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 $\kappa$ 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 $\kappa$. 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


Version française abrégée

La pression hydrostatique $u$ dans un milieu poreux de porosité $\kappa$ 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, $\kappa$ 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 $\kappa$ varie tout en restant constant par morceaux.
Problem statement. – More precisely, consider a bounded open set \( \Omega \) of \( \mathbb{R}^2 \) and a family of closed curves \( a \mapsto \Sigma(a) \) strictly inside \( \Omega \) and function of a scalar parameter \( a \) separating \( \Omega \) into two nonoverlapping sets \( \Omega_i(a) \), \( i = 1, 2 \), with Lipschitz continuous boundaries:

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

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 \( \mathbb{R}^2 \) and \( \mathbb{R}^3 \).

Let \( \kappa(a) \) be piecewise constant and equal to \( k_i \) 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 \( a \) of \( C^1(\Sigma) \) and the following local variation in the “direction” \( \alpha \) around \( \Sigma(0) \) taken as a reference curve:

\[
\Sigma(a) = \{ x + a\alpha(x)n(x) : x \in \Sigma(0) \},
\]

where \( n \) is the unit normal to \( \Sigma(0) \) which points outside \( \Omega_1 \). Let \( L^2(\Omega) = L^2(\Omega) \cap \mathbb{R}^2 \) and

\[
H(\div, \Omega) = \{ W \in L^2(\Omega)^d : \div W \in L^2(\Omega) \}, \quad X = \{ V \in H(\div, \Omega) : V \cdot n = 0 \text{ on } \partial \Omega \}.
\]

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

Find \( (U, u) \in X \times L^2(\Omega) \) with

\[
\forall w \in L^2(\Omega) \int_{\Omega} (\nabla \cdot U) w = \int_{\Omega} f w, \quad \forall W \in X \int_{\Omega} \frac{1}{\kappa} U \cdot W + \int_{\Omega} u \nabla \cdot W = 0.
\]

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

Next we observe that with a piecewise constant \( \kappa \)

\[
\frac{1}{\kappa(a)}(x) = \frac{1}{\kappa_1} + \left[ \frac{1}{\kappa} \right] I_{\Omega_1}, \quad \text{therefore } \frac{d}{da} \left( \frac{1}{\kappa} \right) = \alpha \delta_\Sigma \frac{1}{\kappa}
\]

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

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

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

\[
\left[ \frac{1}{\kappa} U \cdot W \right] = \left[ \frac{1}{\kappa} U \right] \cdot n W \cdot n = \left[ \frac{1}{\kappa} U \right] U \cdot n W \cdot n
\]
and so it seems that $U \cdot n \in L^2(\Sigma)$ 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

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

**Remark 1.** In the distribution sense (5) is $\nabla \cdot V = 0$. To eliminate $V$ we see that $\kappa$ does not have meaning on account of the discontinuity of $\kappa$ on $\Sigma$.

**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 $C^1$. Let $\Sigma$ be a smooth closed curve inside $\Omega$. Let $\kappa > 0$ be piecewise constant discontinuous across $\Sigma$ 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 $\Sigma$ in $H^{-1/2}(\Sigma)$. We need to show that $U \cdot n \in H^{1/2}(\Sigma)$.

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

For clarity the proof is given in dimension 2. Assume that $\Sigma$ is sufficiently regular so that in a neighborhood $O$ of $\Sigma$ we can define a coordinate system $\sigma, \nu$ in which the equation of $\Sigma$ is $\nu = 0$, $n$ the normal to $\Sigma$, is tangent to the curves $\sigma = $ constant and $\sigma$ is its curvilinear abscissa. Taking $u$ such that $\nabla \cdot \nabla w \in L^2(\Omega)$, $w = \partial w'/\partial \sigma$ in (3) in variational form, and by integrating by part in $\sigma$ we find that

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

because $\kappa$ is not a function of $\sigma$. This shows that if $f$ is regular all partial derivatives in $\sigma$ of $u$ are in $H^1(\Omega)$. Therefore $U \cdot \tilde{\sigma}$ has the same regularity. Now $\partial U / \partial \sigma = \kappa \tau^2 u / \partial \sigma^2$ belongs to $L^2(\Omega)$, so by $\nabla \cdot U = 0$ we see that $\nabla U / \partial \sigma|_{\Omega}$ is in $L^2(\Omega)$ for any open set $\Omega \subset \Omega$ not intersecting $\Sigma$.

Similarly, $U \cdot \tilde{\sigma} \in H^1(\Omega)$ implies $\partial U / \partial \sigma \in L^2(\Omega)$, i.e. $\partial U / \partial \sigma \in L^2(\Omega)$. Therefore $\nabla U / \partial \sigma = \kappa \tau^2 u / \partial \sigma^2$ is in $L^2(\Omega)$. Hence $U$ is in $H^1(\Omega)$.

**Corollary 3.2.** If $\Sigma$ is regular and $f \in W^{1,\infty}(\Omega)$ then $U \cdot n$ is continuous in $\Omega \setminus \Sigma$ and $U$ is in $L^\infty(\Omega)$.

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

4. Continuity

In order to study the changes $\delta u, \delta U$ 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

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

2. For the second equation we have

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The results are displayed in Fig. 1. Decreasing both \( n_\sigma \) and \( \alpha \), the numerical solution is calculated with \textit{freefem++} [6] and the mesh size gives convergence. The support \( \Sigma(a) \) of \( \delta \eta \) is a thin strip around \( \Sigma \) of width \( a \alpha \), and \( \eta + \delta \eta \) is either \( \kappa_{\max}^{-1} \) or \( \kappa_{\min}^{-1} \), therefore \( \| \delta \eta \| \leq C_1 (1/\kappa) \) for some constant \( C_1 \).

So we have the following result.

**Theorem 5.2.** – If \( U \in L^\infty(\Omega) \), the solution \( \{ \delta u, \delta U \} \) in \( \{ u, U \} \) due to \( a \) is bounded in \( L^2(\Omega) \times H(\text{div}, \Omega) \), verifies \( \nabla \cdot \delta U = 0 \) and \( \| \delta u \|_0 + \| \delta U \|_{H(\text{div}, \Omega)} \leq C_2 \| \alpha \|_0 \| \delta \eta \|_0 \).

5. Differentiability

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

\[
\lim_{a \to 0} \left\| \frac{\delta(\eta U)}{a} \right\| = 0.
\]

**Proof.** – See [4].

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

6. Discretization and numerical test

6.1. Discretization

Consider a regular family of triangulations of \( \Omega \) of maximum edge length \( h \) and two finite element spaces \( X_h \) and \( L_h \) to approximate \( \text{div}(\mathbf{V}) \) and \( L^2(\Omega) \). Although precision is increased when the triangulations approximate \( \Sigma \) 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

\[
\forall q \in L_h \int_\Omega (\mathbf{V} \cdot \mathbf{v}) q = 0, \quad \forall W \in X_h \int_\Omega \left[ \frac{1}{\kappa} V_h \cdot W + v_h \nabla \cdot W \right] = \int_\Sigma s \mathbf{v} \cdot n. \tag{10}
\]

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 satisfies the discrete inf-sup condition as shown in Achdou et al. [1], Proposition 3.14, when \( \mathbf{v} \in (H^s(\Omega))^2 \times H^s(\Omega), 0 < s \leq 1 \):

\[
\| \mathbf{V} - V_h \|_0 + \| v - v_h \|_0 \leq c h^s \left( \| \mathbf{V} \|_{H^s} + \| v \|_{H^s} \right).
\]

6.2. Numerical simulation

The numerical solution is calculated with \textit{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 \( \Omega = (-5.5) \times (-2.5, 2.5), \kappa = 6 \) inside an ellipse in the middle of the rectangle and 1 outside (Fig. 1). Then the ellipse is changed by \( \varepsilon \) according to

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

yielding a new solution \( u_\varepsilon \) 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 \( \varepsilon \) and the mesh size gives convergence:
7. Identification of a discontinuity

Consider an “observed” data $u_d$ on an observation set $S$ and the problem of finding the best $\kappa$ (i.e., the best $\Sigma$) 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 $\Sigma$ induces a change in $J$ and it is not hard to show that the derivative $J' = dJ/da$ is given by

$$J'(\kappa) = -\int_{\Sigma} \alpha \left[ \frac{1}{\kappa} \left( \kappa \frac{\partial u}{\partial n} \right) \left( \kappa \frac{\partial p}{\partial n} \right) \right]$$

with $p$ solution of $-\nabla \cdot (\kappa \nabla p) = 2(u - u_d)\delta_{S,p}$, $p|_\Gamma = 0$.

Assume that $\alpha = \alpha(r_1, r_2, \ldots, r_m)$. A gradient method on the position of $\Sigma$ with step size $\rho$, via the parameters $\{ r_i \}_{i=1}^m$ 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

$$\Omega = (-5, 5) \times (-2.5, 2.5), \quad D = \{ (x, y) : (x + 2)^2 + y^2 < 1 \},$$

$$\Sigma(r_1, r_2) = \{ (x, y) : x = (r_1 + r_2 \cos t) \cos t, \quad y = (r_1 + r_2 \cos t) \sin t \}$$

Figure 1. – The coefficient $\kappa$ is constant on $\Omega_1$ and constant on $\Omega_2$ and discontinuous across $\Sigma$. When $\Sigma$ becomes $\Sigma(\alpha)$, the distance from $\Sigma(\alpha)$ to $\Sigma$ is $a\|a\|_\infty$, the solution of the partial differential equation changes. We wish to find the derivative with respect to $a$ for a given function $\alpha$.

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

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 \( r_1 - \sqrt{2} \), 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 \( \Sigma \) and 6 inside. We chose \( u_d \) to be the solution of the PDE for \( \kappa \) 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 \( \Sigma \). Now we move \( D \) to the right and \( \Sigma \) 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 \( \Sigma \) 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