

Project 2020

July 31, 2020

1 Project 1

We consider the numerical solution of Poisson-Nernst-Planck system with steric effects:

$$\begin{aligned}\frac{\partial u}{\partial t} &= \nabla \cdot (d_1 \nabla u + \nu_1 u \nabla \phi) + \nabla \cdot (g_{11} u \nabla u + g_{12} u \nabla v) \\ \frac{\partial v}{\partial t} &= \nabla \cdot (d_2 \nabla v + \nu_2 v \nabla \phi) + \nabla \cdot (g_{21} v \nabla u + g_{22} v \nabla v) \\ -\Delta \phi &= \gamma_1 u + \gamma_2 v\end{aligned}\tag{1.1}$$

where $u = u(x, t) > 0$ and $v = v(x, t) > 0$ are the concentration of two ion species carrying charges $\gamma_1 > 0$ and $\gamma_2 < 0$ respectively; $d_1, d_2 > 0$ denote the diffusion rates; the sign of the constant ν_1 (and ν_2) should follow the sign of the charge γ_1 (and γ_2), and $T > 0$ is the absolute temperature; $\phi = \phi(x, t)$ is the electrostatic potential; the coupling constants $g_{11}, g_{12}, g_{21}, g_{22}$ are assumed to be positive; and ρ_0 is the permanent charge.

We use FDM to solve (1.1) with $g_{11}g_{22} - g_{12}g_{21} \geq 0$, and boundary condition

$$\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = \frac{\partial \phi}{\partial n} = 0\tag{1.2}$$

and initial condition

$$u(x, 0) = u_0(x) \quad \text{and} \quad v(x, 0) = v_0(x)\tag{1.3}$$

We note that the third equation exist the solution ϕ when

$$\gamma_1 \int_{-1}^1 u_0(x) dx + \gamma_2 \int_{-1}^1 v_0(x) dx = 0.\tag{1.4}$$

2 Project 2

We consider transport equation:

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2} - c_f u^2 \quad \forall (x, t) \in [a, b] \times [0, T].\tag{2.1}$$

where $c_f \geq 0$, $\mu \geq 0$ and a is constant. Along with this equation we need initial conditions at time 0

$$u(x, 0) = u_0(x),\tag{2.2}$$

and also boundary conditions if we are working on a bounded domain, e.g., the Dirichlet conditions

$$\begin{aligned}u(a, t) &= g_1(t), \\ u(b, t) &= g_2(t).\end{aligned}\tag{2.3}$$

3 Project 3

We consider nonlinear Schrodinger equation:

$$i\frac{\partial\varphi}{\partial t} + \frac{\partial\varphi}{\partial x^2} + 2\varphi|\varphi|^2 = 0 \quad \forall (x, t) \in [a, b] \times [0, T] \quad (3.1)$$

with boundary condition

$$\varphi(a, t) = \varphi(b, t) = 0 \quad \forall t \in [0, T]$$

and initial condition

$$\varphi(x, 0) = \varphi_0(x)$$