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Numerical Analysis/Calculus of Variations

A penalty/Newton/conjugate gradient method for the solution of obstacle problems

Sur une méthode de pénalité/Newton et gradient conjugué pour la résolution de problèmes d'obstacles

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Abstract

Motivated by the search for non-negative solutions of a system of Eikonal equations with Dirichlet boundary conditions, we discuss in this Note a method for the numerical solution of parabolic variational inequality problems for convex sets such as $K = \{v \mid v \in H_0^1(\Omega), v \ge \psi \text{ a.e. on } \Omega\}$. The numerical methodology combines penalty and Newton's method, the linearized problems being solved by a conjugate gradient algorithm requiring at each iteration the solution of a linear problem for a discrete analogue of the elliptic operator $I - \mu \Delta$. Numerical experiments show that the resulting method has good convergence properties, even for small values of the penalty parameter. *To cite this article: R. Glowinski et al., C. R. Acad. Sci. Paris, Ser. I* 336 (2003).

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Résumé

Motivé par la recherche des solutions non négatives d'un système d'équations eiconales, avec conditions aux limites de Dirichlet, on étudie dans cette Note une méthode pour la résolution numérique de problèmes d'inéquations variationnelles paraboliques pour des ensembles convexes du type $K = \{v \mid v \in H_0^1(\Omega), v \ge \psi \text{ p.p. sur } \Omega\}$. La méthode numérique combine pénalité et algorithme de Newton, les problèmes linéarisés étant résolus par un algorithme de gradient conjugué qui demande à chaque iteration la résolution d'un problème linéaire pour un analogue discret de l'opérateur elliptique $I - \mu \Delta$ avec $\mu > 0$. Les essais numériques montrent que la méthode ainsi obtenue a de bonnes propriétés de convergence, même pour des petites valeurs du paramètre de pénalité. *Pour citer cet article : R. Glowinski et al., C. R. Acad. Sci. Paris, Ser. I 336 (2003).* © 2003 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS. Tous droits réservés.

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1. Introduction

In [4] it has been shown that *non-negative* solutions to the following system of Eikonal equations, with Dirichlet boundary conditions,

$$u \in H_0^1(\Omega), \quad \left| \frac{\partial u}{\partial x_i} \right| = 1 \quad \text{a.e., } \forall i = 1, \dots, d,$$
 (1)

could be obtained via an algorithm requiring at each iteration (and among other things) the solution of an *obstacle problem* of the following type:

$$\int_{\Omega} \nabla u \cdot \nabla (v - u) \, \mathrm{d}x \ge \int_{\Omega} \mathbf{p} \cdot \nabla (v - u) \, \mathrm{d}x \quad \forall v \in K^+; \ u \in K^+,$$
(2)

in (1), (2), Ω is a bounded domain of \mathbb{R}^d ($d \ge 1$), **p** is a given vector-valued function of $(L^2(\Omega))^d$ and $K^+ = \{v \mid v \in H_0^1(\Omega), v \ge 0$ a.e. on $\Omega\}$. After the over-relaxation methods with projection and Uzawa type algorithms discussed in, e.g., [8] and [7] proved too slow in the context of problem (1), it was decided to give a chance to an approach combining (exterior) *penalty* and *Newton's method*. Actually, with this combination, we have been able to simulate (see [1,5] for details) the vibrations, *with obstacles*, of strings and beams; however, those were obstacle problems in *one space dimension*, where the linear systems resulting from penalty/Newton (after appropriate finite element discretizations) could be solved easily by *direct methods* taking advantage of the sparsity and band structure of the corresponding matrices. Since some of the *finite element* (or *finite difference*) *meshes* associated to the solution of problem (1) involve more than 10⁶ grid points (1023² to be precise) it is clear that, as of today, direct methods are not a feasible option (for most practitioners, at least) as components of the penalty/Newton solution of problem (2). It will be shown in this note that replacing the above direct methods by a well-chosen *conjugate gradient algorithm* leads to a *fast converging* iterative method, the only requirement being the access to a *fast solver for linear elliptic boundary value problems*. Since vector **p** in (2) is provided by the solution of an initial value problem coupled – in some sense – to (2), we shall take as model problem the *parabolic variational inequality* below

for
$$t > 0$$
, find $u(t) \in K$ such that

$$\int_{\Omega} \frac{\partial}{\partial t} u(t) (v - u(t)) dx + \int_{\Omega} \nabla u(t) \cdot \nabla (v - u(t)) dx \ge \langle f(t), v - u(t) \rangle \quad \forall v \in K,$$
(3)
$$u(0) = u_0 (\in K),$$
(4)

in (3), (4), $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $H^{-1}(\Omega)$ and $H^1_0(\Omega)$, $f(t) \in H^{-1}(\Omega)$, and the convex K is defined by

$$K = \{ v \mid v \in H_0^1(\Omega), \ v \ge \psi \text{ a.e. on } \Omega \},$$
(5)

with $\psi \in H^1(\Omega)$ and $\psi \leq 0$ on the boundary Γ of Ω . It follows from, e.g., [6] that the dynamical obstacle problem (3), (4) has a unique solution.

2. Backward Euler time discretization of problem (3), (4)

Let Δt (>0) be a time discretization step. The *backward Euler time discretization* of problem (3), (4) leads to

$$u^0 = u_0; \tag{6}$$

436

then, for $n \ge 0$, u^n being known, we obtain u^{n+1} from the solution of

$$\begin{cases} u^{n+1} \in K; \ \forall v \in K \\ \int_{\Omega} \frac{u^{n+1} - u^n}{\Delta t} (v - u^{n+1}) \, \mathrm{d}x + \int_{\Omega} \nabla u^{n+1} \cdot \nabla (v - u^{n+1}) \, \mathrm{d}x \geqslant \langle f^{n+1}, v - u^{n+1} \rangle. \end{cases}$$
(7)

The *elliptic variational inequality* problem (7) has a unique solution. Problem (7) is, $\forall n \ge 0$, of the following type

$$\int_{\Omega} u(v-u) \,\mathrm{d}x + \mu \int_{\Omega} \nabla u \cdot \nabla (v-u) \,\mathrm{d}x \ge \langle f, v-u \rangle \quad \forall v \in K; \ u \in K,$$
(8)

with μ a *positive constant*. From now on, we are going to focus on the solution of problem (8).

3. Penalty approximation of problem (8)

Let ε be a *positive parameter* and denote max(0, -v) by v_- . We approximate problem (8) by

$$\int_{\Omega} u^{\varepsilon} v \, \mathrm{d}x + \mu \int_{\Omega} \nabla u^{\varepsilon} \cdot \nabla v \, \mathrm{d}x - \varepsilon^{-1} \int_{\Omega} (u^{\varepsilon} - \psi)^{2}_{-} v \, \mathrm{d}x = \langle f, v \rangle \quad \forall v \in H^{1}_{0}(\Omega); \ u^{\varepsilon} \in H^{1}_{0}(\Omega).$$
(9)

We can show that problem (9) has a unique solution and, in addition, have $\lim_{\varepsilon \to 0^+} \|u^{\varepsilon} - u\|_{H^1(\Omega)} = 0$, with *u* the solution of (8).

4. Newton's method for the solution of problem (9)

Let us drop the superscript ε ; problem (9) can also be written as:

$$F_{\varepsilon}(u) = 0, \tag{10}$$

where $F_{\varepsilon}: H_0^1(\Omega) \to H^{-1}(\Omega)$ is defined by

$$F_{\varepsilon}(v) = v - \mu \Delta v - \varepsilon^{-1} (v - \psi)_{-}^{2} - f \quad \forall v \in H_{0}^{1}(\Omega).$$

$$\tag{11}$$

Applying Newton's method to the solution of problem (10) leads (with obvious notation) to:

 u_0 given in $H_0^1(\Omega)$ (in K if possible);

$$r m \ge 0$$
, u_m being known, compute u_{m+1} via

$$u_{m+1} = u_m - F_{\varepsilon}'(u_m)^{-1} F_{\varepsilon}(u_m), \tag{13}$$

where

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$$\left\langle F_{\varepsilon}'(u_m)v, w \right\rangle = \int_{\Omega} vw \, \mathrm{d}x + \mu \int_{\Omega} \nabla v \cdot \nabla w \, \mathrm{d}x + 2\varepsilon^{-1} \int_{\Omega} \left((u_m - \psi)_{-} \right) vw \, \mathrm{d}x \quad \forall v, w \in H_0^1(\Omega).$$
(14)

It follows from (11), (14) that (13) is equivalent to the following (well posed) linear variational problem:

$$\begin{cases} u_m - u_{m+1} \in H_0^1(\Omega); \ \forall v \in H_0^1(\Omega) \\ \int (u_m - u_{m+1})v \, \mathrm{d}x + \mu \int_{\Omega} \nabla (u_m - u_{m+1}) \cdot \nabla v \, \mathrm{d}x + 2\varepsilon^{-1} \int_{\Omega} ((u_m - \psi)_-)(u_m - u_{m+1})v \, \mathrm{d}x \\ = \int_{\Omega} u_m v \, \mathrm{d}x + \mu \int_{\Omega} \nabla u_m \cdot \nabla v \, \mathrm{d}x - \varepsilon^{-1} \int_{\Omega} (u_m - \psi)_-^2 v \, \mathrm{d}x - \langle f, v \rangle. \end{cases}$$
(15)

(12)

The *finite element* implementation of Newton's algorithm (12), (15) and the *conjugate gradient solution* of the discrete analogues of problem (15) will be discussed in the following section.

5. Finite element implementation of the Newton's algorithm (12), (15). Conjugate gradient solution of the discrete linearized problem

From now on, we suppose that Ω is a polygonal domain of \mathbb{R}^2 ; following, e.g., [7, Appendix 1], [2,3] we introduce a *finite element triangulation* \mathcal{T}_h of Ω and approximate $H_0^1(\Omega)$, K, (8), (9) and the Newton's algorithm (12), (15) by, respectively,

$$V_{0h} = \left\{ v_h \mid v_h \in C^0(\overline{\Omega}), \ v_h \mid_T \in P_1, \ \forall T \in \mathcal{T}_h, \ v_h = 0 \text{ on } \Gamma \right\}$$
(16)

(with P_1 the space of polynomials in two variables of degree ≤ 1),

$$K_h = \left\{ v_h \mid v_h \in V_{0h}, \ v_h(P) \geqslant \psi(P), \ \forall P \in \Sigma_{0h} \right\}$$
(17)

(we suppose here that $\psi \in C^0(\overline{\Omega}) \cap H^1(\Omega)$),

$$\int_{\Omega} u_h(v_h - u_h) \, \mathrm{d}x + \mu \int_{\Omega} \nabla u_h \cdot \nabla (v_h - u_h) \, \mathrm{d}x \ge \langle f, v_h - u_h \rangle \quad \forall v_h \in K_h; \ u_h \in K_h,$$

$$\left\{ \begin{array}{l} u_h^\varepsilon \in V_{0h}; \ \forall v_h \in V_{0h} \end{array} \right\}$$

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$$\left\{ \begin{array}{l} u_h^\varepsilon \in V_{0h}; \ \forall v_h \in V_{0h} \end{array} \right\}$$

$$\begin{cases} \int_{\Omega} u_h^{\varepsilon} v_h \, \mathrm{d}x + \mu \int_{\Omega} \nabla u_h^{\varepsilon} \cdot \nabla v_h \, \mathrm{d}x - \frac{\varepsilon^{-1}}{3} \sum_{P \in \Sigma_{0h}} A_P \big(u_h^{\varepsilon}(P) - \psi(P) \big)_-^2 v_h(P) = \langle f, v_h \rangle, \end{cases}$$
(19)

and (dropping some of the subscripts h)

$$u_0 \text{ is given in } V_{0h} \quad (\text{in } K_h \text{ if possible});$$

$$(20)$$

for $m \ge 0$, u_m being known, denote $u_m - u_{m+1}$ by \bar{u}_m and solve

$$\begin{cases} \bar{u}_m \in V_{0h}; \ \forall v \in V_{0h} \\ \int_{\Omega} \bar{u}_m v \, \mathrm{d}x + \mu \int_{\Omega} \nabla \bar{u}_m \cdot \nabla v \, \mathrm{d}x + \frac{2\varepsilon^{-1}}{3} \sum_{P \in \Sigma_{0h}} A_P \left(\left(u_m(P) - \psi(P) \right)_- \right) \bar{u}_m(P) v(P) \\ = \int_{\Omega} u_m v \, \mathrm{d}x + \mu \int_{\Omega} \nabla u_m \cdot \nabla v \, \mathrm{d}x - \frac{\varepsilon^{-1}}{3} \sum_{P \in \Sigma_{0h}} A_P \left(u_m(P) - \psi(P) \right)_-^2 v(P) - \langle f, v \rangle; \end{cases}$$
(21)

in (17), (19) and (21), $\Sigma_{0h} = \{P \mid P \text{ is a vertex of } \mathcal{T}_h, P \notin \Gamma\}$ and A_P is the measure of the polygonal, union of the triangles of \mathcal{T}_h which have P as a common vertex (the penalty related terms in (19) and (21) have been obtained by approximating $\int_{\Omega} (u^{\varepsilon} - \psi)^2 v \, dx$ and the other similar integrals by the *trapezoidal rule*, in order to "diagonalize" the matrices associated to the penalty treatment of the condition $u \ge \psi$ on Ω ; actually the trapezoidal rule can also be employed to approximate the various $L^2(\Omega)$ -scalar products encountered in (18), (19), and (21)). Problem (21) is equivalent to a linear system of the following form

$$AX + \varepsilon^{-1}DX = b, (22)$$

where *A* is a $N \times N$ matrix, symmetric and positive definite, *D* is a $N \times N$ diagonal matrix, positive semi-definite, and $b \in \mathbb{R}^N$. Define *Y* by $Y = \varepsilon^{-1} D^{1/2} X$; system (22) can be rewritten as:

$$\varepsilon Y + D^{1/2} A^{-1} D^{1/2} Y = D^{1/2} A^{-1} b.$$
(23)

Matrix $\varepsilon I + D^{1/2}A^{-1}D^{1/2}$ being symmetric and positive definite it makes sense to attempt solving problem (23) by a *conjugate gradient algorithm*. Without preconditioning, such an algorithm can be written as follows (where $V \cdot W = \sum_{i=1}^{N} V_i W_i$):

$$Y^0 \text{ is given in } \mathbb{R}^N \quad (Y^0 = 0, \text{ for example});$$
(24)

solve

$$Ar^0 = D^{1/2}Y^0 - b, (25)$$

and set

$$g^{0} = \varepsilon Y^{0} + D^{1/2} r^{0}, \tag{26}$$

$$w^0 = g^0. (27)$$

For $k \ge 0$, assuming that Y^k , g^k , w^k are known, solve

$$A\bar{r}^k = D^{1/2} w^k, \tag{28}$$

and set

$$\bar{g}^k = \varepsilon w^k + D^{1/2} \bar{r}^k. \tag{29}$$

Compute

$$\rho_k = g^k \cdot g^k / \bar{g}^k \cdot w^k, \tag{30}$$

$$Y^{k+1} = Y^k - \rho_k w^k, (31)$$

$$g^{k+1} = g^k - \rho_k \bar{g}^k.$$
(32)

If $\|g^{k+1}\|_{\mathbb{R}^N} / \|g^0\|_{\mathbb{R}^N} \leq \eta$ take $X = A^{-1}(D^{1/2}Y^{k+1} - b)$; else, compute

$$\gamma_k = g^{k+1} \cdot g^{k+1} / g^k \cdot g^k, \tag{33}$$

$$w^{k+1} = g^{k+1} + \gamma_k w^k. ag{34}$$

Do k = k + 1 and return to (28).

It follows from (25), (28) that each iteration of algorithm (24)–(34) requires the solution of a linear system associated to matrix *A*, i.e., in the context of the discrete obstacle problem (18), of a linear system associated to the discrete analogue of operator $I - \mu \Delta$ with Dirichlet boundary conditions, a classical problem indeed. Concerning the speed of convergence of algorithm (24)–(34) it can be shown that, in the neighborhood of the solution of problem (19), the *condition number* ν of the corresponding matrix $\varepsilon I + D^{1/2}A^{-1}D^{1/2}$ is $O(\varepsilon^{-1/2})$ implying (from the relation $||Y^k - Y|| \leq C((\sqrt{\nu} - 1)/(\sqrt{\nu} + 1))^k ||Y^0 - Y||$) that the speed of convergence is controlled by $\varepsilon^{-1/4}$, a not so small number, even if ε is small (of the order of 10^{-4} , for example). From this observation, we can expect a fast convergence for algorithm (24)–(34) if, in (20), (21), u_0 is not too far from the solution u_h^{ε} of problem (19); numerical experiments confirm this prediction.

Remark 5.1. The methodology discussed in Sections 3, 4, and 5 can be easily modified to handle (2). Actually, it has been quite successful at finding non-negative solutions to problem (1).

6. Numerical experiments

In order to validate the methodology discussed in Sections 2–5, we consider the variant of problem (3), (4) with $\Omega = (0, 1) \times (0, 1)$, f = C, and $K = \{v \mid v \in H_0^1(\Omega), v(x) \leq \delta(x, \Gamma), \text{ a.e., on } \Omega\}$; here $\delta(x, \Gamma) = \text{distance from}$

439

Table 1

Calculation results			
ε	N _{Newton}	NCG	L^2 -error
0.0032	4	3	8.9604339×10^{-2}
0.0016	5	3	6.9899789×10^{-2}
0.0008	5	4	5.3565620×10^{-2}
0.0004	5	4	4.0485722×10^{-2}
0.0002	6	4	3.0261847×10^{-2}
0.0001	6	5	2.2398988×10^{-2}
0.00005	7	5	1.6440081×10^{-2}
0.000025	9	6	1.1985428×10^{-2}
0.0000125	11	6	8.6906453×10^{-3}

x to the boundary Γ of Ω . The above problem is well documented and related to the elasto-plastic torsion of a infinitely long cylinder of cross section Ω , *C* being a torsion angle per unit length (see, e.g., [7,8] for details). To approximate the solution of this problem we have used a finite element approximation like the one discussed in Section 5, with V_{0h} and K_h defined from a uniform triangulation \mathcal{T}_h of Ω , allowing the use of fast elliptic solvers in algorithm (24)–(34).

All calculations have been done with $\Delta t = 2.5 \times 10^{-4}$, h = 1/256, and C = 10. The Newton's iterations have been stopped when $\sum_{i,j} |\bar{u}_{m,ij}| \leq 10^{-4}$. In the conjugate gradient algorithm we have taken 10^{-6} for η in the stopping criterion. Finally concerning the time discretization scheme itself, we consider that a steady state has been reached when $\sum_{i,j} |u_{ij}^{n+1} - u_{ij}^n| \leq 10^{-4}$. In Table 1, we have shown the maximal numbers of iterations in the Newton's iteration and the conjugate gradient algorithm and the L^2 -error (compared with the solution obtained with same parameters by the relaxation method discussed in [7]) with different choices of the penalty parameter ε . It is clear from Table 1 that both the Newton's and conjugate gradient methods have fast convergence properties. There is no doubt that the fact that we initialize Newton's method with the solution obtained at the previous time step is an important factor of this good convergence property. However, when applying a similar initialization strategy for SOR projection when solving problem (1) the convergence is quite slow while the penalty/Newton/conjugate gradient approach performs very efficiently: the good initial guess does not explain everything. Our final comment is that the L^2 -error in Table 1 behaves essentially like $\sqrt{\varepsilon}$ which is a result we were expecting.

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