)}, g^{(j)}, u^{0,(j)}, \lambda^{0,(j)}, v h_j^p] \rightarrow (u^{(j)}, \lambda^{(j)})$
- (3) If  $j = J$  return  $u := u^{(J)}$ .
- (4) Set  $j := j + 1$  and go to step (1).

**6 Numerical examples**

We will assess experimentally two aspects analyzed in the article. Firstly, we will illustrate the higher accuracy and improved convergence properties of the fictitious domain method with  $\gamma \not\equiv \Gamma$  compared to this one with  $\gamma \equiv \Gamma$ . Secondly, we shall demonstrate the computational efficiency of the algorithm *ActiveSet* combined with the projected Schur complement method.

We solve three model examples with the same geometry (see Fig. 3):

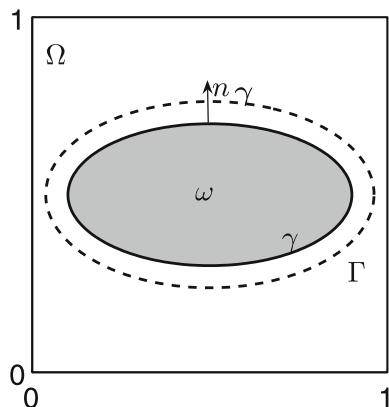
$$\omega = \{(x, y) \in \mathbb{R}^2 \mid (x - 0.5)^2/0.4^2 + (y - 0.5)^2/0.2^2 < 1\},$$

$$\Omega = (0, 1) \times (0, 1).$$

We replace  $H_0^1(\Omega)$  by  $H_{per}^1(\Omega)$  in the fictitious domain formulation  $\hat{\mathcal{P}}(\Gamma)$ . As mentioned before the theoretical results of Sect. 3 remain valid also in this case. The advantage of this new choice consists in the fact that the resulting stiffness matrix  $A$  in (4.6) has a block circulant structure which allows us to use the highly efficient Poisson like solver [13] based on the discrete Fourier transform.

The space  $V_h$  consists of piecewise bilinear functions constructed over a uniform rectangulation of  $\bar{\Omega}$ . Further,  $\Lambda_H(\gamma)$  and  $\Lambda_H(\Gamma)$  are given by piecewise constant functions on partitions of polygonal approximations of  $\gamma$  and  $\Gamma$ , respectively. The stepsizes  $H$  on  $\gamma$  and  $\Gamma$  are chosen in such a way that the condition (5.5) and  $\dim \Lambda_H(\gamma) = \dim \Lambda_H(\Gamma)$  are satisfied.

**Fig. 3** Geometry of  $\omega$



The nodal gradient value  $(\tilde{\nabla}\hat{u}_h)_j$  used in (4.4) for the smooth variant is defined as the arithmetic mean of the gradient values of the finite element solution at the common  $j$ th node [15].

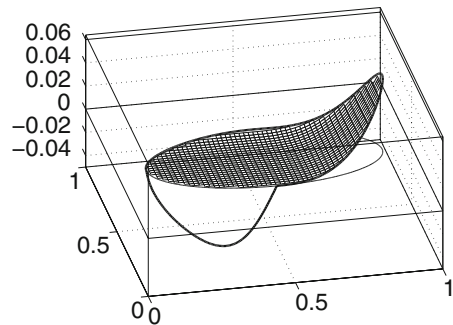
In Tables below we report the number of primal variables ( $n$ ), the number of indices in the active ( $m_{\mathcal{A}} = |\mathcal{A}|$ ) and inactive ( $m_{\mathcal{I}} = |\mathcal{I}|$ ) set, the number of the outer (Newton) iterations, the total number of the inner (BiCGSTAB) iterations, the computational time and the relative errors of approximate solutions in the indicated norms (the comparisons are done with respect to the exact solution  $u_{ex}$  (Example 6.1) or to the reference solution  $u_{ref}$  (Examples 6.2 and 6.3) computed by the smooth variant on the fine mesh with  $h = 1/8,192$  which corresponds to the system with more than 67 millions of equations). From the errors, we determine the convergence rates of our fictitious domain approaches. The terminating tolerance in the algorithm *ActiveSet* is  $\varepsilon_u = 10^{-5}$ .

*Example 6.1 (smooth solution, one contact zone)* Let us consider problem (2.1) with the exact solution

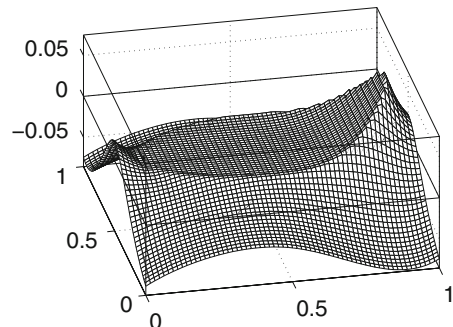
$$u_{ex}(x, y) = ((x - 0.5)^+)^3 + 0.5((y - 0.5)^+)^3, \quad (x, y) \in \mathbb{R}^2,$$

i.e. the right-hand side  $f$  is given by  $f = -\Delta u_{ex} + u_{ex}$  in  $\mathbb{R}^2$  and the obstacle  $g$  is defined by  $g|_{\gamma_1} = u_{ex}|_{\gamma_1}$  on  $\gamma_1$ ,  $\gamma_1 = \gamma \setminus \bar{\gamma}_2$ ,  $\gamma_2 = \{(x, y) \in \gamma \mid x < 0.5, y < 0.5\}$ , and by  $g(x, y) = \sin(-2\varphi)$  for  $(x, y) \in \gamma_2$ , where  $(\varphi, r)$  is the polar coordinate of the point  $(x - 0.5, y - 0.5)$  (see Figs. 3, 4). The computed

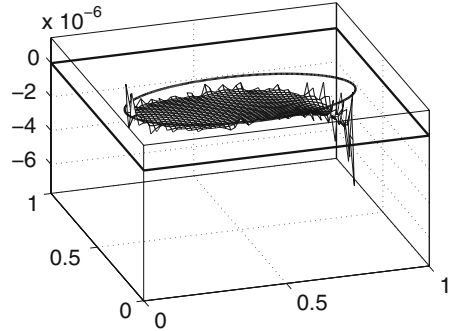
**Fig. 4** Ex. solution  $u_{ex}$



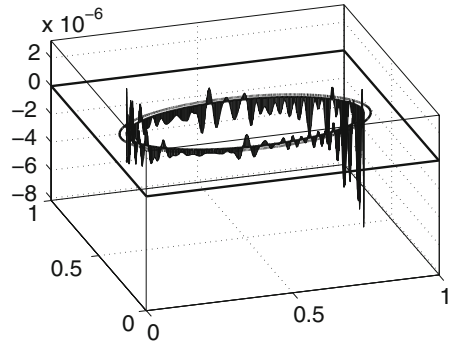
**Fig. 5** Comp. sol.  $\hat{u}_h$



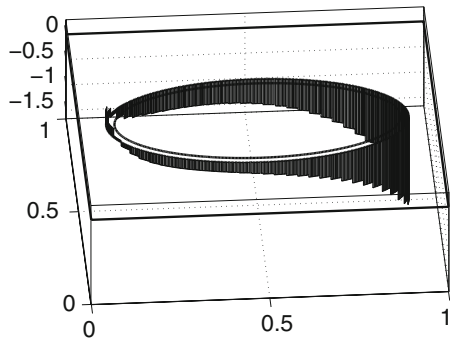
**Fig. 6** Differ.  $\hat{u}_h - u_{ex}$  in  $\omega$



**Fig. 7** Differ.  $\hat{u}_h - u_{ex}$  on  $\gamma$



**Fig. 8** Control variable  $\lambda_H$  on  $\Gamma$



solution by the smooth variant is shown in Fig. 5. Differences between the numerical and exact solutions inside  $\omega$  and on the boundary  $\gamma$  are depicted in Figs. 6 and 7, respectively. Finally, the corresponding control variable  $\lambda_H$  on  $\Gamma$  is shown in Fig. 8. Tables 1 and 2 summarize the results of the non-smooth and smooth fictitious domain formulation, respectively. The boundary  $\Gamma$  for the smooth variant is constructed by shifting  $\gamma$  six  $h$  units in the direction of the outward normal vector  $n_\gamma$  and  $H/h = |\log_2(h)|$ . The computed relative errors and the convergence rates confirm the prediction of Sect. 3. Table 3 illustrates the acceleration of convergence as well as saving of the computational time when the nested iterations

**Table 1** Non-smooth fictitious domain formulation ( $\gamma \equiv \Gamma$ )

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{T}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/24/10	5/24	0.31	4.1007e-02	3.3325e+00	1.7029e-02
1/256	66,049/41/21	6/45	1.81	2.0074e-02	2.3310e+00	8.5208e-03
1/512	263,169/77/33	7/69	13.07	9.7866e-03	1.6275e+00	4.2527e-03
1/1,024	1,050,625/140/58	7/93	74.65	4.8435e-03	1.1449e+00	2.0830e-03
1/2,048	4,198,401/261/99	7/115	432.6	2.2777e-03	7.8540e-01	1.0952e-03
1/4,096	16,785,409/484/178	8/131	2,328	1.1353e-03	5.5449e-01	7.2174e-04
Convergence rates:				1.0374	0.5186	0.9346

**Table 2** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ )

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{T}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/26/8	5/48	0.47	3.2409e-04	2.9532e-01	5.0704e-04
1/256	66,049/46/16	5/69	2.56	6.3196e-05	1.3041e-01	9.1074e-05
1/512	263,169/81/29	5/112	20.89	1.5917e-05	6.5444e-02	2.6525e-05
1/1,024	1,050,625/147/51	7/162	150.6	4.3527e-06	3.4223e-02	1.1771e-05
1/2,048	4,198,401/270/90	6/190	674.1	1.3812e-06	1.9278e-02	5.1861e-06
1/4,096	16,785,409/494/168	9/296	5,000	8.0760e-07	1.4741e-02	2.2854e-06
Convergence rates:				1.7617	0.8809	1.5012

**Table 3** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ ) with nested iterations

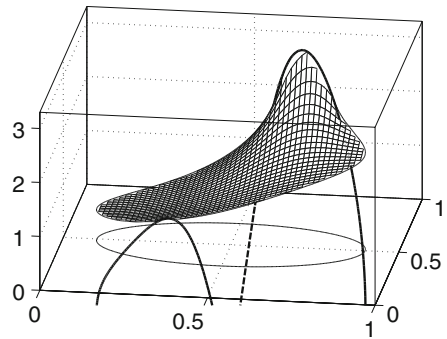
Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{T}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/28/8	4/30	0.55	2.9459e-04	2.8156e-01	3.1239e-04
1/256	66,049/48/16	4/56	2.45	6.2674e-05	1.2987e-01	6.9933e-05
1/512	263,169/84/28	5/90	18.94	1.6119e-05	6.5858e-02	2.6928e-05
1/1,024	1,050,625/147/49	4/92	93.34	4.3720e-06	3.4299e-02	1.1827e-05
1/2,048	4,198,401/271/93	4/152	582.1	1.3465e-06	1.9035e-02	4.7873e-06
1/4,096	16,785,409/494/166	4/204	3,980	7.9822e-07	1.4655e-02	2.2902e-06
Convergence rates:				1.7469	0.8735	1.3786

are used. Finally, Table 4 illustrates a smoothing effect of  $\delta := \text{dist}(\gamma, \Gamma)$ . If  $\Gamma$  is shifted far enough from  $\gamma$  (expressed in multiples of  $h$ ), the smoothness of the computed solution increases inside  $\omega$  which in turn results in smaller discretization errors. On the other hand we shall show in the next examples that the condition number of  $P_1 B_2 A^\dagger B_1$  on  $\mathbb{N}(G_2)$  becomes larger for increasing  $\delta$ . The value  $\delta = 6h$  used in our examples (and found experimentally) turned out to be a good compromise.

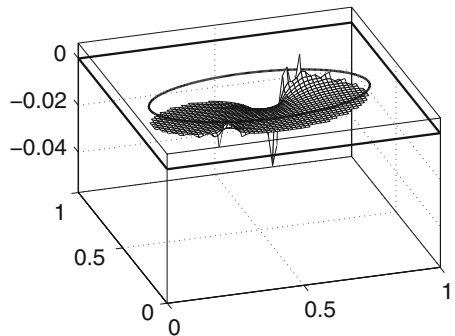
**Table 4** Dependence of the convergence rate on  $\delta := \text{dist}(\gamma, \Gamma)$ ,  $h = 1/256$

Param. $\delta$	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
0 $h$	66,049/41/21	6/45	1.81	2.0074e-02	2.3310e+00	8.5208e-03
2 $h$	66,049/44/18	5/42	1.68	1.6031e-03	6.5682e-01	1.4522e-03
4 $h$	66,049/46/16	5/56	2.06	8.8714e-05	1.5451e-01	1.6632e-04
6 $h$	66,049/46/16	5/69	2.56	6.3196e-05	1.3041e-01	9.1074e-05
8 $h$	66,049/46/16	5/101	3.62	6.0014e-05	1.2708e-01	5.1199e-05

**Fig. 9** Comp. sol.  $\hat{u}_h$

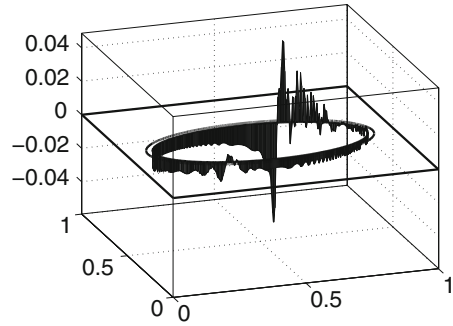


**Fig. 10** Differ.  $\hat{u}_h - u_{ref}$  in  $\omega$



*Example 6.2 (two contact zones)* We solve (2.1) with the right hand-side  $f = -10$  and the obstacle  $g$  given by  $g(x, y) = 5 \sin(2\varphi)(r^2 + r(\cos \varphi + \sin \varphi) + 0.5)^{1/2} - 1.5$  on  $\gamma$ , where  $(\varphi, r)$  is the polar coordinate of the point  $(x - 0.5, y - 0.5)$  (see Fig. 9). The behavior of  $\hat{u}_h - u_{ref}$  inside  $\omega$  and on the boundary  $\gamma$  is depicted in Figs. 10 and 11. Tables 5 and 6 summarize the results of the non-smooth and smooth fictitious domain formulation, respectively. The construction of  $\Gamma$  and the ratio  $H/h$  are as in Example 6.1 and also the conclusions are the same. Table 7 illustrates the acceleration of convergence and saving of the computational time when the nested iterations are used. As the behavior of solvers (BiCGSTAB, e.g.) depends on the condition number or in case of non-symmetric matrices on the normality declination, these characteristics for the matrix  $K := P_1 B_2 A^\dagger B_1$  on  $\mathbb{N}(G_2)$  during the Newton

**Fig. 11** Differ.  $\hat{u}_h - u_{\text{ref}}$  on  $\gamma$



**Table 5** Non-smooth fictitious domain formulation ( $\gamma \equiv \Gamma$ )

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/5/31	5/24	0.31	5.7782e-03	7.3554e-02	9.9305e-03
1/256	66,049/8/54	5/30	1.34	4.1129e-03	5.2790e-02	4.0288e-03
1/512	263,169/12/98	7/56	14.79	1.1455e-03	3.4829e-02	2.1000e-03
1/1,024	1,050,625/23/175	8/83	75.4	1.2240e-03	3.5068e-02	9.9925e-04
1/2,048	4,198,401/41/319	9/123	457.4	5.7576e-04	2.7780e-02	5.7557e-04
1/4,096	16,785,409/75/587	12/194	3,342	4.7758e-04	2.0726e-02	6.8034e-04
Convergence rates:				0.7542	0.3402	0.8237

**Table 6** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ )

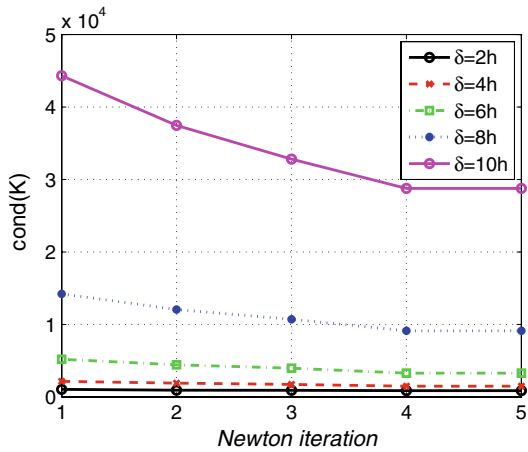
Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/5/31	5/62	0.63	1.5977e-02	1.4851e-01	1.6659e-02
1/256	66,049/8/54	6/80	3.17	3.6103e-03	8.1444e-02	4.7115e-03
1/512	263,169/13/97	7/149	25.24	3.2593e-03	4.4551e-02	3.7531e-03
1/1,024	1,050,625/23/175	8/207	195.8	3.2977e-04	1.0043e-02	4.6532e-04
1/2,048	4,198,401/41/319	9/294	1,075	6.9140e-05	3.8364e-03	9.7680e-05
1/4,096	16,785,409/75/587	10/393	6,509	9.1815e-06	1.5589e-03	3.2264e-05
Convergence rates:				2.1214	1.3784	1.8528

iterations are depicted, see Figs. 12 and 13 (for  $h = 1/256$  and different shifts  $\delta$ ). Each of these iterations corresponds to a mixed Dirichlet–Neumann problem. In all tests, one can see that these characteristics approach the respective value determined by the mixed Dirichlet–Neumann problem satisfied by the solution of the original unilateral problem. Finally, from Fig. 14 we see that the condition number of  $K$  increases if  $h$  tends to zero when  $\delta$  is fixed. For this reason  $\delta$  is not fixed but is taken as a function of  $h$ .

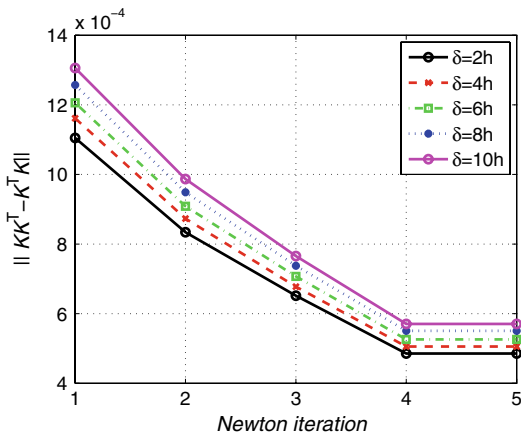
**Table 7** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ ) with nested iterations

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/5/31	4/29	0.53	1.5977e-02	1.4851e-01	1.6659e-02
1/256	66,049/8/56	4/38	1.87	5.4942e-03	8.4101e-02	6.7655e-03
1/512	263,169/13/99	3/43	10.86	8.7074e-04	3.5163e-02	1.4525e-03
1/1,024	1,050,625/23/177	3/59	64.47	1.6465e-04	7.4974e-03	2.5333e-04
1/2,048	4,198,401/41/319	3/78	366.9	6.9135e-05	3.8363e-03	9.7678e-05
1/4,096	16,785,409/76/588	3/118	2,526	2.4750e-05	2.1603e-03	2.8003e-05
1/8,192	67,125,249/140/1080	3/191	23,370	'ref'	'ref'	'ref'
Convergence rates:				1.9432	1.3174	1.9127

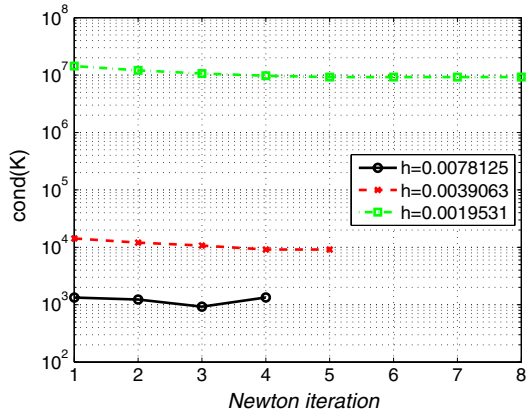
**Fig. 12** Condition number



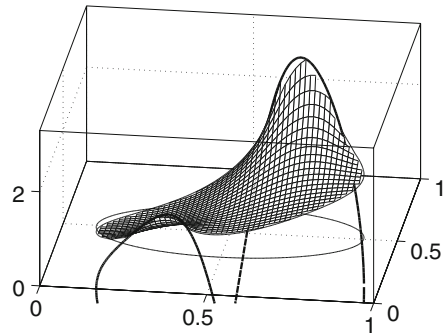
**Fig. 13** Normality declination



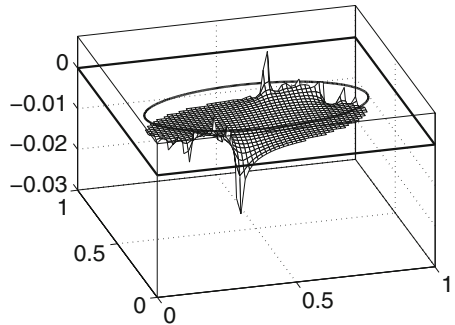
**Fig. 14** Condition number  
( $\delta = 1/32$ )



**Fig. 15** Comp. sol.  $\hat{u}_h$



**Fig. 16** Differ.  $\hat{u}_h - u_{ref}$  in  $\omega$



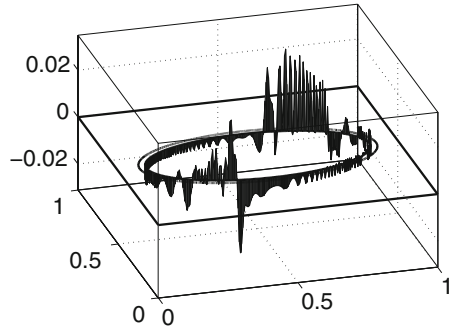
*Example 6.3* (*Example 6.2 without the absolute term  $u$* ) The equation in  $\omega$  now reads as follows:

$$\Delta u = 20 \text{ in } \omega.$$

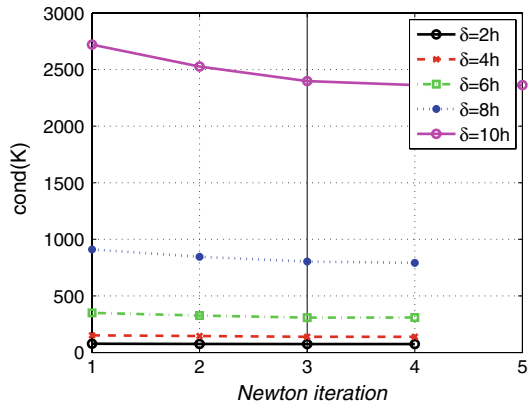
Other data are the same as in Example 6.2. The problem is semicoercive but due to the sign of the right hand-side, it has a unique solution  $u$ . The results are summarized in Figs. 15, 16, 17, 18, 19 and 20 and in Tables 8, 9 and 10. They are similar to those computed in Example 6.2.



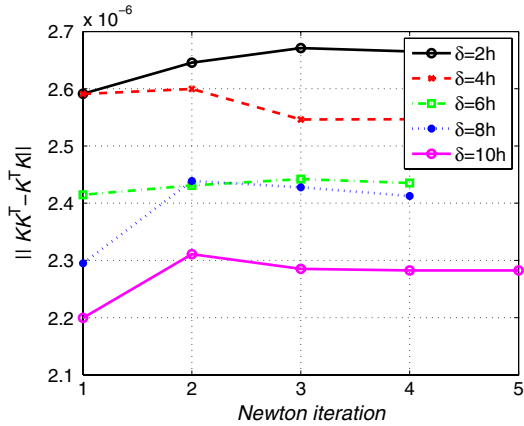
**Fig. 17** Differ.  $\hat{u}_h - u_{\text{ref}}$  on  $\gamma$



**Fig. 18** Condition number



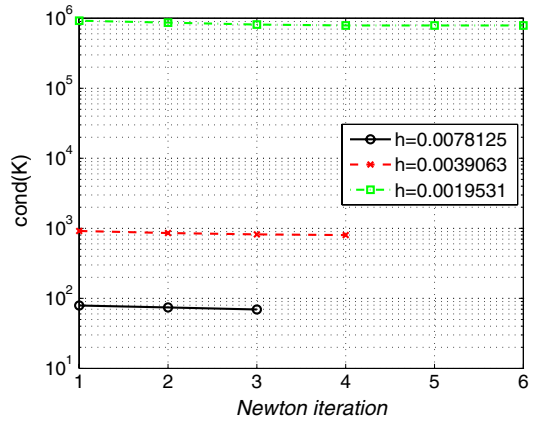
**Fig. 19** Normality declination



### 7 Conclusions and comments

Two variants of a fictitious domain formulation of unilateral boundary value problems are analyzed in this article. The first (non-smooth) approach enforces the satisfactions of unilateral boundary conditions by Lagrange multipliers defined on the boundary  $\gamma$

**Fig. 20** Condition number ( $\delta = 1/32$ )



**Table 8** Non-smooth fictitious domain formulation ( $\gamma \equiv \Gamma$ )

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	Out./ $\sum$ inn. its.	C.time (s)	$Err_{L^2(\omega)}$	$Err_{H^1(\omega)}$	$Err_{L^2(\gamma)}$
1/128	16,641/7/29	6/31	0.39	1.3521e-02	9.1807e-02	2.2136e-02
1/256	66,049/13/49	6/54	2.3	7.0716e-03	6.0371e-02	6.9435e-03
1/512	263,169/23/87	7/69	13.71	4.5768e-03	3.6564e-02	3.1013e-03
1/1,024	1,050,625/41/157	9/127	106.3	2.7119e-03	3.8892e-02	1.6530e-03
1/2,048	4,198,401/74/286	10/166	639.6	9.9011e-04	3.0425e-02	8.3333e-04
1/4,096	16,785,409/136/526	11/241	4,205	8.0521e-04	2.2513e-02	1.0264e-03
Convergence rates:				0.8461	0.3719	0.9211

**Table 9** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ )

Step $h$	$n/m_{\mathcal{A}}/m_{\mathcal{J}}$	Out./ $\sum$ inn. its.	C.time (s)	$Err_{L^2(\omega)}$	$Err_{H^1(\omega)}$	$Err_{L^2(\gamma)}$
1/128	16,641/7/29	4/44	0.48	3.3419e-02	1.6955e-01	3.4271e-02
1/256	66,049/14/48	5/86	3.58	6.5415e-03	8.8017e-02	7.9521e-03
1/512	263,169/23/87	6/119	23.35	2.6697e-03	4.0197e-02	2.8341e-03
1/1,024	1,050,625/41/157	7/221	174.9	3.2798e-04	8.3563e-03	4.7836e-04
1/2,048	4,198,401/74/286	7/276	976.6	1.5904e-04	4.5718e-03	2.1104e-04
1/4,096	16,785,409/136/526	9/442	7,544	2.0672e-05	1.7129e-03	4.8686e-05
Convergence rates:				2.0687	1.3775	1.8734

of the original domain  $\omega$ . Therefore the fictitious domain solution has a singularity on  $\gamma$  that can result in an intrinsic error of the computed solution. In the second (smooth) approach the singularity is moved away from  $\bar{\omega}$  so that the fictitious domain solution keeps the regularity of the original solution in  $\omega$ . Numerical experiments illustrate the efficiency of the smooth variant giving almost the same convergence rates as the classical Ritz–Galerkin method provided that the original solution is smooth enough. From the above examples we see that the numerical solution oscillates in a vicinity of

**Table 10** Smooth fictitious domain formulation ( $\gamma \neq \Gamma$ ) with nested iterations

Step $h$	$n/m \setminus m \mathcal{I}$	Out./ $\sum$ inn. its.	C.time (s)	$\text{Err}_{L^2(\omega)}$	$\text{Err}_{H^1(\omega)}$	$\text{Err}_{L^2(\gamma)}$
1/128	16,641/7/29	4/30	0.61	3.3413e-02	1.6954e-01	3.4267e-02
1/256	66,049/14/50	3/33	1.75	3.9598e-03	8.7142e-02	6.3479e-03
1/512	263,169/24/88	3/51	12.45	1.1261e-03	3.7856e-02	1.9881e-03
1/1,024	1,050,625/42/158	3/69	73.44	9.4370e-04	1.2378e-02	1.0656e-03
1/2,048	4,198,401/74/286	3/110	496.3	1.5906e-04	4.5720e-03	2.1105e-04
1/4,096	16,785,409/135/525	3/115	2,626	3.6853e-05	2.1328e-03	5.9375e-05
1/8,192	67,125,249/249/971	3/187	23,110	'ref'	'ref'	'ref'
Convergence rates:				1.8083	1.3124	1.7570

transition points where contact zones change into non-contact ones. It is worth noticing that the errors in Example 6.1 on the coarsest grid (16,641 of primal variables) used in the smooth approach are smaller than the ones on the finest grid (more than 16 millions of primal variables) in the non-smooth approach.

The algebraic system arising from a finite element discretization is represented by a system of piecewise affine functions. The structure of this system makes it possible to apply the semismooth Newton method in the outer iterative loop which is equivalent to an active-set strategy. Let us note that the computations benefit from the superlinear convergence rate of the semismooth Newton method [3, 11]. Each Newton step requires to solve a non-symmetric saddle-point system with a possibly singular diagonal block. To this end, we use the projected Schur complement method [10] employing the projected BiCGSTAB algorithm as the inner iterative loop. In order to accelerate iterations (outer and inner) a non-linear version of nested iterations is used [12]. This preconditioning technique links theoretical results on convergence rates of finite element discretizations with the terminating criterions for both Newton and BiCGSTAB methods. The numerical experiments demonstrate a higher efficiency of computations.

**Acknowledgments** Supported by the grant 201/07/0294 of the Grant Agency of the Czech Republic and by the Research Project MSM6198910027 of the Czech Ministry of Education. The second author acknowledges the support of the project IAA100750802 of the Grant Agency of the Czech Academy of Science.

## References

1. Benzi M, Golub GH, Liesen J (2005) Numerical solution of saddle point systems. *Acta Numer* 1–137
2. Brezis H (1972) Problèmes unilatéraux. *J Math Pure Appl* 51:1–168
3. Chen X, Nashed Z, Qi L (2000) Smoothing methods and semismooth methods for nondifferentiable operator equation. *SIAM J Numer Anal* 38:1200–1216
4. Facchinei F, Pang J-S (2003) Finite-dimensional variational inequalities and Complementarity problems. Springer, New York
5. Farhat C, Mandel J, Roux F (1994) Optimal convergence properties of the FETI domain decomposition method. *Comput Methods Appl Mech Eng* 115:365–385

6. Girault V, Glowinski R (1995) Error analysis of a fictitious domain method applied to a Dirichlet problem. *Jpn J Indust Appl Math* 12:487–514
7. Glowinski R, Pan T, Periaux J (1994) A fictitious domain method for Dirichlet problem and applications. *Comput Methods Appl Mech Eng* 111:283–303
8. Haslinger J, Klarbring A (1995) Fictitious domain/mixed finite element approach for a class of optimal shape design problems. *M2AN* 29: 815–834
9. Haslinger J, Kozubek T (2000) A fictitious domain approach for a class of Neumann boundary value problems with applications in shape optimization. *East-West J Numer Math* 8:1–26
10. Haslinger J, Kozubek T, Kučera R, Peichl G (2007) Projected Schur complement method for solving non-symmetric systems arising from a smooth fictitious domain approach. *Lin Algebra Appl* 14: 713–739
11. Ito K, Kunisch K (2003) Semi-smooth methods for variational inequalities of the first kind. *M2AN* 37:41–62
12. Kronsjö L, Dahlquist G (1972) On the design of nested iterations for elliptic difference equations. *BIT Numer Math* 12:63–71
13. Kučera R (2005) Complexity of an algorithm for solving saddle-point systems with singular blocks arising in wavelet-Galerkin discretizations. *Appl Math* 50:291–308
14. Van der Vorst HA (1992) BiCGSTAB: a fast and smoothly converging variant of BiCG for solution of nonsymmetric linear systems. *SIAM J Sci Statist Comput* 13:631–644
15. Zhu Q (1998) A survey of superconvergence techniques in finite element methods. *Lect Notes Pure Appl Math Ser* 196:287–302