Charge induced deformation of scanning electrolyte before contact

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Dynamic grid by conformal map

The Laplace Equation in 2D cylindrical coordinates with axial symmetry is expressed as:

$$\frac{\partial^2\phi}{\partial R^2}+\frac{1\partial\phi}{R\partial R}+\frac{\partial^2\phi}{\partial Z^2}=0 \quad (Eq.\ \text{S1})$$

where R and Z are dimensionless normalized to the radius of capillary r_c, and ϕ is normalized to φ_{appl}. The simulation space is $R\in[0,R_{max}]$, $Z\in[0,Z_{max}]$. Note that here Z_{max} depends on the electrolyte boundary, so it is dynamic for $R\in[0,1]$.

A convenient way is to transform the coordinates by defining:

$$X=R \quad (Eq.\ \text{S2})$$

$$Y=\frac{Z}{Z_{max}(R)} \quad (Eq.\ \text{S3})$$

Thus,

$$\frac{\partial X}{\partial R}=1 \quad (Eq.\ \text{S4})$$

$$\frac{\partial^2 X}{\partial R^2}=0 \quad (Eq.\ \text{S5})$$

$$\frac{\partial Y}{\partial R}=Z\frac{\partial\left(\frac{1}{Z_{max}(R)}\right)}{\partial R} \quad (Eq.\ \text{S6})$$

$$\frac{\partial^2 Y}{\partial R^2}=Z\frac{\partial^2\left(\frac{1}{Z_{max}(R)}\right)}{\partial R^2} \quad (Eq.\ \text{S7})$$

$$\frac{\partial X}{\partial Z}=0 \quad (Eq.\ \text{S8})$$

$$\frac{\partial^2 X}{\partial Z^2} = 0 \quad (Eq.\ \text{S9})$$

$$\frac{\partial Y}{\partial Z} = \frac{1}{Z_{max}(R)} \quad (Eq.\ \text{S10})$$

$$\frac{\partial^2 Y}{\partial Z^2} = 0 \quad (Eq.\ \text{S11})$$

Applying the chain rule:

$$\frac{\partial \phi}{\partial R} = \frac{\partial \phi \partial X}{\partial X \partial R} + \frac{\partial \phi \partial Y}{\partial Y \partial R} = \frac{\partial \phi}{\partial X} + \frac{\partial \phi \partial Y}{\partial Y \partial R} \quad (Eq.\ \text{S12})$$

$$\frac{\partial^2 \phi}{\partial R^2} = \frac{\partial^2 \phi}{\partial X^2} + 2\frac{\partial^2 \phi}{\partial X \partial Y}\frac{\partial Y}{\partial R} + \frac{\partial^2 \phi}{\partial Y^2}\left(\frac{\partial Y}{\partial R}\right)^2 + \frac{\partial \phi \partial^2 Y}{\partial Y \partial R^2} \quad (Eq.\ \text{S13})$$

$$\frac{\partial^2 \phi}{\partial Z^2} = \frac{\partial^2 \phi}{\partial Y^2}\left(\frac{\partial Y}{\partial Z}\right)^2 = \frac{1}{Z_{max}^2(R)}\frac{\partial^2 \phi}{\partial Y^2} \quad (Eq.\ \text{S14})$$

The boundary conditions can also be converted:

At $X = 0$, $\frac{\partial \phi}{\partial X} = 0$, considering $\left.\frac{\partial Z_{max}(R)}{\partial R}\right|_{R=0} = 0$

At $X = X_{max}$, $\phi = 0$

At $Y = 0$, $\phi = 0$

At $Y = 1$, $\phi = 1$ for $X \in [0,1]$ and $\frac{\partial \phi}{\partial Y} = 0$ for $X \in [1, X_{max}]$

In this case, one may discretize R and Y in the range of $X \in [0, X_{max}]$ and $Y \in [0,1]$. In this work, shrinking grid is considered for $X \in [0,1]$ and expanding grid is taken for $X \in [1, X_{max}]$, so that the most details are around $X = 1$. In Y axis, the grid is expanding from 0 to 0.5 and shrinking symmetrically from 0.5 to 1. Such treatment gives m × n grid which can be solved by ADI method using Thomas algorithm. For the deformation of electrolyte boundary, only the expression of $Z_{max}(R)$ is varying, while the grid always keeps m × n. This requires dynamic modification of the sparse Jacobi matrix for each iteration step, but allows taking the previous solution of ϕ as initial value for the next solution after changing the boundary. It may lead to faster convergence than taking an arbitrarily chosen initial value such as $\phi = 0.5$ for all iterations.