Numerical approximation of a nonlinear problem with a Signorini boundary condition

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Abstract

The aim of this work is to find a numerical approximation of the solution to an elliptic problem arising in electrochemical modelling. The non-linearity arising from the Signorini boundary condition is handled through an iterative procedure, for which we prove the convergence on the discrete problem obtained by a discretization by the finite volume method for a given "admissible" mesh.

KEYWORDS: Signorini condition, free boundary, finite volune, iterative methods.

1 Introduction

Signorini boundary conditions may be encountered in fluid mecanichs and heat transfer problems when modelling, for instance, the flow through semipermeable boundaries. They are also encountered in the contact problems in elasticity. The Signorini boundary conditions, which we have to deal with, here arise from modelling the so called "triple point" of an electrochemical reaction (see [5]).

The first rigorous analysis of a class of Signorini problems was published in 1963 by Fichera. Details of the mathematical analysis such as existence, uniqueness, and regularity of the solution can be found in [1] and references therein. Signorini problems are classically discretized by finite element formulated in [8]. The approximate problem can be solved by a duality method [4], [9]. In [4], a point overrelaxation method with projection is also studied and found to be cheaper in terms of computational than the duality method. Another candidate for the resolution of the approximated Signorini problem is the penalty method [8] and references therein.

In this work, we are interested by obtaining a precise approximation of the flux at the boundaries, in order to couple the equation of interest here to another problem (see [5]); we shall therefore discretize the problem by the finite volume method [2].

The discrete problem will then solved by an iterative algorithm which seems to be computationnally efficient, and which is inspired from a procedure used for multiphase flow modelling [3].

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2 The continuous and discrete problem

Let us consider the following problem:

$$\begin{aligned} -\Delta(u(\mathbf{x})) &= 0, \quad \mathbf{x} \in \Omega, && (1)\\ u(\mathbf{x}) &= 0, \quad \mathbf{x} \in \Gamma^1, && (2)\\ \nabla u(\mathbf{x}) \cdot \mathbf{n} &= 0, \quad \mathbf{x} \in \Gamma^2, && (3) \end{aligned}$$

with the following Signorini boundary condition:

$$\left.\begin{aligned} u(\mathbf{x}) &\geq a,\\ \nabla u(\mathbf{x}) \cdot \mathbf{n} &\geq b,\\ (u(\mathbf{x}) - a)(\nabla u(\mathbf{x}).\mathbf{n} - b) &= 0, \end{aligned}\right\} \quad \mathbf{x} \in \Gamma^3, \qquad (4)$$

Assumption 2.1 *Let Ω be a bounded open polygonal subset of $\mathbb{R}^2$, and $\partial\Omega$, the boundary of Ω, is composed of three non empty, disjoint connex sets Γ^1, Γ^2 and Γ^3, such that $\overline{\Gamma^1} \cup \overline{\Gamma^2} \cup \overline{\Gamma^3} = \overline{\partial\Omega}$. Let $a \leq 0$ and $b \in \mathbb{R}$ and let $\mathbf{n}$ be the unit normal vector to $\partial\Omega$ outward to the domain Ω.*

Under some regularity assumptions, Problem (1)-(4) is equivalent to the following variational problem (see e.g. [5]):

$$\left\{\begin{array}{l} u \in \mathcal{K} = \{v \in H^1(\Omega),\ v_{|\Gamma^1} = 0,\ v_{|\Gamma^3} \geq a \text{ a.e}\},\ \text{satisfying :}\\ \quad \displaystyle\int_\Omega \nabla u(\mathbf{x}) \cdot \nabla(v-u)(\mathbf{x}) d\mathbf{x} \geq \int_{\Gamma^3} b(\gamma(v) - \gamma(u))(s) ds, \quad \forall v \in \mathcal{K}, \end{array}\right. \qquad (5)$$

with $v_{|\Gamma^i} = \gamma(v)_{|\Gamma^i}$ $(i = 1, 3)$, where γ is the trace operator from $H^1(\Omega)$ to $L^2(\partial\Omega)$. By Stampacchia's Theorem, Problem (5) admits a unique solution. In order to obtain a numerical approximation of the solution to (5), let us define a discretization mesh over Ω, which is assumed (following [2]) to be admissible in the following sense:

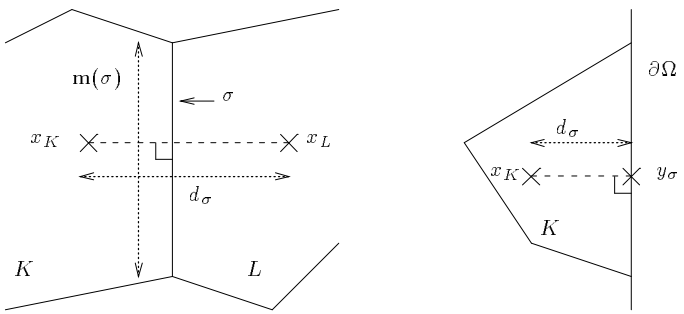

Figure 1: admissible meshes

Definition 2.1 (Admissible meshes) *Let Ω be an open bounded polygonal domain of $\mathbb{R}^2$. Let us denote by $\mathcal{T}$, an admissible mesh of Ω, $\mathcal{T}$ is the set of control volums K, convex, polygonal subsets of Ω such that $\bigcup_{K\in\mathcal{T}} \overline{K} = \overline{\Omega}$. Let us define $\mathcal{E}$ the set of the "edges" of the mesh, $\mathcal{E}_{\text{int}} = \{\sigma \in \mathcal{E};\ \sigma \not\subset \partial\Omega\}$ (resp. $\mathcal{E}_{\text{ext}} = \{\sigma \in \mathcal{E};\ \sigma \subset \partial\Omega\}$) and $\mathcal{E}_K = \{\sigma \in \mathcal{E};\ \sigma \subset \partial K\}$. The transmissivity through σ is defined by $\tau_\sigma = \text{m}(\sigma)/d_\sigma$ if $d_\sigma \neq 0$.*

Let us now define a "discrete" functional space and a "discrete" norm.

Definition 2.2 *Let Ω be an open bounded polygonal domain of $\mathbb{R}^2$, and $\mathcal{T}$ be an admissible mesh in the sense of Definition 2.1. Define $X(\mathcal{T})$ as the set of the functions defined a.e. from $\Omega \cap \Gamma^3$ to $\mathbb{R}$ which are constant over each control volume of the mesh, and which are constant over each edge in $\mathcal{E}_{\rm ext}$, inclued in Γ^3.*

Let $u \in X(\mathcal{T})$, we shall denote by u_K the value taken by u on the control volume K, and by u_σ the value taken by u on the edge $\sigma \in \mathcal{E}_{\rm ext}$, $\sigma \subset \Gamma^3$. Let us define the discrete H^1_{0,Γ^1} norm by $\|u\|^2_{1,\mathcal{T}} = \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma u)^2$, *with $|D_\sigma u| = |u_K - u_L|$ if $\sigma \in \mathcal{E}_{\rm int}$, $\sigma = K/L$, $D_\sigma u = -u_K$ if $\sigma \subset \Gamma^1$, $\sigma \in \mathcal{E}_K$, $D_\sigma u = 0$ if $\sigma \subset \Gamma^2$, and $D_\sigma u = u_\sigma - u_K$ if $\sigma \subset \Gamma^3$, $\sigma \in \mathcal{E}_K$.*

A discretization by a "classical" finite volume method yields the following "discrete problem":

$$\sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma} = 0 \quad \forall K \in \mathcal{T}, \tag{6}$$

$$\begin{aligned}
F_{K,\sigma} &= -\tau_\sigma (u_L - u_K) \quad \forall \sigma \in \mathcal{E}_{\rm int} \text{ if } \sigma = K/L, && (7)\\
F_{K,\sigma} &= \tau_\sigma u_K \quad \forall \sigma \subset \Gamma^1,\ \sigma \in \mathcal{E}_K && (8)\\
F_{K,\sigma} &= 0 \quad \forall \sigma \subset \Gamma^2,\ \sigma \in \mathcal{E}_K && (9)\\
F_{K,\sigma} &= -\tau_\sigma (u_\sigma - u_K) \quad \forall \sigma \subset \Gamma^3,\ \sigma \in \mathcal{E}_K && (10)
\end{aligned}$$

and on the Signorini boundary:

$$\begin{aligned}
u_\sigma &\geq a \quad \forall \sigma \subset \Gamma^3, && (11)\\
-F_{K,\sigma} &\geq {\rm m}(\sigma)\, b \quad \forall \sigma \subset \Gamma^3, && (12)\\
(u_\sigma - a)\left(\frac{F_{K,\sigma}}{{\rm m}(\sigma)} + b\right) &= 0 \quad \forall \sigma \subset \Gamma^3. && (13)
\end{aligned}$$

In order to show the existence and uniqueness of $U = ((u_K)_{K\in\mathcal{T}},\ (u_\sigma)_{\sigma\subset\Gamma^3})$ where $(u_K)_{K\in\mathcal{T}}$ and $(u_\sigma)_{\sigma\subset\Gamma^3}$ is solution to (6)-(13), let us give an equivalent "variational" formulation to (6)-(13) (see [7] for the proof):

Lemma 2.1 *Under Assumptions 2.1, Let $\mathcal{T}$ be an admissible finite volume mesh in the sense of Definition 2.1; and $u_\mathcal{T} \in X(\mathcal{T})$ (see Definition 2.2) defined by $u_\mathcal{T}(x) = u_K$ for $x \in K$, for all $K \in \mathcal{T}$ and by $u_\mathcal{T}(x) = u_\sigma$ for $x \in \sigma$, for all $\sigma \in \mathcal{E}_{\rm ext}$, $\sigma \subset \Gamma^3$.*

Then $(u_K)_{K\in\mathcal{T}}$, $(u_\sigma)_{\sigma\subset\Gamma^3}$ is solution to Problem (6)-(13) if and only if $u_\mathcal{T}$ is solution to the following Problem:

$$\left\{\begin{array}{l} u_\mathcal{T} \in \mathcal{K}_\mathcal{T} = \{v \in X(\mathcal{T}),\ s.t.\ v_\sigma \geq a\ \forall \sigma \subset \Gamma^3\} \text{ such that :} \\ \mathcal{A}(u_\mathcal{T}, v - u_\mathcal{T}) \geq \mathcal{L}(v - u_\mathcal{T}) \quad \forall v \in \mathcal{K}_\mathcal{T}, \end{array}\right. \tag{14}$$

with $\mathcal{A}(u,v) = \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma u)(D_\sigma v)$ *and* $\mathcal{L}(u) = \sum_{\sigma\subset\Gamma^3} b u_\sigma {\rm m}(\sigma) \quad \forall u,\ v \in \mathcal{K}_\mathcal{T}$.

Lemma 2.1 and Stampacchia's Theorem are used to obtain the following result:

Proposition 2.1 (Existence) *Under Assumptions 2.1, let $\mathcal{T}$ be an admissible finite volume mesh in the sense of Definition 2.1; there exists an unique solution $(u_K)_{K\in\mathcal{T}}$, $(u_\sigma)_{\sigma\subset\Gamma^3}$ to Problem (6)-(13).*

Remark 2.1 *Under regularity assumptions on the exact solution, we obtain an estimate of order 1 for the "discrete" H^1 norm and L^2 norm of the error on the solution to (6)-(13). From this result, we deduce the convergence in $L^2(\Omega)$ of the approximate solution to the exact one (see [6] for the proof).*

3 The iterative algorithm

This section is devoted to the construction of an algorithm which yields iterates which converge, hopefully, to the (unique) solution of Problem (6)-(13).

Indeed, the continuous problem which we wish to solve is non linear because of the Signorini condition (4). Hence the need for an iterative method, which we present now, and which adapts an idea which was used for two phase flows in porous media [3].

Let us notice that the set $\{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3\}$ can be decomposed into two disjoint sets $\mathcal{E}_a$ and $\mathcal{E}_b$, where $\mathcal{E}_a = \{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3$ s.t. $u_\sigma = a$ and $-F_{K,\sigma} \geq {\rm m}(\sigma)\, b\}$ and $\mathcal{E}_b = \{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3$ s.t. $u_\sigma > a$ and $-F_{K,\sigma} = {\rm m}(\sigma)\, b\}$. Hence, Problem (6)-(13) is equivalent to the problem composed of equations (6)-(10) and :

$$u_\sigma = a \quad \forall \sigma \in \mathcal{E}_a, \tag{15}$$

$$-F_{K,\sigma} = {\rm m}(\sigma)\, b \quad \forall \sigma \in \mathcal{E}_b. \tag{16}$$

The algorithm determines $\mathcal{E}_a$ and $\mathcal{E}_b$ by the following steps:

- Initialization: $\mathcal{E}_a^{(0)} = \{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3\}$ and $\mathcal{E}_b^{(0)} = \emptyset$
- step (j): Assume the sets $\mathcal{E}_a^{(j)}$ and $\mathcal{E}_b^{(j)}$ are known.

let $U^{(j)} = ((u_K^{(j)})_{K\in\mathcal{T}}, (u_\sigma^{(j)})_{\sigma\subset\Gamma^3})$ be the solution to the set of equations (6)-(10) and :

$$u_\sigma^{(j)} = a \quad \forall \sigma \in \mathcal{E}_a^{(j)}, \tag{17}$$

$$F_{K,\sigma}^{(j)} = -{\rm m}(\sigma)\, b \quad \forall \sigma \in \mathcal{E}_b^{(j)}, \tag{18}$$

Let $\mathcal{E}_a^{(j+1)}$ and $\mathcal{E}_b^{(j+1)}$ be defined in the following way:

$$\begin{array}{lll} \text{for any } \sigma \in \mathcal{E}_a^{(j)}, \quad \text{if} \quad -F_{K,\sigma} \geq {\rm m}(\sigma)\, b & \text{then } \sigma \in \mathcal{E}_a^{(j+1)}, \\ & \text{else } \sigma \in \mathcal{E}_b^{(j+1)}, \\ \text{for any } \sigma \in \mathcal{E}_b^{(j)}, \quad \text{if} \quad u_\sigma^{(j)} \geq a & \text{then } \sigma \in \mathcal{E}_b^{(j+1)}, \\ & \text{else } \sigma \in \mathcal{E}_a^{(j+1)}. \end{array}$$

Remark 3.1 *If there exists j such that $-F_{K,\sigma}^{(j)} \geq {\rm m}(\sigma)\, b$ for all $\sigma \in \mathcal{E}_a^{(j)}$ and $u_\sigma^{(j)} \geq a$ for all $\sigma \in \mathcal{E}_b^{(j)}$, then the method has converged; in which case $\mathcal{E}_a^{(j+1)} = \mathcal{E}_a^{(j)}$, $\mathcal{E}_b^{(j+1)} = \mathcal{E}_b^{(j)}$, $U^{(j+1)} = U^{(j)}$, hence we define $\mathcal{E}_a = \mathcal{E}_a^{(j)}$ and $\mathcal{E}_b = \mathcal{E}_b^{(j)}$ and $U = U^{(j)}$. Then U satisfies the set of equations (6)-(10) and $u_\sigma = a$, $-F_{K,\sigma} \geq {\rm m}(\sigma)\, b$ for all $\sigma \in \mathcal{E}_a$ and $-F_{K,\sigma} = {\rm m}(\sigma)\, b$, $u_\sigma \geq a$ for all $\sigma \in \mathcal{E}_b$, so U is the (unique) solution to (6)-(13).*

Note that (6)-(10), (17) and (18) lead, after an easy elimination of the auxiliary unknowns, to a linear system of N equations with N unknowns, namely the $(u_K^{(j)})_{K\in\mathcal{T}}$ and $(u_\sigma^{(j)})_{\sigma\subset\Gamma^3}$ with N =cardT+card($\{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3\}$). Let us write this system as:

$$A^{(j)} U^{(j)} = B^{(j)}, \tag{19}$$

where $U^{(j)} \in \mathbb{R}^N$ is the vector with components $(u_K^{(j)})_{K\in\mathcal{T}}$ and $(u_\sigma^{(j)})_{\sigma\subset\Gamma^3}$.

The following maximum principle holds (see [7] for the proof):

Lemma 3.1 *Let $\mathcal{T}$ be an admissible finite volume mesh in the sense of Definition 2.1, and $A^{(j)}$ the matrix defined by (6)-(10), and (17)-(19). Let $U \in \mathbb{R}^N$ such that $A^{(j)}U \geq 0$ then $U \geq 0$.*

Corollary 3.1 *This result immediately yields the existence and uniqueness of the solution of the numerical scheme (6)-(10), (17) and (18).*

Let us now state that $U^{(j)}$ is non decreasing, it is bounded and converges to the solution to (6)-(16) (the proof of which may be found in [7]).

Theorem 3.1 *Under Assumptions 2.1, let $\mathcal{T}$ be an admissible finite volume mesh in the sense of Definition 2.1 and $N = card\mathcal{T} + card(\{\sigma \in \mathcal{E}_{\rm ext},\ \sigma \subset \Gamma^3\})$; let $U^{(j)}$, $j \in \mathbb{N}$ denote the vector of $\mathbb{R}^N$, the components of which are $(u_K^{(j)})_{K\in\mathcal{T}}$ and $(u_\sigma^{(j)})_{\sigma\subset\Gamma^3}$ solution to (6)-(10), (17) and (18). Then:*

$$U^{(j)} \leq U^{(j+1)} \quad \text{and} \quad U^{(j)} \leq U \quad \forall j \in \mathbb{N}, \tag{20}$$

where $U = ((u_K)_{K\in\mathcal{T}},\ (u_\sigma)_{\sigma\subset\Gamma^3})$ is a vector of the components of which, are solution to (6)-(16); futhermore, $U^{(j)}$ converges to U as j tends to $+\infty$.

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