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Analysis of Curvature Influence on Effective Boundary Conditions

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Abstract. The aim of this work is the construction of effective boundary conditions (wall laws) for elliptic problems defined in domains with curved, rough boundaries with periodic wrinkles. We present error estimates for first and second order approximations, and a numerical test.

Analyse de l'Influence de la Courbure sur les Conditions aux Limites Équivalentes

Résumé. *Ce travail a pour objectif le développement de conditions aux limites équivalentes (lois de paroi) pour des problèmes elliptiques définis dans un domaine courbe ayant une interface rugueuse avec des rugosités périodiques. On présente des estimations d'erreur pour les approximations au premier et deuxième ordres. L'approche est validée par un test numérique.*

Version française abrégée

Dans ce travail, on s'intéresse au développement et à l'analyse de conditions aux limites équivalentes (CLE) ou lois de paroi pour des problèmes elliptiques définis dans un domaine courbe ayant une interface oscillante. On s'inspire des techniques de décompostion de domaines (Lemme 0.1) proposées dans [1] et [4] pour traiter des domaines arbitrairement courbes et rugueux (figure 1). L'approche permet de remplacer l'interface oscillante par une surface régulière sur laquelle on impose les lois de paroi. Les CLEs prennent en compte de façon homogénéisé l'influence des échelles rapides, par la résolution de problèmes locaux contenant la géométrie de la rugosité (8), (9), (10), (17) et (18). L'influence de la courbure du domaine sur la forme des CLEs est explicitée par le changement de variables (5). Cela nous permet de reproduire la loi de paroi d'ordre un (11) presentée dans [1] et d'introduire une nouvelle loi de paroi d'ordre deux (15)

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contenant des termes dépendents de la courbure. Des Théorèmes de convergence 1.1 et 2.1 sont démontrés et sont basés sur les Lemmes auxiliaires 1.2, 1.3 et 2.2. Un test numérique montre l'importance de l'utilisation des CLEs (figures 2 et 3).

The presence of wrinkles on curved boundaries have a great influence on solutions of PDEs, depending on the form of the roughness elements and on the interface curvature—see [3] for interesting experimental results in aerodynamics. The use of effective boundary conditions (wall laws) reduces the high computational costs associated with numerical discretizations. One of the authors (Valentin) introduced several boundary conditions for different PDEs in domains limited by rough but otherwise straight boundaries [4]. Concerning curved boundaries, a worthy work was done by Achdou and Pironneau [1], where they obtained a first order approximation for the Poisson problem. We employ here a completely different strategy, that allows the construction of higher order approximations for elliptic problems in domains with quite arbitrary curved rough boundaries.

The outline of this paper is as follows. We conclude this introduction by characterizing the domain, defining a related PDE problem, and stating a lemma upon which we base our estimates. Section 1 includes the development of a first order approximation that is based on a combination of domain decomposition techniques and a suitable change of coordinates. In Section 2, similar ideas help the development of a second order approximation. Finally, Section 3 contains a numerical example.

Let Ω^ε be a two-dimensional domain, where $\mathbf{x}$ is a typical point in it. We define a smooth "baseline" Γ_b, which we arc-length parametrize by a smooth, injective, ε-independent function $\boldsymbol{\psi}_b : (0, L) \to \Gamma_b$. The bottom boundary of Ω^ε is the rough curve Γ_r^ε, where ε indicates the length scale of the rugosity, and $\varepsilon = L/N$ for some positive integer N. The curve Γ_r^ε is defined as a perturbation of Γ_b, and parametrized by $\boldsymbol{\psi}^\varepsilon(\theta) = \boldsymbol{\psi}_b(\theta) - \varepsilon\psi_r(\varepsilon^{-1}\theta)\mathbf{n}(\theta)$, where $\mathbf{n}$ is the outward normal to Γ_b. The function $\psi_r : \mathbb{R} \to \mathbb{R}$ is independent of ε, Lipschitz-continuous with $\psi_r(0) = 0$, and periodic of period 1. For technical reasons we impose $\varepsilon\|\psi_r\|_{L^\infty(\mathbb{R})}$ to be smaller than the minimum radius of curvature of the baseline Γ_b.

The lateral boundaries of Ω^ε are straight lines, which are normal to the baseline Γ_b. Finally, the top boundary is given by another injective, Lipschitz-continuous curve. The theory is quite similar if Γ_r^ε defines an inner border limited by a Lipschitz-continuous outer boundary.

Consider the problem

$$\begin{aligned} -\Delta u^\varepsilon &= f \quad \text{in } \Omega^\varepsilon, \\ u^\varepsilon &= 0 \quad \text{on } \partial\Omega^\varepsilon. \end{aligned} \tag{1}$$

We define now subdomains of Ω^ε (figure 1), one "smooth", the other "rough". Let δ be smaller than the minimum radius of curvature of Γ_b, but $\delta > \varepsilon\|\psi_r\|_{L^\infty(\mathbb{R})}$. Let

$$\Omega_s = \{\, \mathbf{x} \in \Omega^\varepsilon : \operatorname{dist}(\mathbf{x}, \Gamma_b) > \delta \,\}, \qquad \Omega_r^\varepsilon = \{\, \mathbf{x} \in \Omega^\varepsilon : \operatorname{dist}(\mathbf{x}, \Gamma_b) < \delta \,\},$$
$$\Gamma = \{\, \mathbf{x} \in \Omega^\varepsilon : \operatorname{dist}(\mathbf{x}, \Gamma_b) = \delta \,\}.$$

For simplicity, we assume that the support of f does not intercept Γ or Ω_r^ε. It is possible to withdraw this restriction at the expense of including a few extra terms in our computations.

Let $u_s : \Omega_s \to \mathbb{R}$, and $u_r : \Omega_r^\varepsilon \to \mathbb{R}$ be approximations of u^ε in their respective domains, and define the corresponding error by

$$e = \begin{cases} u^\varepsilon - u_s & \text{in } \Omega_s, \\ u^\varepsilon - u_r & \text{in } \Omega_r^\varepsilon. \end{cases} \tag{2}$$

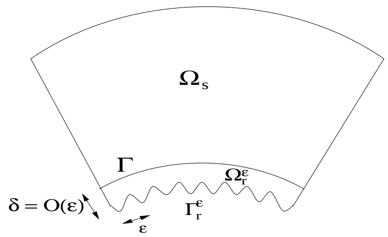

Figure 1: Domain decomposition strategy.

The error estimates will be based on the following lemma [1].

LEMMA 0.1. – *Let Ω be a domain of $\mathbb{R}^2$ and Γ an interface dividing Ω in two subdomains Ω^- and Ω^+. If $e = 0$ on $(\partial\Omega^-\backslash\Gamma) \cup (\partial\Omega^+\backslash\Gamma)$, there exists a constant c such that*

$$\|e\|^2_{1,\Omega^-} + \|e\|^2_{1,\Omega^+} \leqslant -\int_{\Omega^-\cup\Omega^+} e\,\Delta\, e\, d\mathbf{x} + c\left(\|[e]\|_{\frac{1}{2},\Gamma}\|e\|_{1,\Omega^+} + \left\|\left[\frac{\partial e}{\partial n}\right]\right\|_{-\frac{1}{2},\Gamma}\|e\|_{1,\Omega^-}\right),$$

where $[\cdot]$ represents the jump function over Γ.

1. First Order Approximation

Assume that u_s satisfies the following equations:

$$-\Delta\, u_s = f \quad \text{in } \Omega_s, \qquad u_s = 0 \quad \text{on } \partial\Omega_s\backslash\Gamma. \tag{3}$$

Ideally, u_r would satisfy similar restrictions, that is,

$$-\Delta\, u_r = 0 \quad \text{in } \Omega_r^\varepsilon, \qquad u_r = 0 \quad \text{on } \partial\Omega_r^\varepsilon\backslash\Gamma. \tag{4}$$

We do not impose (4) exactly though, only up to powers of ε. To fully understand the influence of the curvature and of the small parameter ε, we rewrite (4) using boundary fitted coordinates in Ω_r^ε.

We digress then to introduce these coordinates [2]. For a given $\theta \in (0, L)$, and $\rho = \operatorname{dist}(\mathbf{x}, \Gamma_b) \in (\psi_r(\theta), \delta)$, a point $\mathbf{x}(\rho,\theta) = \boldsymbol{\psi}_b(\theta) - \rho\mathbf{n}(\theta)$ in Ω_r^ε. Note that for δ small enough, the above map is reversible. Let κ be the curvature of Γ_b, defined by the identity $\mathbf{n}' = \kappa\mathbf{s}$, where $\mathbf{s} = \boldsymbol{\psi}_b'$, and let $J(\rho,\theta) = 1 - \rho\kappa(\theta)$. The expression for the Laplacian in these new coordinates follows:

$$\partial_{11}U + \partial_{22}U = \partial_{\rho\rho}U - \frac{\kappa}{J}\partial_\rho U + \frac{1}{J^2}\partial_{\theta\theta}U + \frac{\rho\kappa'}{J^3}\partial_\theta U = \partial_{\rho\rho}U + \sum_{j=0}^{\infty}\rho^j\left(a_1^j\partial_\rho U + a_2^j\partial_{\theta\theta}U + a_3^j\partial_\theta U\right), \tag{5}$$

where we formally replace each coefficient with its respective Taylor expansion, and $a_1^j = -[\kappa(\theta)]^{j+1}$, $a_2^j = (j+1)[\kappa(\theta)]^j$, $a_3^j = j(j+1)[\kappa(\theta)]^{j-1}\kappa'(\theta)/2$. To make the influence of ε in (5) explicit, we define new variables $\hat\rho = \varepsilon^{-1}\rho$, and $\hat\theta = \varepsilon^{-1}\theta$, and add hats to functions in the new coordinates, for instance, $\hat U(\hat\rho,\hat\theta) = U(\mathbf{x}(\varepsilon\hat\rho,\varepsilon\hat\theta))$.

Motivated by the geometry of the rough domain Ω_r^ε, we assume that

$$u_r(\mathbf{x}) = -\varepsilon\hat\chi^0(\hat\rho,\hat\theta)\phi(\theta), \tag{6}$$

where we define $\hat\chi^0$ and ϕ further below. Using (5) and (6), we rewrite equation (4) as

$$\begin{aligned}\partial_{11}u_r + \partial_{22}u_r &= -\varepsilon^{-1}\left(\partial_{\hat\rho\hat\rho}\hat\chi^0 + \partial_{\hat\theta\hat\theta}\hat\chi^0\right)\phi + \kappa\partial_{\hat\rho}\hat\chi^0\phi - 2\partial_{\hat\theta}\hat\chi^0\phi' - 2\kappa\hat\rho\partial_{\hat\theta\hat\theta}\hat\chi^0\phi \\ &- \sum_{j=0}^{\infty}\varepsilon^{j+1}\hat\rho^j\left(a_2^j\hat\chi^0\phi'' + a_3^j\hat\chi^0\phi' + \hat\rho a_1^{j+1}\partial_{\hat\rho}\hat\chi^0\phi + 2a_2^{j+1}\hat\rho\partial_{\hat\theta}\hat\chi^0\phi' + a_3^{j+1}\hat\rho\partial_{\hat\theta}\hat\chi^0\phi + a_2^{j+2}\hat\rho^2\partial_{\hat\theta\hat\theta}\hat\chi^0\phi\right).\end{aligned} \tag{7}$$

Based on (7), we impose

$$\partial_{\hat\rho\hat\rho}\hat\chi^0 + \partial_{\hat\theta\hat\theta}\hat\chi^0 = 0 \quad \text{in } \Omega_r. \tag{8}$$

Such domain Ω_r occupies the region limited by straight lateral boundaries at $\hat\theta = 0$ and $\hat\theta = 1$, and by the lower and upper boundaries $\Gamma_r^- = \{\, (\psi_r(\hat\theta), \hat\theta) : \hat\theta \in (0,1)\,\}$, and $\Gamma_r^+ = \{\, (\delta/\varepsilon, \hat\theta) : \hat\theta \in (0,1)\,\}$. The choice $\delta = l_0\varepsilon$, where the ε-independent constant $l_0 > \|\psi_r\|_{L^\infty(0,1)}$ renders Ω_r independent of ε as well. From (1) and (6), and motivated by the periodic geometry, we impose

$$\hat\chi^0 = 0 \quad \text{on } \Gamma_r^-, \qquad \hat\chi^0 \text{ is } \hat\theta\text{-periodic.} \tag{9}$$

We want now to use Lemma 0.1. Since, from (6),

$$\left[\frac{\partial e}{\partial n}\right] = \frac{\partial u_s}{\partial n} - \partial_{\hat\rho}\hat\chi^0\phi \quad \text{on } \Gamma,$$

we define

$$\partial_{\hat\rho}\hat\chi^0 = 1 \quad \text{on } \Gamma_r^+, \qquad \phi = \frac{\partial u_s}{\partial n} \quad \text{on } \Gamma, \tag{10}$$

and the jump on Γ of the normal derivative of the error vanishes. Since $\partial u_s/\partial n$ is defined on Γ, we shall describe this function as depending on θ only. Next, using (6), $[e] = u_s + \varepsilon\hat\chi^0\partial u_s/\partial n$, and defining $\langle\hat\chi^0\rangle = \int_{\Gamma_r^+}\hat\chi^0\,ds$, we set

$$u_s + \varepsilon\langle\hat\chi^0\rangle\frac{\partial u_s}{\partial n} = 0 \quad \text{on } \Gamma. \tag{11}$$

From the weak maximum principle, $\hat\chi^0$ is nonnegative, and then $\langle\hat\chi^0\rangle$ is positive. We conclude that

$$[e] = (\hat\chi^0 - \langle\hat\chi^0\rangle)\frac{\partial u_s}{\partial n} \quad \text{on } \Gamma. \tag{12}$$

To sum up, the approximations of u^ε are then defined as follows. From (6), and (10), we have $u_r = -\varepsilon\hat\chi^0(\hat\rho,\hat\theta)\partial u_s(\theta)/\partial n$, where the function $\hat\chi^0$ is $\hat\theta$-periodic with period equal to 1, and satisfies (8), (9), (10). Finally, (3), (11) define u_s. The following convergence result holds.

Theorem 1.1 (first order) *Let e be defined as in* (2)*, where u^ε solves* (1)*, u_s satisfies* (3), (11)*, and u_r is as in* (6)*. Then there exists a constant c independent of ε such that*

$$\|e\|_{1,\Omega_s} + \|e\|_{1,\Omega_r^\varepsilon} \leqslant c\varepsilon^{3/2}.$$

The proof of the above theorem uses Lemma 0.1, and the two lemmas below.

LEMMA 1.2. – *Let $\hat\chi^0$ be defined by* (8), (9), (10)*. Then there exists a constant c independent of ε, δ and l_0 such that $\left\|\hat\chi^0 - \langle\hat\chi^0\rangle\right\|_{\frac{1}{2},\Gamma_r^+} \leqslant c\exp(-2\pi\delta/\varepsilon)$.*

LEMMA 1.3. – *For all $m \in \mathbb{N}$, there exists a constant c independent of ε such that $\|u_s\|_{W^{m,\infty}(\Gamma)} \leqslant c\varepsilon$.*

2. Second Order Approximation

In several instances, a first order approximation is not close enough to the exact solution, and it is desirable to have higher order approximations [4]. We show here how this is done in the case of a Poisson problem. From the previous definition of u_r, equations (6), (7), (8), and the identity

$$\partial_\theta\frac{\partial u_s}{\partial n} = (1 - \delta\kappa)\frac{\partial^2 u_s}{\partial n\partial s} \quad \text{on } \Gamma,$$

it follows that

$$\partial_{11}u_r + \partial_{22}u_r = \kappa\partial_{\hat\rho}\hat\chi^0\frac{\partial u_s}{\partial n} - 2\partial_{\hat\theta}\hat\chi^0\frac{\partial^2 u_s}{\partial n\partial s} - 2\kappa\hat\rho\partial_{\hat\theta\hat\theta}\hat\chi^0\frac{\partial u_s}{\partial n} + R\big(\hat\chi^0, \frac{\partial u_s}{\partial n}\big), \tag{13}$$

where the remainder R satisfies $\|R\|_{L^\infty(\Omega_r^\varepsilon)} \leqslant c\varepsilon$. Motivated by (13), we redefine u_r as

$$u_r(\mathbf{x}) = -\varepsilon\hat{\chi}^0(\hat{\rho},\hat{\theta})\frac{\partial u_s}{\partial n}(\theta) - \varepsilon^2\kappa(\theta)\hat{\chi}^1(\hat{\rho},\hat{\theta})\frac{\partial u_s}{\partial n}(\theta) - \varepsilon^2\hat{\chi}^2(\hat{\rho},\hat{\theta})\frac{\partial^2 u_s}{\partial n\partial s}(\theta), \tag{14}$$

where we choose the functions $\hat{\chi}^1$ and $\hat{\chi}^2$ such that $\hat{\chi}^1 = \hat{\chi}^2 = 0$ on Γ_r^- and

$$-\partial_{\hat{\rho}\hat{\rho}}\hat{\chi}^1 - \partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^1 = -\partial_{\hat{\rho}}\hat{\chi}^0 + 2\hat{\rho}\partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^0 \quad \text{in } \Omega_r, \qquad -\partial_{\hat{\rho}\hat{\rho}}\hat{\chi}^2 - \partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^2 = 2\partial_{\hat{\theta}}\hat{\chi}^0 \quad \text{in } \Omega_r.$$

Using again Lemma 0.1, we proceed to minimize the error jump at the interface. From (14),

$$\left[\frac{\partial e}{\partial n}\right] = \frac{\partial u_s}{\partial n} - \partial_{\hat{\rho}}\hat{\chi}^0\frac{\partial u_s}{\partial n} - \varepsilon\kappa\partial_{\hat{\rho}}\hat{\chi}^1\frac{\partial u_s}{\partial n} - \varepsilon\partial_{\hat{\rho}}\hat{\chi}^2\frac{\partial^2 u_s}{\partial n\partial s}.$$

Hence, since (10) holds, $[\partial e/\partial n]$ vanishes if $\partial_{\hat{\rho}}\hat{\chi}^1 = \partial_{\hat{\rho}}\hat{\chi}^2 = 0$ on Γ_r^+. In addition,

$$[e] = u_s + \varepsilon\hat{\chi}^0\frac{\partial u_s}{\partial n} + \varepsilon^2\kappa\hat{\chi}^1\frac{\partial u_s}{\partial n} + \varepsilon^2\hat{\chi}^2\frac{\partial^2 u_s}{\partial n\partial s} \quad \text{on } \Gamma.$$

Choosing

$$u_s + \varepsilon\left(\left\langle\hat{\chi}^0\right\rangle + \varepsilon\kappa\left\langle\hat{\chi}^1\right\rangle\right)\frac{\partial u_s}{\partial n} + \varepsilon^2\left\langle\hat{\chi}^2\right\rangle\frac{\partial^2 u_s}{\partial n\partial s} = 0 \quad \text{on } \Gamma, \tag{15}$$

the jump error of the solution is

$$[e] = \varepsilon\left(\hat{\chi}^0 - \left\langle\hat{\chi}^0\right\rangle\right)\frac{\partial u_s}{\partial n} + \varepsilon^2\kappa\left(\hat{\chi}^1 - \left\langle\hat{\chi}^1\right\rangle\right)\frac{\partial u_s}{\partial n} + \varepsilon^2\left(\hat{\chi}^2 - \left\langle\hat{\chi}^2\right\rangle\right)\frac{\partial^2 u_s}{\partial n\partial s} \quad \text{on } \Gamma. \tag{16}$$

Motivated by the periodicity of the roughness elements we impose that $\hat{\chi}^1$ and $\hat{\chi}^2$ are $\hat{\theta}$-periodic. So, the functions $\hat{\chi}^1$ and $\hat{\chi}^2$ are the solution of the following Poisson problems:

$$\begin{gathered} -\partial_{\hat{\rho}\hat{\rho}}\hat{\chi}^1 - \partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^1 = -\partial_{\hat{\rho}}\hat{\chi}^0 + 2\hat{\rho}\partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^0 \quad \text{in } \Omega_r, \\ \hat{\chi}^1 = 0 \quad \text{on } \Gamma_r^-, \qquad \partial_{\hat{\rho}}\hat{\chi}^1 = 0 \quad \text{on } \Gamma_r^+, \qquad \hat{\chi}^1 \text{ is } \hat{\theta}\text{-periodic,} \end{gathered} \tag{17}$$

and

$$\begin{gathered} -\partial_{\hat{\rho}\hat{\rho}}\hat{\chi}^2 - \partial_{\hat{\theta}\hat{\theta}}\hat{\chi}^2 = 2\partial_{\hat{\theta}}\hat{\chi}^0 \quad \text{in } \Omega_r, \\ \hat{\chi}^2 = 0 \quad \text{on } \Gamma_r^-, \qquad \partial_{\hat{\rho}}\hat{\chi}^2 = 0 \quad \text{on } \Gamma_r^+, \qquad \hat{\chi}^2 \text{ is } \hat{\theta}\text{-periodic.} \end{gathered} \tag{18}$$

From (3) and (15), u_s is well-defined, and the following error estimate follows.

Theorem 2.1 (second order) *Let e be defined as in* (2)*, where u^ε solves* (1)*, u_s satisfies (3), (15), and u_r is as in* (14)*. Then there exists a constant c independent of ε such that*

$$\|\, e\|_{1,\Omega_s} + \|\, e\|_{1,\Omega_r^\varepsilon} \leqslant c\varepsilon^{5/2}.$$

The proof is based on Lemmas 0.1, 1.2, 1.3 and on the following result.

LEMMA 2.2. – *Let $\hat{\chi}^1$ and $\hat{\chi}^2$ be defined by* (17) *and* (18) *respectively. Then there exist positive constants c and α, both independent of ε, δ and l_0, such that $\left\|\hat{\chi}^1 - \langle\hat{\chi}^1\rangle\right\|_{\frac{1}{2},\Gamma_r^+} + \left\|\hat{\chi}^2 - \langle\hat{\chi}^2\rangle\right\|_{\frac{1}{2},\Gamma_r^+} \leqslant c\exp(-\alpha\delta/\varepsilon)$.*

Remark 1. – *It is convenient, in terms of implementation, to introduce another second order wall law, which is equivalent to* (15)*, up to higher order powers of ε. Its derivation comes from taking the tangential derivative of* (15)*, and replacing the computed value of $\partial^2 u_s/\partial n\partial s$ back in* (15)*. The result is*

$$u_s + \varepsilon\left(\left\langle\hat{\chi}^0\right\rangle + \varepsilon\kappa\left\langle\hat{\chi}^1\right\rangle\right)\frac{\partial u_s}{\partial n} - \varepsilon\frac{\left\langle\hat{\chi}^2\right\rangle}{\langle\hat{\chi}^0\rangle + \varepsilon\kappa\left\langle\hat{\chi}^1\right\rangle}\frac{\partial u_s}{\partial s} = 0 \quad \textit{on } \Gamma. \tag{19}$$

To the best of our knowledge, the second order wall law (15) is new in the literature. In our numerical tests (next section) it improved the results, and the presence of the curvature term was essential. The importance of second order laws was already investigated by Valentin [4] in the flat case (zero curvature).

3. Numerical Validation: Rough Cylinder

We consider a squared domain of size 4, having as inner boundary a rough circle of unitary radius, with periodically distributed roughness elements of height 0.1. We test a variation of (1), imposing $f = 0$, but with $u = 1$ at the outer boundary. We obtain an "exact" solution by fully discretizing the rough domain with a very refined mesh. The approximate solutions are defined in a similar, but wrinkle-free domain with $\delta = 0.15$. The first order solution employs the wall law (11), and the second order solution is based on (19). Figure 2 shows the isolines and profiles of the solutions for the cell problems (8), (9), (10), and (17). In figure 3 we compare the exact solution, with the first and second order approximations. As we can see in the profile depicted, close to the rough boundary the second order approximation yields better results.

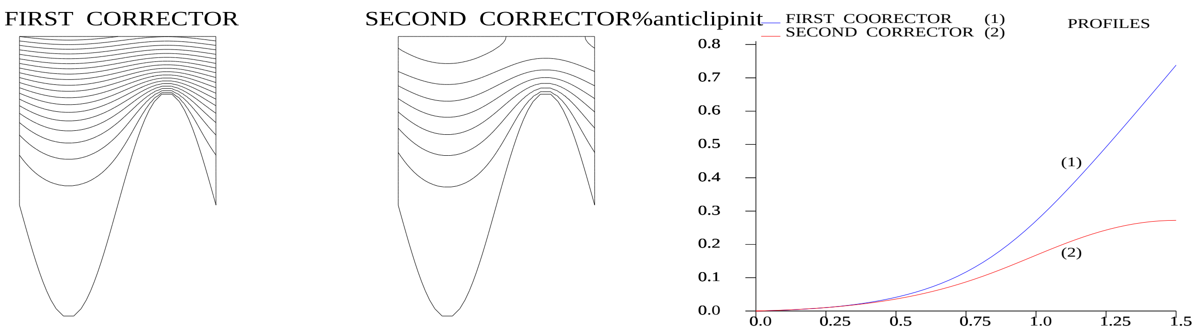

Figure 2: Isovalues and profiles at $\hat{\theta} = 0.78$ for the first and second order cell problem solutions.

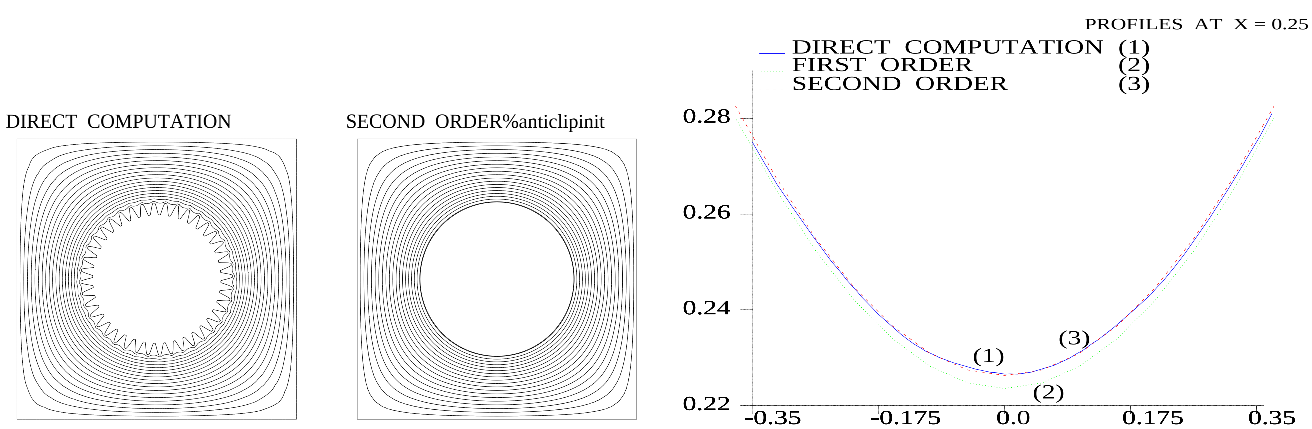

Figure 3: Second order approximation solves accurately the original problem.

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