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Laplacian transfer across a rough interface: Numerical resolution in the conformal plane

Damien Vandembroucq and Stéphane Roux*

*Surface du Verre et Interfaces,
Unité Mixte de Recherche CNRS/Saint-Gobain,
39 Quai Lucien Léfranc,
93303 Aubervilliers cedex, France.*

We use a conformal mapping technique to study the Laplacian transfer across a rough interface. Natural Dirichlet or Von Neumann boundary condition are simply read by the conformal map. Mixed boundary condition, albeit being more complex can be efficiently treated in the conformal plane. We show in particular that an expansion of the potential on a basis of evanescent waves in the conformal plane allows to write a well-conditioned 1D linear system. These general principle are illustrated by numerical results on rough interfaces.

I. INTRODUCTION

Various physical phenomena such as the diffusion of oxygen molecules through lungs, the complex impedance of a rough electrode, the heterogeneous catalysis on a rough or porous substrate can be described by the simple model of Laplacian transport across irregular boundaries[1]. Although very simple in the case of plane or smooth interfaces, the resolution of the problem becomes extremely arduous as soon as the geometry of the boundary is irregular. The interest for this question was stimulated when it appeared that the irregularity of numerous surfaces could be mathematically modelled as fractal and in the last two decades a large number of works have been devoted to this question, notably by Sapoval and coworkers, who clarified these different problems through seminal contributions.

The fractal description of rough or porous electrodes allowed them to obtain exact results in the case of deterministic fractal electrodes[2] and more generally this motivated the use of scaling arguments [3, 4] in the study of the constant phase angle (CPA) behavior of rough electrodes. More recently, they showed that the frequential behavior of a rough electrode could be obtained by studying the spectral properties of the so-called self-transport operator[5, 6]. The latter measures the probability for two given sites of an interface to be linked by random walk through the electrolyte. One of the difficulty raised by the Laplacian transport through irregular interfaces comes from the nature of a physically sound boundary condition (b.c.). Neither Dirichlet nor Neumann type do apply, but rather a mixed b.c. holds quite generally, namely $V = \Lambda \partial_n V$ where V is the potentiel and \vec{n} the outward normal to the interface. The length Λ is the ratio of the surface resistance of the electrode to the resistivity of the electrolyte. To overcome this difficulty Sapoval [7] proposed to replace the mixed b.c. by a Dirichlet condition on an equivalent interface obtained by coarse graining at the scale Λ from the original interface.

In the same spirit one can also think of replacing the b.c. on the rough interface by a derived one on a plane interface. In two dimensions, this can be easily performed by a conformal map[8, 9]. For a simple b.c. such as Dirichlet (constant potentiel) or Von Neumann (constant flux), the harmonic problem is entirely solved once the conformal map has been determined: the solutions are precisely given by the real and imaginary parts of the map from the rough electrode to the plane one. However, in case of a mixed b.c., the situation becomes more complex: the “simple” mixed b.c. on a rough interface has to be replaced by a “heterogeneous” b.c. on the equivalent plane interface. The “heterogeneity” of the b.c. simply reflects the harmonic measure on the original interface. A related difficulty arises when studying a Stokes flow along a rough boundary[9], the conformal map thus transforms the original bi-Laplacian equation into a more complex equation where the derivative of the conformal map acts as a non constant coefficient. In the last two cases, however, one can show that the use of a conformal map helps computing the potential in spite of the complexity of the equivalent equation or boundary condition. Expanding the potential on a basis of evanescent waves in the conformal plane allows us to write a well conditioned linear system, a much more laborious work in the original geometry. Let us emphasize that the conditioning (and hence precision) of the formulation is the most salient interest of the approach.

In the following, we recall how to compute a conformal map onto a two-dimensional domain bounded by a single valued interface; then we write down the equivalent linear system corresponding to the resolution of the Laplacian transfer across a rough interface. We finally present numerical results.

*Electronic address: damien.vandembroucq@saint-gobain.com; stephane.roux@saint-gobain.com

II. CONFORMAL MAP

The conformal half-plane and the physical domain are referenced by the complex coordinates $z = x + iy$ and $w = u + iv$ respectively and defined by $y < 0$ and $v < h(u)$, where h is a known function periodic of period 2π . There exists a map $w = \Omega(z)$ such that the image of the axis $y = 0$, is the rough interface. Equivalently, we can write $\Im[\Omega^{-1}(u + ih(u))] = 0$.

The map Ω is chosen under the form: $\Omega(z) = z + 2 \sum_{k=0}^N \bar{a}_k e^{-ikz}$, coordinate by coordinate, we have:

$$\begin{cases} u &= x + \sum_{k=0}^N \bar{a}_k e^{-ikx} + \sum_{k=0}^N a_k e^{ikx} = x + \sum_{k=-N}^N c_k e^{ikx} \\ h(u) &= \sum_{k=0}^N (\bar{ia}_k) e^{-ikx} + \sum_{k=0}^N (ia_k) e^{ikx} = \sum_{k=-N}^N b_k e^{ikx} \end{cases} \quad (1)$$

with $b_k = ia_k$ for $k > 0$, $b_k = -i\bar{a}_{-k} = \bar{b}_{-k}$ for $k < 0$, and $b_0 = i(a_0 - \bar{a}_0)$. Simultaneously $c_k = a_k$ with $k > 0$, $c_k = \bar{a}_{-k}$ for $k < 0$, and $c_0 = a_0 + \bar{a}_0$. Thus $c_k = -i \text{sign}(k) b_k$

The computation of a_k is made through the following steps: let us assume as a starting hypothesis $x \approx u$. Then from Eq. 1, b_k is given by the Fourier transform of $h(x)$. We construct the c_k as the Hilbert transform of h , and thus we have access to a first corrected estimate of $u(x)$. Therefore for an arithmetic sequence of x , an *unevenly* distribution sequence of u results, which is used to sample $h(u(x))$. The iteration of this step can be shown to converge as soon as the maximum local slope of the interface is lower than unity[8], and the latter constraint can be relaxed using under-relaxation at the expense of computational efficiency.

III. USE OF THE MAP FOR HARMONIC PROBLEM SOLUTIONS

The determination of the conformal map gives a direct solution for the equipotential condition $V = V_0$ along the boundary and a prescribed gradient $\partial_y V = \alpha$ far from the interface: $V = V_0 + \alpha y = V_0 + \alpha \Im[\Omega^{-1}(w)] q$. Similarly, the solution for zero flux flowing out of the boundary is obtained from the real part of the inverse conformal map. Other b.c. require some more work. In the case of a prescribed inhomogeneous potential, Dirichlet condition, the field in the entire domain is obtained from a single 1D Fourier transform of the imposed potential. The extension of the solution to the bulk is naturally provided by using evanescent modes in the conformal domain.

In the case of inhomogeneous Neumann b.c., one should take into account the fact that in the mapping the gradients are transformed. Let us first introduce the following notation concerning the gradient of a scalar real function A . The gradient is a vector of coordinates $(\partial_u A, \partial_v A)$, can be represented as a complex number $\partial_u A + i\partial_v A = \partial_{\bar{w}} A$. In the transformed domain, we have

$$\partial_{\bar{z}} A = \overline{\Omega'(z)} \partial_{\bar{w}} A \quad (2)$$

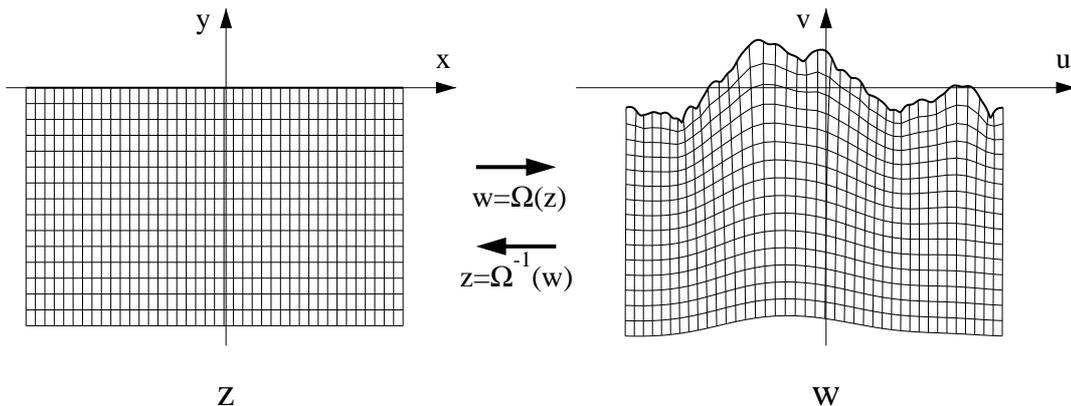


FIG. 1: Conformal map from the lower half-plane onto a domain bounded by an arbitrary (single valued) rough interface. The image of the regular mesh gives a direct access to the equipotential and current lines in the rough geometry.

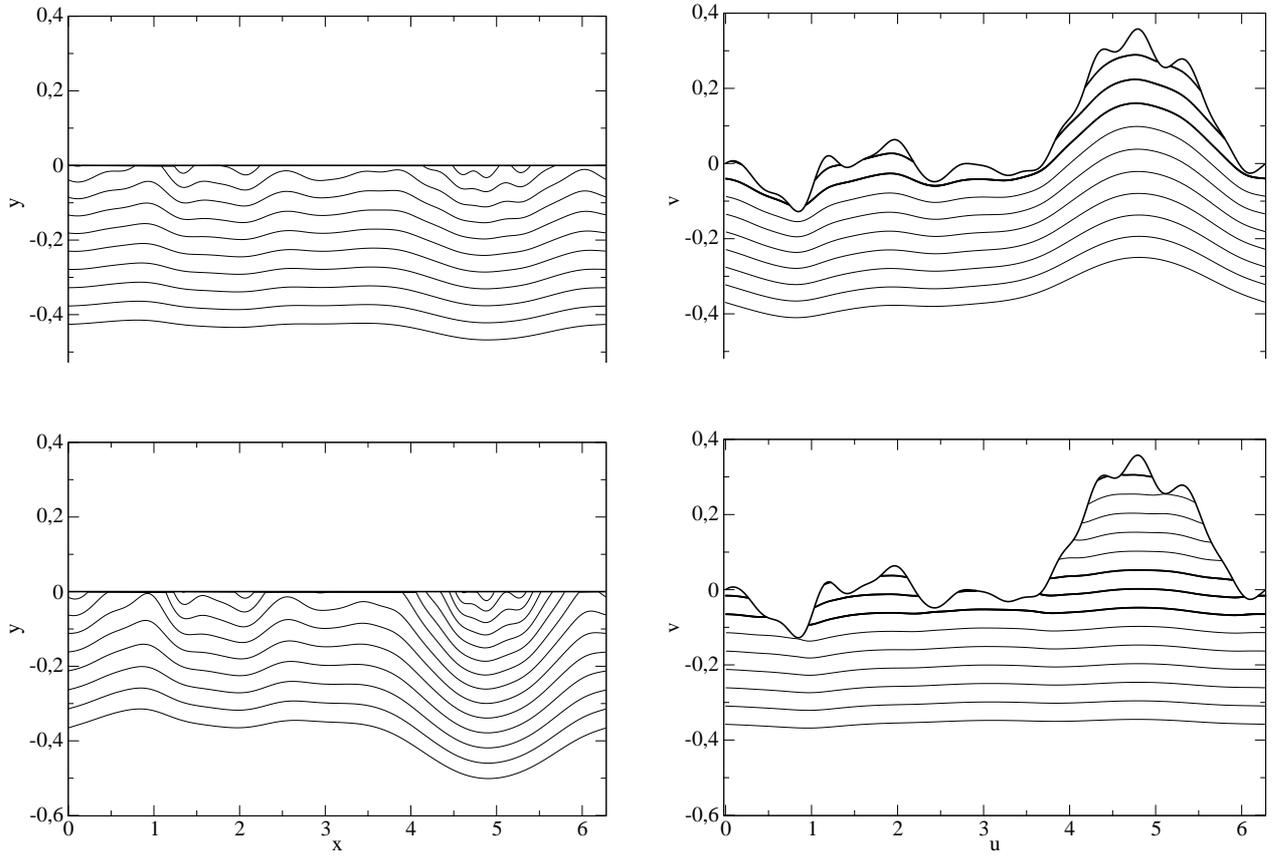


FIG. 2: Equipotential lines in the conformal geometry (left) and in the physical domain (right) for two mixed boundary conditions: $\Lambda = 0.25$ (above) and $\Lambda = 4$ (below). The bold curve represents the interface.

For a prescribed flux, once the conformal map has been obtained, the transformed flux in the z plane is obtained from the above formula. Again looking for a decomposition of the potential over a basis of exponential functions gives a straightforward answer. For the case of mixed boundary conditions, the problem appears to be somewhat more complicated. We will consider a simple case of a boundary condition written as

$$V = \Lambda(\vec{\nabla}V)\vec{n} \quad (3)$$

where \vec{n} is the unit normal to the boundary, and where Λ is a characteristic length scale. In the far field, $y \rightarrow -\infty$, we impose $\vec{\nabla}V \rightarrow \vec{e}_y$. In the reference plane z , the normal component of the gradient is along the y axis, since the conformal map preserves angles. The boundary condition written in the reference plane is thus

$$|\Omega'(z)|V(z) = \Lambda(\partial_y V) \quad (4)$$

We search $V(z)$ as the real part of a sum of evanescent modes:

$$V(z) = y + \alpha_0 + \Re \left[\sum_{n \geq 1} 2\alpha_n e^{-inz} \right] \quad (5)$$

Because the conformal map has been determined in a first step, the $|\Omega'(z)|$ is known. We naturally introduce its Fourier transform, so that

$$|\Omega'(x, 0)| = \beta_0 + \Re \left[\sum_{n \geq 1} 2\beta_n e^{-inx} \right] = \beta_0 + \sum_{n=1}^N \beta_n e^{-inx} + \sum_{n=1}^N \overline{\beta_n} e^{inx} . \quad (6)$$

The satisfaction of the boundary condition (4) thus leads to:

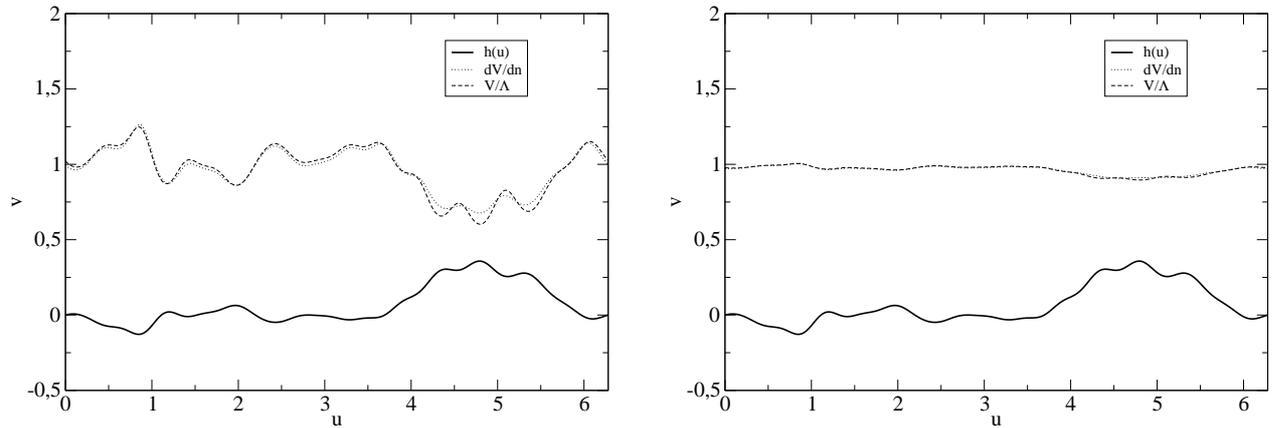


FIG. 3: Satisfaction of the mixed boundary condition along the rough interface for the two mixed boundary conditions $\Lambda = 0.25$ (left) and $\Lambda = 4$ (right).

$$\alpha_0\beta_0 + \sum_{k=1}^N (\alpha_k\overline{\beta_k} + \overline{\alpha_k}\beta_k) = \Lambda \quad \text{and} \quad (A_{nk} - 2\pi n\delta_{nk})\alpha_k = 0 \quad (n \geq 1) \quad (7)$$

where $A_{nk} = \beta_{n-k}$ if $k \leq n$ and $A_{nk} = \overline{\beta_{k-n}}$ if $k > n$.

IV. NUMERICAL RESULTS

We present here results obtained for a mixed boundary condition on a rough interface characterized by a self-affine scaling of roughness exponent $\zeta = 0.8$ (with a lower cut-off $=2\pi/16$) and of maximum local slope $s_{max} = 0.75$ (Note that we only consider here an intermediate self-affine scaling: the interface remains regular at short scales). The Laplacian potential is written on a basis of 512 evanescent modes. Figure 2 shows the equipotential lines obtained in the conformal half-plane (x, y) and their images in the physical domain (u, v) for two different b.c. with $\Lambda = 0.25$ and $\Lambda = 4$ respectively. In Fig. 3 we represent the normal derivative of the potential and the surface potential sealed by the length Λ . The satisfaction of the b.c. corresponds to the equality of these two quantities. We obtain very nice results except for the lowest values of the potential for $\Lambda = 0.25$. This is attributed to the truncation of the high frequency modes performed in writing the linear system. Let us note that the equipotential lines shown in Fig. 2 define precisely the effective Dirichlet b.c. giving rise to the same behavior (including near field). This object is the one for which B. Sapoval [7] proposed a geometrical construction based on coarse graining.

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