Implementation of the Poisson-Nernst-Planck equations in FEniCS

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Abstract

We will show how to implement the Poisson-Nernst-Planck (PNP) equations in FEniCS.

1 Introduction

We will study the dynamics of ions in a medium. We will consider a system of two ions. One positive ion with valency, indexed by 1, and one negative ion with valency -1, indexed by 2. We can think of the positive ion as potassium and the negative ion as chloride, although the spesific ion types will not be important in this text

2 The equations

The ion concentration dynamics are influenced by two principles:

1. The ions will move by diffusion, from areas of with high concentration to areas of low concentration.
2. As the ions are charged, they will be influenced if there is an electric field present. For the same reason, the ions themselves will create an electric field.

We assume that these concentration currents are additive. Starting with the continuity equation, we get

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \mathbf{J}_i + f_i, \tag{1}$$

where c_i is the concentration of ion type i, $\mathbf{J}_i$ is the concentration current of ion type i, and f_i is a source term

$$\mathbf{J}_i = \mathbf{J}_i^{\text{diff}} + \mathbf{J}_i^{\text{field}}, \tag{2}$$

$$= -D_i \nabla c_i - \frac{D_i z_i}{\psi} c_i \nabla \phi, \tag{3}$$

where D_i is the diffusion coefficient, z_i is the valency of ion type i, ψ is a physical constant, and ϕ is the electric field. This equation is called the *Nernst-Planck* equation. The electric field is found by the Poisson equation:

$$\nabla^2\phi = -\frac{\rho}{\epsilon} = -\frac{F}{\epsilon}\sum_i z_i c_i, \tag{4}$$

where ρ is the charge concentration, F is Faradays constant, ϵ is the permittivity of the medium (in this case the extracellular space). Together, these equations form the *Poisson-Nernst-Planck* (PNP) system of equations. We present the full set of equations:

$$\frac{\partial c_1}{\partial t} = \nabla\cdot\left[D_1\nabla c_1 + \frac{D_1 z_1}{\psi}c_1\nabla\phi\right] + f_1 \tag{5}$$

$$\frac{\partial c_2}{\partial t} = \nabla\cdot\left[D_2\nabla c_2 + \frac{D_2 z_2}{\psi}c_2\nabla\phi\right] + f_2 \tag{6}$$

$$\nabla^2\phi = -\frac{F}{\epsilon}(z_1 c_1 + z_2 c_2) \tag{7}$$

3 Boundary Conditions

We will use Dirichlet boundary conditions for the concentrations, and a pure von Neumann boundary condition for the field:

$$c_1 = c_1^D \qquad \text{on } \partial\Omega \tag{8}$$

$$c_2 = c_2^D \qquad \text{on } \partial\Omega \tag{9}$$

$$\nabla\phi\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega \tag{10}$$

4 Units and dimensions

Note that in terms of natural constants, $\psi = RT/F$, where R is the gas constant, F is Faradays constant and T is the temperature.

symbol	explanation	units
x	position	μm
t	time	ms
ϕ	potential	V
c_i	concentration	mmol/ml
D_i	diffusion coefficient	μm^2/ms
f_i	source term	mmol/(ml$\times$ms)
z_i	valency	(none)
ψ	see text	J/C
F	Faradays Constant	C/mol
ϵ	permittivity	pF/m

5 FEniCS implementation

5.1 Time discretization

We use a finite difference time discretization scheme, which means that we discretetize the time into equispaced points, t^n, were

$$t^n = n\Delta t \tag{11}$$

where Δt is the space between adjacent time points. We let c_i^n denote the value of c_i at time t^n. In order to discretize equations eqs. (8) to (10) in time, we can set the left hand sides as

$$\frac{\partial c_i}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}, \tag{12}$$

$$\nabla^2 \phi = \nabla^2 \phi^{n+1}. \tag{13}$$

One the right hand side, we can enter concentrations at either time n or $n+1$. We can also enter a combination of the two. Generally, we can define

$$c^\theta = (1-\theta)c^n + \theta c^{n+1}, \tag{14}$$

we then set the right hand side as

$$\nabla \cdot \left[D_i \nabla c_i + \frac{D_i z_i}{\psi} c_i \nabla \phi \right] + f_i = \nabla \cdot \left[D_i \nabla c_i^\theta + \frac{D_i z_i}{\psi} c_i \nabla \phi^\theta \right] + f_i^\theta. \tag{15}$$

The Poisson equation is not time dependent, so we should solve for all elements at the same time step,

$$\nabla^2 \phi^{n+1} = -\frac{F}{\epsilon}(z_1 c_1^{n+1} + z_2 c_2^{n+1}) \tag{16}$$

5.2 Weak form

6 Method of Manufactured Solution

In order to test the implementation, we use the method of manufactured solution. We set the solution of the system of equations, and then modify the source term to make the chosen solution correct. Since we only have two source terms, we can only freely choose the solution of two of the equations, and then chose the last one so that the solutions are consistent. If we set the solution for c_1 and ϕ, then we can find the solution of c_2 from Equation (7). We also have to set ϕ so that it is consistent with the boundary conditions, as well as the additional condition $\int_\Omega \phi \, \mathrm{d}x = 0$. We set the following set of solutions:

$$c_1 = \cos^3(x)\sin(t) \tag{17}$$

$$\phi = (\sin^2(\pi x) - 0.5)\cos^2(t) \tag{18}$$

$$c_2 = -\frac{1}{z_2}\left(\frac{F}{\epsilon}\nabla^2\phi + z_1 c_1\right) \tag{19}$$

From this we get the following demands for the source terms:

$$f_1 = \frac{\partial c_1}{\partial t} - \nabla \cdot \left[D_1 \nabla c_1 + \frac{D_1 z_1}{\psi} c_1 \nabla \phi \right] \tag{20}$$

$$f_2 = \frac{\partial c_2}{\partial t} - \nabla \cdot \left[D_2 \nabla c_2 + \frac{D_2 z_2}{\psi} c_2 \nabla \phi \right] \tag{21}$$

7 Example 1: Ions in a box: Liquid Junction Potential

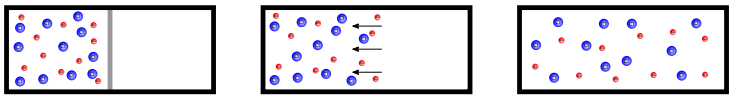

Figure 1: The figure illustrates the Ions in a box example. The ions start out locked in the left side of the box. At $t = 0$, the box is opened and the ions are allowed to move freely. The difference in diffusion constants creates an electric field.

8 Example 2: Neuron in a dish