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Derivative with respect to discontinuities in the porosity

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Abstract We investigate the sensitivity of hydrostatic pressure of flows through porous media with respect to the position of the soil layers. Indeed, these induce discontinuities of the porosity which is a piecewise constant coefficient κ of the partial differential equation satisfied by the pressure u and it leads to the computation of the derivative of u with respect to changes in position of discontinuity surfaces of κ. The analysis relies on a mixed formulation of the problem. Preliminary numerical simulations are given to illustrate the theory. An application to a simple inverse problem is also given. ***To cite this article: C. Bernardi, O. Pironneau, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 661–666.***

Dérivée par rapport aux discontinuités du coefficient de porosité

Résumé Nous étudions la dérivabilité de la solution de l'équation de Darcy par rapport à la porosité dans le cas où celle-ci est constante par morceaux. La variable est donc la position de la ligne de discontinuité de la porosité. Nous montrons que la dérivée existe et que pour la calculer le problème doit être posé sous forme variationnelle mixte. La dérivée est solution d'un problème identique avec une masse de Dirac au second membre. Des calculs numériques préliminaires sont donnés pour illustrer le résultat théorique et un problème d'identification de porosité discontinue est résolu par une méthode de gradient. ***Pour citer cet article : C. Bernardi, O. Pironneau, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 661–666.***

Version française abrégée

La pression hydrostatique u dans un milieu poreux de porosité κ peut être obtenue, dans les cas simples, en résolvant l'équation de Darcy :

$$-\nabla\cdot(\kappa\nabla u)=f. \tag{1}$$

Lorsque le milieu poreux est fait de couches de matériaux quasi-homogènes, ce qui est souvent le cas en géologie, κ est presque constant dans chaque couche mais discontinu d'une couche à l'autre. Pour l'identification de paramètre en géologie par des méthodes d'optimisation différentiable, il est donc important de savoir calculer la variation de u lorsque κ varie tout en restant constant par morceaux.

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Ce problème pourrait être traité par les méthodes d'optimisation topologique (cf. [2]), mais celles-ci ne prennent pas en compte le fait que les discontinuités de κ sont sur des lignes/surfaces Σ bien définies. Par ailleurs tout résultat de différentiabilité de u par rapport à κ dans une topologie autre que $\mathrm{L}^1(\Omega)$, (comme dans [5]) ne permet pas de résoudre le problème.

Le résultat central de cette Note est le Théorème 1.1. Pour l'obtenir il faut remplacer (1) par la formulation mixte (3), et utiliser le fait que $U \cdot n$ est continu aux discontinuités de κ. Ensuite, et c'est la principale difficulté technique, il faut montrer que $U \cdot n$ admet une trace assez régulière sur Σ.

Pour les tests numériques, une discrétisation par éléments finis mixtes standard est utilisée. On a comparé la solution de (5) avec une différence finie entre deux solutions pour deux paramètres a voisins faisant varier Σ. Enfin un calcul inverse montre qu'on peut retrouver les discontinuités de la porosité par une méthode de moindres carrés associée à un algorithme d'optimisation de type gradient.

Problem statement. – More precisely, consider a bounded open set Ω of $\mathcal{R}^2$ and a family of closed curves $a \mapsto \Sigma(a)$ strictly inside Ω and function of a scalar parameter a separating Ω into two nonoverlapping sets $\Omega_i(a),\ i = 1, 2$, with Lipschitz continuous boundaries:

$$\overline{\Omega} = \overline{\Omega}_1(a) \cup \overline{\Omega}_2(a), \quad \Omega_1(a) \cap \Omega_2(a) = \emptyset, \quad \overline{\Sigma}(a) = \overline{\Omega}_1(a) \cap \overline{\Omega}_2(a).$$

Note that we do not allow $\Sigma(a)$ to touch $\partial\Omega$. This is for mathematical convenience only and it is conjectured that the following results apply also to the general case both in $\mathcal{R}^2$ and $\mathcal{R}^3$.

Let $\kappa(a)$ be piecewise constant and equal to κ_i on $\Omega_i(a)$ and consider (1) with Dirichlet or Neumann conditions on $\Gamma = \partial\Omega$. We wish to compute the derivative u' of $u(a)$ with respect to a at $a = 0$.

1. The result

From now on we work with curves $\Sigma(a)$ which depend on a via a given function α of $\mathcal{C}^1(\Sigma)$ and the following local variation in the "direction" α around $\Sigma(0)$ taken as a reference curve:

$$\Sigma(a) = \big\{x + a\alpha(x)n(x) : x \in \Sigma(0)\big\}, \tag{2}$$

where n is the unit normal to $\Sigma(0)$ which points outside Ω_1. Let $\mathrm{L}^2_0(\Omega) = L^2(\Omega)/\mathcal{R}$ and

$$H(\mathrm{div}, \Omega) = \big\{W \in \mathrm{L}^2(\Omega)^d : \nabla \cdot W \in \mathrm{L}^2(\Omega)\big\}, \qquad X = \big\{V \in H(\mathrm{div}, \Omega) : V \cdot n = 0 \text{ on } \partial\Omega\big\}.$$

Let $f \in \mathrm{L}^2(\Omega)$. Consider the mixed formulation with $U = \kappa\nabla u$.

$$\text{Find } (U, u) \in X \times \mathrm{L}^2_0(\Omega) \text{ with}$$
$$\forall w \in \mathrm{L}^2_0(\Omega) \quad \int_\Omega (\nabla \cdot U)w = \int_\Omega fw, \qquad \forall W \in X \quad \int_\Omega \frac{1}{\kappa} U \cdot W + \int_\Omega u\nabla \cdot W = 0. \tag{3}$$

This is a slight departure from the standard mixed formulation (see Azaïez et al. [3]) in that we have divided by κ.

Next we observe that with a piecewise constant κ

$$\frac{1}{\kappa(a)}(x) = \frac{1}{\kappa_1} + \left[\frac{1}{\kappa}\right] I_{\Omega_2} \quad \text{therefore } \frac{\mathrm{d}}{\mathrm{d}a}\left(\frac{1}{\kappa}\right) = \alpha\delta_\Sigma \left[\frac{1}{\kappa}\right]$$

with δ_Σ defined by $\forall f \in \mathrm{H}^{1/2+\varepsilon}(\Omega)$ $\int_\Omega f\delta_\Sigma = \int_\Sigma f$. So differentiating (3) yields

$$\int_\Omega (\nabla \cdot U')w = 0, \qquad \int_\Omega \left(\frac{1}{\kappa} U' \cdot W + u'\nabla \cdot W\right) = -\int_\Sigma \alpha \left[\frac{1}{\kappa} U\right] \cdot W, \tag{4}$$

assuming that the trace of $U \cdot W$ on Σ exist. Note, however, that if s, n denotes a tangent vector and a normal vector to Σ, $U \cdot n/\kappa$ jumps across Σ but $U \cdot s/\kappa = \partial u/\partial s$ does not because $[u]_\Sigma = 0$. Hence

$$\left[\tfrac{1}{\kappa} U \cdot W\right] = \left[\tfrac{1}{\kappa} U\right] \cdot nW \cdot n = \left[\tfrac{1}{\kappa}\right] U \cdot nW \cdot n$$

and so it seems that $U \cdot n \in \mathrm{L}^2(\Sigma)$ could be sufficient. We can justify this computation and prove the following result:

THEOREM 1.1. – *The derivative* $(V, v) \equiv (U', u')$ *of* (U, u) *solution of* (3) *is given by*

$$\text{Let } g = -\alpha\left[\frac{1}{\kappa}\right] U \cdot n. \text{ Find } (V, v) \in X \times \mathrm{L}_0^2(\Omega) \text{ with}$$

$$\forall w \in \mathrm{L}_0^2(\Omega) \quad \int_\Omega (\nabla \cdot V) w = 0, \qquad \forall W \in X \quad \int_\Omega \left(\frac{1}{\kappa} V \cdot W + v \nabla \cdot W\right) = \int_\Sigma g W \cdot n. \tag{5}$$

Remark 1. – In the distribution sense (5) is $\nabla \cdot V = 0$, $\frac{1}{\kappa} V - \nabla v = \delta_\Sigma g n$, $V \cdot n|_\Gamma = 0$. Note then that it is not possible to eliminate V and write a single equation for v because $\kappa \delta_\Sigma$ has no meaning on account of the discontinuity of κ on Σ.

Remark 2. – Note also that (5) can be obtained by differentiating directly the partial differential equation written in strong form and the jump condition at the interface. Such a computation is of course quite formal and requires more regularity than used here.

2. Existence and uniqueness

Assume $\Gamma = \partial\Omega$ of class $\mathrm{C}^{1,1}$. Let Σ be a smooth closed curve inside Ω. Let $\kappa > 0$ be piecewise constant discontinuous across Σ only. Then, *provided that* $W \mapsto \int_\Sigma g W \cdot n$ *is continuous on* X. Existence and uniqueness can be shown by adapting the proof of Theorem 2.1 in [3] to the case $\kappa \neq 1$.

3. Regularity

In (5) $U \cdot n|_\Sigma$ appears in an integral. We need to show that the integral exists. Functions of V have their normal component traces $V \cdot n$ on Σ in $\mathrm{H}^{-1/2}(\Sigma)$. So we need to show that $U \cdot n \in \mathrm{H}^{1/2}(\Sigma)$.

PROPOSITION 3.1. – *If* Σ *is regular and* f *is in* $\mathrm{H}^1(\Omega)$ *then* $U \cdot n$ *belongs to* $\mathrm{H}^{1/2}(\Sigma)$.

For clarity the proof is given in dimension 2. Assume that Σ is sufficiently regular so that in a neighborhood $\mathcal{O}$ of Σ we can define a coordinate system σ, ν in which the equation of Σ is $\nu = 0$, n the normal to Σ, is tangent to the curves $\sigma =$ constant and σ is its curvilinear abscissa. By taking $\operatorname{supp} w' \subset \mathcal{O}$, $w = \partial w'/\partial\sigma$ in (3) in variational form, and by integrating by part in σ we find that

$$\forall w' \in \mathrm{H}_0^1(\mathcal{O}) \quad \int_\mathcal{O} \kappa \nabla \frac{\partial u}{\partial \sigma} \nabla w' = \int_\mathcal{O} \frac{\partial f}{\partial \sigma} w' \tag{6}$$

because κ is not a function of σ. This shows that if f is regular all partial derivatives in σ of u are in $\mathrm{H}^1(\mathcal{O})$. Therefore $U \cdot \vec{s}$ has the same regularity. Now $\partial U \cdot s/\partial\sigma = \kappa \partial^2 u/\partial\sigma^2$ belongs to $\mathrm{L}^2(\mathcal{O})$. So by $\nabla \cdot U = 0$ we see that $\frac{\partial U \cdot n}{\partial \nu}|_{\mathcal{O}_i}$ is in $\mathrm{L}^2(\mathcal{O}_i)$ for any open set $\mathcal{O}_i \subset \mathcal{O}$ not intersecting Σ.

Similarly, $U \cdot \vec{s} \in \mathrm{H}^1(\mathcal{O}_i)$ implies $\frac{\partial}{\partial \nu} U \cdot \vec{s} \in \mathrm{L}^2(\mathcal{O}_i)$, i.e. $\frac{\partial}{\partial \nu} \kappa \frac{\partial u}{\partial \sigma} \in \mathrm{L}^2(\mathcal{O}_i)$. Therefore $\frac{\partial U \cdot n}{\partial \sigma} = \kappa \frac{\partial^2 u}{\partial \nu \partial \sigma}$ is in $\mathrm{L}^2(\mathcal{O}_i)$. Hence U is in $\mathrm{H}^1(\mathcal{O}_i)$.

COROLLARY 3.2. – *If* Σ *is regular and* $f \in \mathrm{W}^{1,\infty}(\Omega)$ *then* U *is continuous in* $\Omega \backslash \Sigma$ *and* U *is in* $\mathrm{L}^\infty(\Omega)$.

This is because (6) shows that $\frac{\partial u}{\partial \sigma}$ satisfies a partial differential equation of the same type as the one of u. So by the proposition above $\kappa \nabla \frac{\partial u}{\partial \sigma} \cdot n$ is in $\mathrm{H}^{1/2}(\Sigma)$. Therefore $U.n$ is in $\mathrm{H}^{3/2}(\Sigma)$, hence it is also continuous and bounded. By the maximum principle (in $\Omega\backslash\Sigma$, ΔU is bounded), U is bounded everywhere.

4. Continuity

In order to study the changes δu, δU of u, U, when $a \to 0$, let

$$\eta = \kappa^{-1}, \quad \delta u = u(a) - u(0), \quad \delta U = U(a) - U(0), \quad \delta\eta = \eta(a) - \eta(0).$$

1. The first equation in (5) is easy to establish because

$$\int_\Omega (\nabla \cdot U) w = 0, \quad \int_\Omega \big(\nabla \cdot (U + \delta U)\big) w = 0 \Rightarrow \int_\Omega (\nabla \cdot \delta U) w = 0. \tag{7}$$

2. For the second equation we have

$$\int_\Omega \big((\eta+\delta\eta)(U+\delta U)\cdot W - \eta U\cdot W + \delta u \nabla\cdot W\big) = 0 \quad \text{which is also}$$

$$\int_\Omega \big((\eta+\delta\eta)\delta U\cdot W + \delta u \nabla\cdot W\big) = -\int_\Omega \delta\eta U\cdot W. \tag{8}$$

Take $W=\delta U$ in (3), and use $w=\delta u$ in (3), then with $\kappa_{\max}=\max(\kappa_1,\kappa_2)$, $\kappa_{\min}=\min(\kappa_1,\kappa_2)$

$$\int_\Omega (\eta+\delta\eta)|\delta U|^2 = -\int_\Omega \delta\eta U\cdot\delta U \leqslant \|\delta U\|_0\|U\|_\infty\|\delta\eta\|_0 \quad\Rightarrow\quad \frac{1}{\kappa_{\max}}\|\delta U\|_0 \leqslant \|U\|_\infty\|\delta\eta\|_0.$$

The support $S(a)$ of $\delta\eta$ is a thin strip around Σ of width αa, and $\eta+\delta\eta$ is either $\kappa_{\max}^{-1}$ or $\kappa_{\min}^{-1}$; therefore $\|\delta\eta\|_0 \leqslant C_1|[1/\kappa]|\sqrt{a\|\alpha\|_\infty}$ for some constant C_1.

So we have the following result,

PROPOSITION 4.1. – *If $U\in L^\infty(\Omega)$, the change $\{\delta u,\delta U\}$ in $\{u,U\}$ due to a is bounded in $L^2_0(\Omega)\times H(\mathrm{div},\Omega)$, verifies $\nabla\cdot\delta U=0$ and $\|\delta u\|_0+\|\delta U\|_{H(\mathrm{div},\Omega)} \leqslant C_2\sqrt{\|\alpha\|_\infty a}\,\|U\|_\infty|[\kappa]|/\kappa_{\min}$.*

5. Differentiability

LEMMA 5.1. – *Let $\mathcal{O}$ be a neighborhood of Σ containing $S(a)$ but sufficiently thin near Σ so as to be able to extend n_σ in $\mathcal{O}$. If U, W are continuous in $\mathcal{O}\backslash\Sigma$ and $U\cdot n$, $W\cdot n$ are continuous in $\mathcal{O}$ then, for a small enough,*

$$\lim_{a\to 0}\left|\int_\Omega \frac{\delta(\eta U)}{a}\cdot W - \int_\Sigma \alpha\left[\frac{1}{\kappa}\right] U\cdot n W\cdot n\right| = 0. \tag{9}$$

Proof. – See [4].

THEOREM 5.2. – *The solution of* (3), $\{u(a),U(a)\}$, *with* $\Sigma(a)=\{x+a\alpha(x)n_\Sigma(x): x\in\Sigma\}$ *is differentiable in a in the sense that $v=\lim_{a\to 0}(u(a)-u(0))/a$ $V=\lim_{a\to 0}(U(a)-U(0))/a$ is solution of* (5) *where the jump $[1/\kappa]$ is*: $x\in\Sigma[\frac{1}{\kappa}](x)=\lim_{a\to 0}(\kappa(x+a\alpha(x)n(x))^{-1}-\kappa(x-a\alpha(x)n(x))^{-1})$.

6. Discretization and numerical test

6.1. Discretization

Consider a regular family of triangulations of Ω of maximum edge length h and two finite element spaces X_h and L_h to approximate $H(\mathrm{div},\Omega)$ and $L^2_0(\Omega)$. Although precision is increased when the triangulations approximate Σ as an internal boundary, the theory works also without this hypothesis. The numerical discretization of problem (5) can be expressed: find $(V_h,v_h)\in X_h\times L_h$ with

$$\forall q\in L_h \quad \int_\Omega(\nabla\cdot V_h)q=0, \qquad \forall W\in X_h \quad \int_\Omega\left(\frac{1}{\kappa}V_h\cdot W + v_h\nabla\cdot W\right) = \int_\Sigma gW\cdot n. \tag{10}$$

Among the various admissible choices, we have selected the Raviart–Thomas element for X_h and the piecewise constant functions for L_h. This couple satifies the discrete inf-sup condition as shown in Achdou et al. [1], Proposition 3.14, when $(V,v)\in(H^s(\Omega))^2\times H^s(\Omega)$, $0<s\leqslant 1$:

$$\|V-V_h\|_0 + |v-v_h|_0 \leqslant ch^s\big(\|V\|_{H^s}+\|v\|_{H^s}\big).$$

6.2. Numerical simulation

The numerical solution is calculated with `freefem++` [6]. To illustrate the theory we have solved the problem

$$-\nabla\cdot(\kappa\nabla u)=0 \quad \text{in } \Omega, \quad u|_\Gamma = xy, \tag{11}$$

where $\Omega=(-5,5)\times(-2.5,2.5)$, κ is 6 inside an ellipse in the middle of the rectangle and 1 outside (Fig. 1). Then the ellipse is changed by ε according to

$$\big\{(x,y): x=(2+\varepsilon)(\sqrt{2}+\varepsilon)\cos t,\ y=(\sqrt{2}+\varepsilon)\sin t,\ t\in(0,2\pi)\big\}$$

yielding a new solution u_ε of (11). Then $u'_\varepsilon=(u_\varepsilon-u)/\varepsilon$ is compared to the numerical solution of (10). The results are displayed in Fig. 1. Decreasing both ε and the mesh size gives convergence:

ε	0.1	0.05	0.025	0.0125
L^2-error	0.96	0.71	0.56	0.46

7. Identification of a discontinuity

Consider an "observed" data u_d on an observation set S and the problem of finding the best κ (i.e., the best Σ) to fit this data. A least square approach leads to $\min_{\kappa\in K}\{J(\kappa)=\int_S \|u-u_d\|^2 : -\nabla\cdot(\kappa\nabla u)=0,\ u|_\Gamma = x+y\}$. In this example the problem is driven by a boundary condition rather than by a right-hand side f. Obviously a normal change $a\alpha$ in the position of Σ induces a change in J and it is not hard to show that the derivative $J' = \mathrm{d}J/\mathrm{d}a$ is given by

$$J'(\kappa) = -\int_\Sigma \alpha\left[\frac{1}{\kappa}\right]\left(\kappa\frac{\partial u}{\partial n}\right)\left(\kappa\frac{\partial p}{\partial n}\right) \quad \text{with } p \text{ solution of } -\nabla\cdot(\kappa\nabla p) = 2(u-u_d)\delta_S,\ p|_\Gamma = 0.$$

Assume that $\alpha = \alpha(r_1, r_2, \dots, r_m)$. A gradient method on the position of Σ with step size ρ, via the parameters $\{r_i\}_1^m$ would be to change r_i according to

$$r_i \leftarrow r_i + \rho\int_\Sigma \frac{\partial\alpha}{\partial r_i}\left[\frac{1}{\kappa}\right]\left(\kappa\frac{\partial u}{\partial n}\right)\left(\kappa\frac{\partial p}{\partial n}\right).$$

(a) We ran a preliminary test by taking

$$\Omega = (-5,5)\times(-2.5,2.5), \quad D = \{(x,y) : (x+2)^2 + y^2 < 1\},$$
$$\Sigma(r_1,r_2) = \{(x,y) : x = (r_1 + r_2\cos t)\cos t,\ y = (r_1 + r_2\cos t)\sin t\}$$

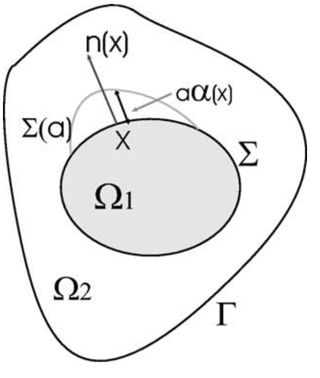

Figure 1. – The coefficient κ is constant on Ω_1 and constant on Ω_2 and discontinuous across Σ. When Σ becomes $\Sigma(a)$, the distance from $\Sigma(a)$ to Σ is $a\|\alpha\|_\infty$,the solution of the partial differential equation changes. We wish to find the derivative with respect to a for a given function α.

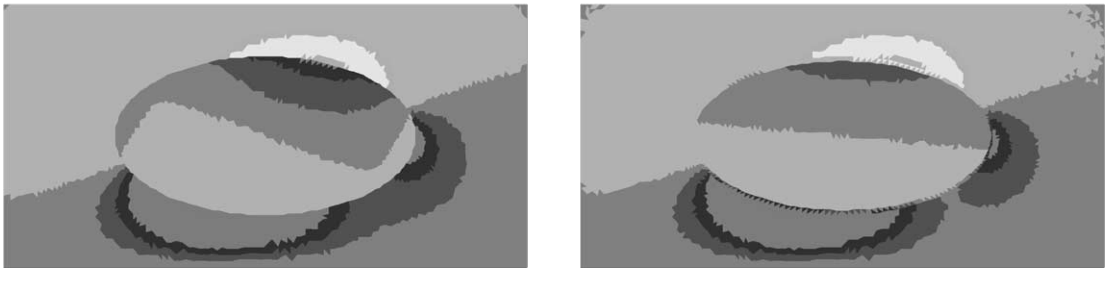

Figure 2. – *Left*: u'. *Right*: u'_ε when $\varepsilon = 0.0125$. Observe that both solutions are clearly discontinuous across Σ.

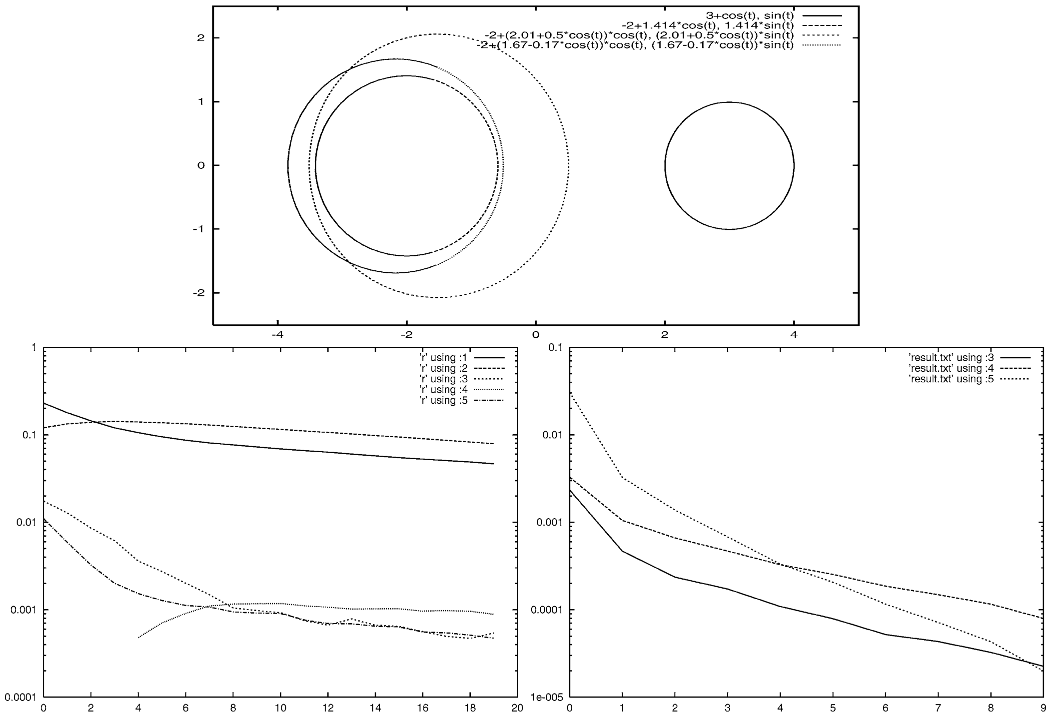

Figure 3. – *Center up*: Geometry of the second example showing the observation set (right circle), the exact and computed solution (inner circle and middle curve) and the initial shape (outer curve). *Bottom left*: Convergence curves for the identification problem: curve 1 and 2 are $r_1 - \sqrt{2}, r_2$, curve 3 and 4 are $\partial J/\partial r_1,\ \partial J/\partial r_2$ and curve 5 is J; all tend to zero; the x-axis is the iteration count (from 1 to 20 here). *Bottom right*: Convergence curves showing the two gradients and the cost function for 10 iterations.

and the reference surface $\Sigma = \Sigma(\sqrt{2}, 0)$. As before $\kappa = 1$ outside Σ and 6 inside. We chose u_d to be the solution of the PDE for κ given by $\Sigma(\sqrt{2}, 0)$. Then we apply the steepest descent method with $\rho = 4$ starting from $\Sigma(0.3, 0.1)$. Fig. 3 shows the convergence curves.

(b) In the previous configuration D intersects Σ. Now we move D to the right and Σ to the left (Fig. 2) and ran the same test with $r_1 = 0.3$ and $r_2 = 0.5$ initially. The method converges but the final shape is close to but different from $\Sigma(\sqrt{2}, 0)$. This is because the numerical approximation does not "see" the right part of Σ which is too far.

(c) In third test where $r_1 = 0$ and the descent is only on r_2, the exact solution was reached in 4 iterations. This indicates that the method is sound but a conjugate gradient is needed for test (b).

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References

[1] Y. Achdou, C. Bernardi, F. Coquel, F. Archambeau, B. Gest, Discrétisation par volumes finis des équations de Darcy, Rapport EDF HI-83/00/043/A, 2001.

[2] G. Allaire, Shape Optimization by the Homogenization Method, Springer-Verlag, New York, 2001.

[3] M. Azaïez, C. Bernardi, M. Grundmann, Méthodes spectrales pour les équations du milieu poreux, East-West J. Numer. Anal. 2 (1994) 91–105.

[4] C. Bernardi, O. Pironneau, Sensitivity of Darcy's law to discontinuities, Chinese Ann. Math., 2002, submitted.

[5] A.M. Bruaset, B.F. Nielsen, On the stability of pressure and velocity computations for heterogeneous reservoirs, SIAM J. Appl. Math. 56 (4) (1996) 991–1007.

[6] F. Hecht, `freefem++`, a general purpose finite element software allowing serval types of finite elements in one program, to appear.

[7] O. Pironneau, Optimal Shape Design of Elliptic Systems, in: Lecture Notes in Comput. Phys., Springer-Verlag, 1983.