Semi-Smooth Newton Method for Solving Unilateral Problems in Fictitious Domain Formulations

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1 Introduction

This contribution deals with the numerical solution of elliptic boundary value problems with unilateral boundary conditions using a fictitious domain method. Any fictitious domain formulation [2] extends the original problem defined in a domain ω to a new (fictitious) domain Ω with a simple geometry (e.g. a box) which contains $\overline{\omega}$. The main advantage consists in possibility to use a uniform mesh in Ω leading to a structured stiffness matrix. This enables us to apply highly efficient multiplying procedures [6].

Fictitious domain formulations of problems with the classical Dirichlet or Neumann boundary conditions lead after a finite element discretization typically to algebraic saddle-point systems. For their solution one can use the algorithm studied in [3] that combines the Schur complement reduction with the null-space method. The situation is not so easy for unilateral problems since their weak formulation contains a non-differentiable projection operator. Fortunately, a resulting algebraic representation is described by a system that is semi-smooth in the sense of [1] so that a generalized Newton method can be applied. This method has been already used in [5] for solving complementarity problems. In our case each Newton step relates to a mixed Dirichlet-Neumann problem and therefore the algorithm from [3] can be used for solving inner linear systems. Due to the *superlinear* convergence rate of the Newton iteration [1], the computations are only slightly more expensive than the solution of pure Dirichlet or Neumann problems.

In this paper we compare two variants of the fictitious domain method. The first one enforces unilateral conditions by Lagrange multipliers defined on the boundary γ of the original domain ω. Therefore the fictitious domain solution has a singularity on γ that can result in an intrinsic error of the computed solution. The second one uses an auxiliary boundary Γ located outside of $\overline{\omega}$ on which we introduce a new control variable in order to satisfy the conditions on γ. In the second approach the singularity is moved away from $\overline{\omega}$ so that the computed solution is smoother in ω. We shall experimentally show that the discretization H^1-error is significantly smaller in this case. For more details we refer to [4, 3].

2 Fictitious domain formulations

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

$$\left.\begin{array}{l} -\Delta u + u = f \quad \text{in } \omega, \\ u \geq g, \ \dfrac{\partial u}{\partial n_\gamma} \geq 0, \ \dfrac{\partial u}{\partial n_\gamma}(u-g) = 0 \quad \text{on } \gamma, \end{array}\right\} \tag{1}$$

where $f \in L^2_{loc}(\mathbb{R}^2)$, $g \in H^{1/2}(\gamma)$ are given functions and $\frac{\partial}{\partial n_\gamma}$ stands for the normal derivative of a function on γ. We assume a sufficiently regular (weak) solution to (1) so that $\frac{\partial u}{\partial n_\gamma} \in L^2_+(\gamma)$. Then the unilateral condition in (1) is equivalent to

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

onto $L^2_+(\gamma)$ and $\rho > 0$ is arbitrary but fixed.

Let us consider a bounded domain Ω having a simple shape such that $\overline{\omega} \subset \Omega$ and let us construct a closed curve $\Gamma \subset \Omega$ surrounding ω. Instead of (1), we propose to solve the extended problem in Ω called the *fictitious domain formulation*:

$$\left.\begin{array}{l} \textit{Find } (\hat{u}, \lambda) \in H^1_0(\Omega) \times H^{-1/2}(\Gamma) \textit{ such that} \\[2mm] (\hat{u}, v)_{1,\Omega} = (f, v)_{0,\Omega} + \langle \lambda, v \rangle_\Gamma \quad \forall v \in H^1_0(\Omega), \\[2mm] \dfrac{\partial \hat{u}_{|\omega}}{\partial n_\gamma} \in L^2(\gamma), \\[2mm] \dfrac{\partial \hat{u}_{|\omega}}{\partial n_\gamma} = P(\dfrac{\partial \hat{u}_{|\omega}}{\partial n_\gamma} - \rho(\hat{u}_{|\omega} - g)), \end{array}\right\} \qquad (2)$$

where $(\cdot\,,\cdot)_{k,\Omega}$ denotes the scalar product in $H^k(\Omega)$, $k \geq 0$ integer ($H^0(\Omega) := L^2(\Omega)$), and $\langle \cdot, \cdot \rangle_\Gamma$ is the duality pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$. We distinguish two cases: *(i)* the non-smooth variant of (2), if $\gamma \equiv \Gamma$; *(ii)* the smooth variant of (2), if $\mathrm{dist}(\gamma, \Gamma) > 0$. In both cases $u = \hat{u}_{|\omega}$ is the (weak) solution to (1), while $\hat{u}$ is the first component of the solution to (2) [4].

3 Semismooth Newton method

We shall use same notation for the discrete analogies of $\hat{u}$, λ, f and g. The algebraic problem resulting from a finite element discretization of (2) reads as follows:

$$F(y) = 0, \qquad (3)$$

where $F : \mathbb{R}^{n+m} \mapsto \mathbb{R}^{n+m}$ is defined by

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

$$G(\hat{u}) := C_\gamma \hat{u} - \max\{0, C_\gamma \hat{u} - \rho(B_\gamma \hat{u} - g)\}$$

and the max-function is understood componentwisely. Here, $A \in \mathbb{R}^{n \times n}$ denotes the standard stiffness matrix, $B_\gamma, B_\Gamma \in \mathbb{R}^{m \times n}$ are the Dirichlet trace matrices related to γ, Γ, respectively, $C_\gamma \in \mathbb{R}^{m \times n}$ is the Neumann trace matrix on γ and $f \in \mathbb{R}^n$, $g \in \mathbb{R}^m$.

The equation (3) is nonsmooth due to the presence of the max-function. Fortunately, it is semismooth in the sense of [1] and, therefore, the semismooth Newton method can be used. It is well-known that the Newton iterations converge superlinearly and that they are equivalent with an active-set type algorithm [5]. To this end we denote $\mathcal{M} := \{1, 2, \ldots, m\}$ and, for $\mathcal{S} \subseteq \mathcal{M}$, we define the diagonal matrix $D(\mathcal{S})$ by

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

Algorithm ASM (Active-Set Method)

(0) Set $k := 0$ and choose $\rho > 0$, $\varepsilon_u > 0$ ($\varepsilon_u = 10^{-5}$). Initialize $u^0 \in \mathbb{R}^n$ and $\lambda^0 \in \mathbb{R}^m$.
(1) Define the inactive and active sets by:

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

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

This algorithm has the finite terminating property provided that all linear systems in the step (2) are solved exactly. Numerical experiments however show that an inexact implementation is more efficient. In order to maintain the finite terminating property, we drive the precision control in solving inner linear systems adaptively [4].

4 Numerical experiments

We illustrate the efficiency of the presented method on the slightly modified problem:

$$\left.\begin{aligned} & -\Delta u = 0 \quad \text{in } \omega, \\ & u = g_d \ \text{ on } \gamma_d, \ \frac{\partial u}{\partial n_\gamma} = 0 \ \text{ on } \gamma_0, \ \frac{\partial u}{\partial n_\gamma} = g_n \ \text{ on } \gamma_n, \\ & u \geq g, \ \frac{\partial u}{\partial n_\gamma} \geq 0, \ \frac{\partial u}{\partial n_\gamma}(u - g) = 0 \quad \text{on } \gamma_c, \end{aligned}\right\} \tag{4}$$

with $\omega = \{(x, y) \in \mathbb{R}^2 | (x-0.5)^2/0.4^2 + (y-0.5)^2/0.2^2 < 1\}$, $\gamma = \gamma_d \cup \gamma_0 \cup \gamma_n \cup \gamma_c$, $g_d = 2\sin(2\varphi)$, $g_n = -10$ and $g = 5\sin(2\varphi)(r^2 + r(\cos\varphi + \sin\varphi) + 0.5)^{1/2} - 1.5$, where (φ, r) denotes the polar coordinate. In the fictitious domain formulation we take $\Omega = (0, 1) \times (0, 1)$; see Figures 1, 2. Our discretization is based on the piecewise bilinear approximation of u over a uniform rectangulation of Ω with a stepsize h and on the piecewise constant approximation of the normal derivative, the Lagrange multiplier and the control variable, respectively, over partitions of γ, Γ with a stepsize H. The curve Γ is constructed by shifting γ three h units in the direction of the outward normal vector n_γ and $H/h = 5$.

In Tables 1, 2 we report the number of primal variables (n), the number of active ($m_{\mathcal{A}} = |\mathcal{A}|$) and inactive ($m_{\mathcal{I}} = |\mathcal{I}|$) control variables, the number of outer (Newton) iterations, the total number of inner (BiCGSTAB) iterations, the computational time and the errors of approximate solutions in the indicated norms (the comparisons are done with respect to the reference solution computed on the fine mesh with $h = 1/2048$). From the errors, we determine the convergence rate of fictitious domain approaches.

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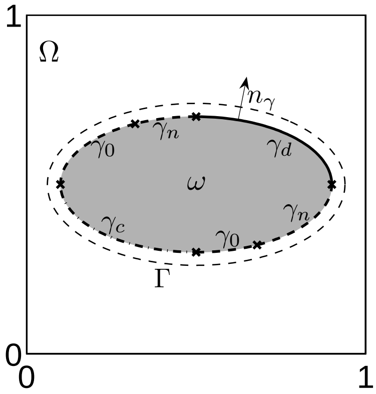

Figure 1: Geometry.

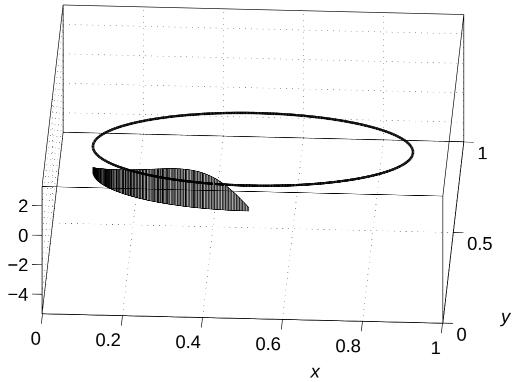

Figure 2: Obstacle g.

Step h	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	out./$\sum$inn. its.	C.time[s]	$\mathrm{Err}_{L^2(\omega)}$	$\mathrm{Err}_{H^1(\omega)}$	$\mathrm{Err}_{L^2(\gamma)}$
1/128	16641/4/8	8/46	0.8	4.8687e-003	2.3282e-001	2.5526e-002
1/256	66049/7/17	11/92	5.2	2.5485e-003	1.6791e-001	1.1830e-002
1/512	263169/14/36	9/123	46.7	1.4337e-003	1.8603e-001	6.6737e-003
1/1024	1050625/28/72	9/242	355.9	5.3726e-004	1.3110e-001	2.8188e-003
Convergence rates:				1.0369	0.2338	1.0362

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

Step h	$n/m_{\mathcal{A}}/m_{\mathcal{I}}$	out./$\sum$inn. its.	C.time[s]	$\mathrm{Err}_{L^2(\omega)}$	$\mathrm{Err}_{H^1(\omega)}$	$\mathrm{Err}_{L^2(\gamma)}$
1/128	16641/4/8	6/40	0.7	6.9482e-003	3.2016e-001	2.7923e-002
1/256	66049/7/17	7/52	3.3	2.4280e-003	1.5623e-001	1.1746e-002
1/512	263169/14/36	8/95	37.0	1.3418e-003	7.1610e-002	5.1939e-003
1/1024	1050625/28/72	9/189	284.5	8.1896e-004	4.4756e-002	2.7937e-003
Convergence rates:				1.0110	0.9641	1.1141

Table 2: Smooth fictitious domain formulation ($\gamma \not\equiv \Gamma$).

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