Numerical modeling of floating potentials in electrokinetic problems

Damien Voyer, Sergio Corridore, Annabelle Collin, Riccardo Scorretti, Clair Poignard

Numerical modeling of floating potentials in electrokinetic problems

D.Voyer[1, 2], S. Corridore[2], A. Collin[2], R. Scorretti[3] and C. Poignard[2]

[1]EIGSI La Rochelle, La Rochelle Cedex F-17041, France, voyer@eigsi.fr
[2]Team MONC, INRIA, CNRS UMR 5251, Bordeaux INP, Talence Cedex F-33405, France
[3]Université de Lyon, Ampère, UMR 5005, Ecully Cedex F-69134, France

Floating potentials appear in electrokinetic problems when isolated domains with high conductivity are introduced. In this paper, an asymptotic development is proposed in order to avoid the direct computation that leads to inaccurate numerical results when the contrast of conductivity is strong. We show that the problem where perfect conductors are assumed is the zero order solution of the initial problem; the solution can then be refined introducing a first order correction that implies two successive problems defined inside and outside the domains with high conductivity. The proposed example deals with a four electrodes system designed to both induce electroporation in a biological tissue sample and measure the resulting impedance. The proposed approach is extended to a nonlinear problem by taking advantage of the iterative scheme that is necessary applied in this case.

Index Terms— **Floating potential, asymptotic method, nonlinear problem, electroporation.**

I. Introduction

Four electrodes systems are often used to measure the impedance of biological tissues [1]. In such a device, internal electrodes are modeled as isolated domains with a high conductivity. The direct solution of this problem requires meshing these electrodes and this can lead to inaccurate results when the contrast in conductivity is very strong. Assuming electrodes as perfect conductors is an alternative solution that proves to be the zero order of an asymptotic development, where the exact solution is expanded using a formal series with respect to the parameter defined by the ratio of conductivities. The accuracy of the solution can then be refined formulating a first order correction derived from the asymptotic development. A study of the numerical convergence shows that the asymptotic approach overcomes the limitations of the direct solution. We propose then to extend this approach to the case of nonlinear materials: as the solution of a nonlinear problem is necessarily performed using an iterative technique, the superposition holds at each step of the iterative solution as it will be discussed here.

II. Formulation of the electrokinetic problem

A. Linear case

A four electrode system is considered with two pair of active and passive electrodes. The problem to solve reads:

$$\begin{cases} -\nabla\cdot(\sigma_e\nabla\varphi_e) = 0 \quad in\,\Omega_e \\ \varphi_{e|\Gamma_g{}^\pm} = \pm\dfrac{V}{2} \qquad \sigma_e\dfrac{\partial\varphi_e}{\partial n}_{|\Gamma_{out}} = 0 \\ -\nabla\cdot(\sigma_i\nabla\varphi_i) = 0 \quad in\,\Omega_i{}^\pm \\ \varphi_i\big|_{\partial\Omega_i{}^\pm} = \varphi_e\big|_{\partial\Omega_i{}^\pm} \qquad \sigma_e\dfrac{\partial\varphi_e}{\partial n}\Big|_{\partial\Omega_i{}^\pm} = \sigma_i\dfrac{\partial\varphi_i}{\partial n}\Big|_{\partial\Omega_i{}^\pm} \end{cases} \tag{1}$$

where $\Gamma_g{}^\pm$ is the border for the positive and negative active electrodes, Γ_{out} the external border of the biological tissue. σ_e is the conductivity of the biological tissue defined inside the domain Ω_e and σ_i the conductivity of the positive and negative passive electrodes defined inside the domains $\Omega_i{}^\pm$.

The solution for φ_e and φ_i is expanded using formal series with respect to the parameter $\varepsilon = \sigma_e/\sigma_i << 1$:

$$\begin{cases} \varphi_e = \varphi_e^0 + \varepsilon\,\varphi_e^1 + O(\varepsilon^2) \\ \varphi_i = \varphi_i^0 + \varepsilon\,\varphi_i^1 + O(\varepsilon^2) \end{cases} \tag{2}$$

Combining (1) and (2) leads to solve sequentially problems by identifying the different orders in the asymptotic expansions: firstly, solution $\{\varphi_i^0, \varphi_e^0\}$ is computed; then, it is exploited to solve $\{\varphi_i^1, \varphi_e^1\}$, and so on. Thus, the first problem to solve

$$\begin{cases} -\nabla.(\sigma_e\nabla\varphi_e^0) = 0 \quad in\,\Omega_e \\ \varphi^0_{e|\Gamma_g{}^\pm} = \pm\dfrac{V}{2} \qquad \sigma_e\dfrac{\partial\varphi_e^0}{\partial n}_{|\Gamma_{out}} = 0 \\ \varphi_e^0\big|_{\partial\Omega_i{}^\pm} = \pm\dfrac{\alpha_0}{2} \quad \text{with } \alpha_0 \text{ such that } \int_{\partial\Omega_i{}^\pm}\sigma_e\dfrac{\partial\varphi_e^0}{\partial n} = 0 \end{cases} \tag{3}$$

appears to be the one formulated when perfect conductive electrodes are considered instead of electrodes with high conductivity. The floating potential $\pm\alpha_0/2$ is computed from the superposition of two problems where the Dirichlet condition $\varphi_e^0 = 0$ is set successively on the boundary $\partial\Omega_i{}^\pm$ of the passive electrodes and on the boundary $\Gamma_g{}^\pm$ of the active electrodes.

Then, the first order correction is obtained solving both following problems:

$$\begin{cases} -\nabla.(\sigma_i\nabla\varphi_i^1) = 0 \quad in\,\Omega_i{}^\pm \\ \dfrac{\partial\varphi_i^1}{\partial n}\Big|_{\partial\Omega_i{}^\pm} = \dfrac{\partial\varphi_e^0}{\partial n}\Big|_{\partial\Omega_i{}^\pm} \qquad \int_{\partial\Omega_i{}^\pm}\varphi_i^1 = 0 \end{cases} \tag{4a}$$

$$\begin{cases} -\nabla\cdot(\sigma_e\nabla\varphi_e^1) = 0 \quad in\,\Omega_e \\ \varphi^1_{e|\Gamma_g{}^\pm} = 0 \qquad \sigma_e\dfrac{\partial\varphi_e^1}{\partial n}_{|\Gamma_{out}} = 0 \\ \varphi_e^1\big|_{\partial\Omega_i{}^\pm} = \varphi_i^1\big|_{\partial\Omega_i{}^\pm} \pm\dfrac{\alpha_1}{2} \text{ with } \alpha_1 \text{ such that } \int_{\partial\Omega_i{}^\pm}\sigma_e\dfrac{\partial\varphi_e^1}{\partial n} = 0 \end{cases} \tag{4b}$$

B. Nonlinear case

Considering a medium with a nonlinear conductivity $\sigma_e(\nabla\varphi_e)$ in (1), the solution $\varphi = \varphi_e + \varphi_i$ can be calculated using Picard's algorithm [2]. From the solution φ^{k-1} computed at the iteration k-1, the problems (3)-(4) are solved with $\sigma_e(\nabla\varphi_e^{k-1})$ to calculate the intermediate solution $\varphi_{e+i}^k = \varphi_e^k + \varphi_i^k$. Then, a relaxation factor K^k is applied to optimize the contribution of the intermediate solution φ_{e+i}^k to the solution computed at the iteration k: $\varphi^k = \varphi^{k-1} + K^k(\varphi_{e+i}^k - \varphi^{k-1})$; at each iteration, K^k is corrected according to how the solution is approached in order to accelerate the convergence [2].

III. Numerical Results

A. Linear case

A 2D problem is solved using the finite element method with a fine and a coarse mesh (see Fig. 1).

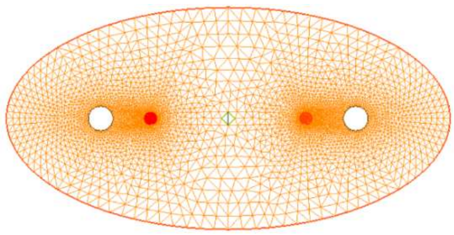

Fig.1: 2D model of the four electrodes system with a coarse mesh. The diameter for the external (respectively internal) electrodes is 0.45 mm (respectively 0.225 mm) and the separation distance between negative and positive electrodes is 4.8 mm (respectively 2.8 mm).The height of the electrodes is 6.3 mm.

The resistance R, defined as the ratio of the potential difference between the passive electrode and the current flowing through the active electrodes, is computed when the tissue is composed of a uniform conductivity $\sigma_e = 0.1$ S/m. Fig.2 reports the relative error of the asymptotic development at the zero and first orders, where the reference value is the one computed using the direct solution.

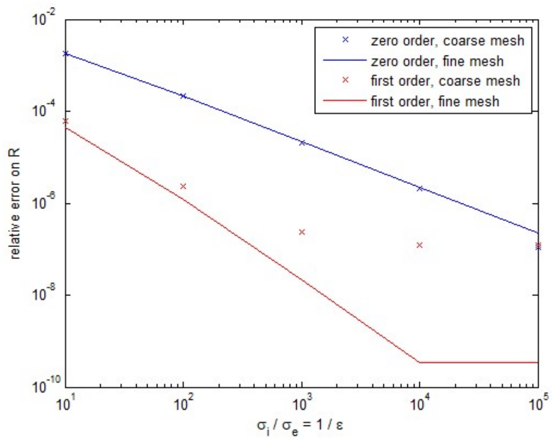

Fig.2: Convergence of the asymptotic approach at the zero and first orders for two different meshes

One observes that the relative error on R decreases for the zero order computation following the rate ε. Adding the first order correction, the relative error decreases following a rate slightly lower than ε^2 until a break point is reached because of the mesh.

B. Nonlinear case

A sigmoid function is introduced to model the dependence of the conductivity with respect to the electric field as it is considered in the electroporation phenomenon [2]:

$$\sigma_e(\nabla\varphi_e) = \sigma_0 + \frac{\sigma_1}{1 + d\,exp\left(-\frac{|\nabla\varphi_e| - a}{b}\right)} \tag{5}$$

where parameters σ_0, σ_1, a; b, c and d depend on the type of biological tissue. When electroporation occurs, the tissue conductivity increases in the area between the electrodes (see Fig. 3 top). Picard's algorithm has been performed to solve the nonlinear problem for both the direct solution and the asymptotic development at the zero order, in the case where the conductivity $\sigma_i = 10^4\sigma_0$ is set for the passive electrodes. The algorithm stops when the relative error between solutions φ^{k-1} and φ^k reaches 10^{-8}: 36 iterations are required for the asymptotic approach and 43 iterations for the direct solution. The relative error on R is 9,3 10^{-5} with the asymptotic development at the zero order, which is 42 times larger than the error obtained in the linear case. Fig. 3 bottom shows that the relative error on the conductivity between the direct solution and the asymptotic approach reaches 10^{-3} in the electropored region.

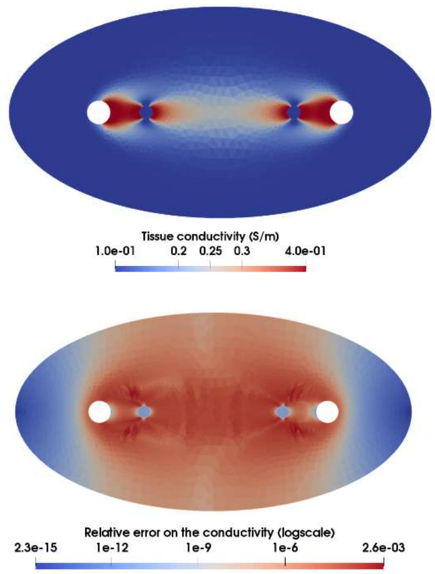

Fig.3: (top) Distribution of the conductivity computed using the asymptotic approach (bottom) Relative error on the conductivity between the asymptotic approach and the direct solution. V = 288 Volts in (1) and the tissue parameters are $\sigma_0 = 0.1$ S/m, $\sigma_1 = 0.3$ S/m, a= $(E_0+E_1)/2$; b = $(E_1-E_0)/c$, c = 8 and d = 10 with $E_0 = 460$ V/cm and $E_1 = 700$ V/cm.

Further discussion on the convergence as well as a 3 D realistic problem will be provided in an extended version of the paper.

References

[1] A Ivorra, B. Al-Sakere, B. Rubinsky and L. M Mir, *In vivo electrical conductivity measurements during and after tumor electroporation: conductivity changes reflect the treatment outcome*, Physics in Biology and Medecine, volume 54, pp. 5949–5963, 2009

[2] M. Breton, F. Buret, L. Krähenbühl, M. Leguèbe, L. M. Mir, et al., *Nonlinear steady-state electrical current modeling for the electropermeabilization of biological tissue*, 16th Biennial IEEE Conference on Electromagnetic Field Computation, 2014.