Nernst-Planck-Poisson

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The Nernst-Planck equation describes the motion of ionic species due to concentration gradients and migration under an applied electric field.

$$\frac{\delta c}{\delta t} = D\left[\nabla^2 c + \frac{zFc}{RT}\nabla^2\Phi\right] \tag{1}$$

The Poisson equation describes the electric field.

$$\nabla^2\Phi = -\rho\epsilon = -\frac{Fzc}{\epsilon} \tag{2}$$

1 Weak formulation and time discretization

1.1 Nernst-Planck

$$\frac{\delta c}{\delta t} - D\left[\nabla^2 c + \frac{zFc}{RT}\nabla^2\Phi\right] = 0 \tag{3}$$

The PDE is multiplied with a test-function w and integrated over space.

$$\int_\Omega \frac{\delta c}{\delta t} \cdot w - D\left[\nabla^2 c + \frac{zFc}{RT}\nabla^2\Phi\right] \cdot wdV = 0 \tag{4}$$

Green's formula is used on the second term to reduce order of derivatives.

$$\int_\Omega -D\left[\nabla^2 c \cdot + \frac{zFc}{RT}\nabla^2\Phi\right] \cdot wdV = \int_\Omega D\left[\nabla c + \frac{zFc}{RT}\nabla\Phi\right] \cdot \nabla wdV \tag{5}$$

The integral becomes,

$$\int_\Omega \frac{\delta c}{\delta t} \cdot w + D\left[\nabla c + \frac{zFc}{RT}\nabla\Phi\right] \cdot \nabla wdV = 0 \tag{6}$$

$$\int_\Omega \frac{\delta c}{\delta t} \cdot wdV = \int_\Omega -D\left[\nabla c + \frac{zFc}{RT}\nabla\Phi\right] \cdot \nabla wdV \tag{7}$$

Forward Euler explicit time stepping

$$\int_\Omega \frac{c^{n+1}-c^n}{\Delta t}\cdot wdV = \int_\Omega -D\Big[\nabla c^n + \frac{zFc^n}{RT}\nabla\Phi^n\Big]\cdot\nabla wdV \tag{8}$$

$$\int_\Omega c^{n+1}\cdot wdV = \int_\Omega c^n + \int_\Omega -D\Delta t\Big[\nabla c^n + \frac{zFc^n}{RT}\nabla\Phi^n\Big]\cdot\nabla wdV \tag{9}$$

The residuals are thus defined as,

$$r_c = c^n \tag{10}$$

$$r_c x = -D\Delta t\Big[\nabla c^n + \frac{zFc^n}{RT}\nabla\Phi^n\Big] \tag{11}$$

1.2 Poisson

The Poisson equation is a time-independent linear PDE.

$$\nabla^2\Phi = -\frac{Fzc}{\epsilon} \tag{12}$$

It is thus solved using Newton's method of iteration.

$$\frac{\delta R(\Phi)}{\delta\phi}\nabla^2\Phi = -R(\Phi_0) \tag{13}$$

Our residual is,

$$R(\Phi) = \nabla^2\Phi + \frac{Fzc}{\epsilon} \tag{14}$$

We start with the LHS.

$$\frac{\delta R(\Phi)}{\delta\phi}\nabla^2\Phi = \nabla^2(\nabla^2\Phi) \tag{15}$$

We multiply with test-function w and integrate over space as well as use Green's formula to decrease order of derivatives.

$$\int_\Omega w\cdot\nabla^2(\nabla^2\Phi)dV = \int_\Omega \nabla w\cdot(-\nabla(\nabla^2\Phi))dV \tag{16}$$

The RHS is,

$$-R(\Phi) = -\nabla^2\Phi - \frac{Fzc}{\epsilon} \tag{17}$$

Once again, the equation is multiplied with a test-function w and integrated over space.

$$\int_\Omega -\nabla^2\Phi\cdot w - \frac{Fzc}{\epsilon}\cdot wdV = \int_\Omega \nabla\Phi\cdot\nabla w - \frac{Fzc}{\epsilon}\cdot wdV \tag{18}$$

The LHS and RHS of the Poisson equation are thus,

$$\int_{\Omega} \nabla w \cdot (-\nabla(\nabla^2 \Phi))dV = \int_{\Omega} \nabla \Phi \cdot \nabla w - \frac{Fzc}{\epsilon} \cdot wdV \tag{19}$$

The residual for the LHS will be,

$$r_{\nabla \phi x} = -\nabla(\nabla^2 \Phi^n) \tag{20}$$

The RHS,

$$r_{\phi} = -\frac{Fzc^n}{\epsilon} \tag{21}$$

$$r_{\phi x} = \nabla \Phi^n \tag{22}$$