Weak form of Poisson-Nernst-Planck model

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Here, I describe how to put the Poisson-Nernst-Planck (PNP) model in the weak formulation for the finite element.

The PNP model is described by the Nernst-Planck equation coupled to the Poisson concentration, where the charge density is linked to the concentration of migrating ions. In addition to this consideration, we have imposed an external (fixed) electric field.

For a single ionic species and, in the absence of a magnetic field,

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla u) + \nabla \cdot \left(\frac{zeDC}{k_B T} \nabla \phi - \mathbf{b} C \right) \tag{1a}$$

$$-\nabla^2 \phi = \frac{zeC}{\varepsilon}, \tag{1b}$$

where C is our trial function for the concentration, C is the trial function for the concentration in the function sub-domain, D is the diffusion coefficient, k_B is the Boltzmann's constant, ϕ is the electric potential. z is the valence of the species, e is the elementary charge, T is the absolute temperature, $\varepsilon = \varepsilon_0 \varepsilon_r$ and,

$$\mathbf{b} = -\frac{zeD}{k_B T} \mathbf{E}, \tag{2}$$

where E is the external field.

Reformatting (1)

$$\frac{\partial C}{\partial t} - \nabla \cdot (D \nabla C) - \nabla \cdot \left(\frac{zeDC}{k_B T} \nabla \phi - \mathbf{b} C \right) = 0 \tag{3a}$$

$$-\nabla^2 \phi + \frac{zeC}{\varepsilon} = 0 \tag{3b}$$

In order to put (1) in the weak form, we have to multiply by a test function v and integrate over the domain Ω. Assuming D is constant

$$L_a u \equiv \int_\Omega \frac{\partial C}{\partial t} v_a d\Omega - D \int_\Omega \nabla^2 C v_a d\Omega - \int_\Omega \nabla \cdot \left(\frac{zeDC}{k_B T} \nabla \phi - \mathbf{b} C \right) v_a d\Omega = 0 \tag{4a}$$

$$L_b C \equiv \int_\Omega \frac{\partial \nabla^2 \phi}{\partial x} v_b d\Omega + \int_\Omega \frac{zeC}{\varepsilon} v_b d\Omega = 0, \tag{4b}$$

with v_a and v_b test functions for of the sub-spaces corresponding to each of the equations. L_a and L_b are then, the differential operators for each system.

We can now integrate by parts the terms containing a Laplacian operators, using (14),

$$\int_\Omega \frac{\partial C}{\partial t} v_a d\Omega + D \int_\Omega (\nabla C \cdot \nabla v_a) d\Omega - D \int_{\partial \Omega_N} (\nabla C \cdot \hat{\mathbf{n}}) v_a dS - \int_\Omega \nabla \cdot \left(\frac{zeDC}{k_B T} \nabla \phi - \mathbf{b} C \right) v_a d\Omega = 0 \tag{5a}$$

$$-\int_\Omega (\nabla \phi \cdot \nabla v_b) d\Omega + \int_{\partial \Omega_N} (\nabla \phi \cdot \hat{\mathbf{n}}) v_b dS + \int_\Omega \frac{zeC}{\varepsilon} v_b d\Omega = 0 \tag{5b}$$

For our problem, the following boundary conditions are defined

$$C(x=0) = C_s \tag{6a}$$

$$\nabla C \cdot \hat{\mathbf{n}} = h\left(C_1 - \frac{C_2}{m}\right) \quad \text{(segregation)} \tag{6b}$$

$$\nabla \phi \cdot \hat{\mathbf{n}} = 0 \tag{6c}$$

1 SUPG estabilization

To construct the additonal term for the *Streamline Upwind Petrov-Galerkin* (SUPG) stabilization, we need to find the skew-symmetric part (L_{SSu}) of the differential operator $L_a u$ for each of the equations (5). These can be obtained from the convective term

$$\nabla \cdot \left[\left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) C\right]$$

For the term $\nabla \cdot (\mathbf{d}u)$ the skew-symmetric term is

$$L_{SSu} = \frac{1}{2}\left[\nabla \cdot (\mathbf{d}u) + \mathbf{d} \cdot \nabla u\right]. \tag{7}$$

In our case,

$$L_{SSu} = \frac{1}{2}\left[\nabla \cdot \left[\left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) C\right] + \left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) \cdot \nabla C\right]. \tag{8}$$

The following rule comes useful

$$\nabla \cdot (f\mathbf{A}) = f\,(\nabla \cdot A) + \mathbf{A} \cdot (\nabla f), \tag{9}$$

applied to the first term in the RHS

$$\nabla \cdot \left[\left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) C\right] = C\nabla \cdot \left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) + \left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) \cdot \nabla C$$

Plugging this result into (8),

$$L_{SSu} = \left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) \cdot \nabla C + \left(\frac{zeDC}{2k_B T}\right) \nabla \cdot \nabla\phi \tag{10}$$

In this case we have considered that $\nabla \cdot \mathbf{b} = 0$. Since $\nabla \cdot \nabla\phi = -zeC/\varepsilon$, we can finally get

$$L_{SSu} = \left(\frac{zeD}{k_B T}\nabla\phi - \mathbf{b}\right) \cdot \nabla C - \left(\frac{D(zeC)^2}{2\varepsilon k_B T}\right) \tag{11}$$

A Intergation by parts

Let's introduce

$$\int_\Omega \nabla \cdot (\nabla u)\, v d\Omega \tag{12}$$

Take the divergence of $v\nabla u$:

$$\nabla \cdot (v\nabla u) = v\nabla \cdot \nabla u + \nabla v \cdot \nabla u.$$

Then,

$$\int_{\Omega} \nabla \cdot (\nabla u)\, v d\Omega = \int_{\Omega} \nabla \cdot (v\nabla u)\, d\Omega - \int_{\Omega} (\nabla v \cdot \nabla u)\, d\Omega$$

Applying the Gauss theorem to the first term on the RHS:

$$\int_{\Omega} \nabla \cdot (v\nabla u)\, d\Omega = \int_{\partial\Omega_D \cup \partial\Omega_N} (\nabla u \cdot \hat{\mathbf{n}})\, v dS, \tag{13}$$

where $\partial\Omega_D \cup \partial\Omega_N$ is the union of the Dirichlet and Neumann surfaces. Typically, v is define such that the integral over the Dirichlet part of the surface vanishes.

Putting it all together:

$$\int_{\Omega} \nabla \cdot (\nabla u)\, v d\Omega = -\int_{\Omega} (\nabla u \cdot \nabla v)\, d\Omega + \int_{\partial\Omega_N} (\nabla u \cdot \hat{\mathbf{n}})\, v dS \tag{14}$$