Scharfetter-Gummel Method

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Abstract

The Scharfetter-Gummel method provides an optimum way to discretize the drift-diffusion (or Nernst-Planck) equation for charged particle transport in semiconductor devices (or ionic flow in biological ion channels). This is an exponential fitting method usually called in the literature of convection-dominated fluid models.

The steady state 1D Nernst-Planck (drift-diffusion) equation of cations (or holes) in an ion channel (or a semiconductor device) is

$$-\frac{d}{dx}J(x) = 0, \quad \forall x \in (0, l) \tag{1}$$

where

$$J(x) = -D\frac{dC(x)}{dx} + \mu E C(x) \tag{2}$$

is the flux density of cations, $C(x)$ is an unknown concentration (distribution) function of cations, $E = -\frac{d\phi(x)}{dx}$ is the electric field, $\phi(x)$ is the electrostatic potential, μ is the hole mobility, and D is the diffusion coefficient of cations. The Einstein relation of charged particles is $D = \mu k_B T/q$, where k_B is the Boltzmann constant, T is absolute temperature, and q is the charge on each particle (cation or anion).

Assuming that μ, E, D, J are constant within the interval $[x_i, x_{i+1}] \subset [0, l]$, we have from (2)

$$\frac{dC(x)}{dx} = \frac{\mu E}{D}C(x) - \frac{J}{D} = bC(x) - \frac{J}{D} \tag{3}$$

which implies that

$$
\begin{aligned}
\frac{1}{C(x)-\frac{J}{bD}}\frac{dC(x)}{dx} &= b, \quad b=\frac{\mu E}{D}\\
\frac{d}{dx}\ln\left|C(x)-\frac{J}{bD}\right| &= b\\
\ln\left|C(x)-\frac{J}{bD}\right| &= bx+c, \quad c \text{ is a constant,}\\
C(x)-\frac{J}{bD} &= \pm e^{bx+c} \quad \text{on} \quad [x_i, x_{i+1}]\,.
\end{aligned}
\tag{4}
$$

Therefore, the flux J at the grid point $x_{i+\frac{1}{2}} = \frac{x_i+x_{i+1}}{2}$ (denoted by $J_{i+\frac{1}{2}}$) can be written as

$$
\frac{C_{i+1}-\frac{J_{i+\frac{1}{2}}}{bD}}{C_i-\frac{J_{i+\frac{1}{2}}}{bD}} = e^{bh_i}, \quad h_i = x_{i+1}-x_i,\, C_i = C(x_i), \tag{5}
$$

$$
\begin{aligned}
C_{i+1}-\frac{J_{i+\frac{1}{2}}}{bD} &= e^{bh_i}\left(C_i-\frac{J_{i+\frac{1}{2}}}{bD}\right)\\
\left(e^{bh_i}-1\right)\frac{J_{i+\frac{1}{2}}}{bD} &= \left(-C_{i+1}+e_i^{bh_i}C_i\right)\\
J_{i+\frac{1}{2}} &= \frac{bD}{(e^{bh_i}-1)}\left(-C_{i+1}+e_i^{bh_i}C_i\right)\\
&= \frac{D}{h_i}\left[\frac{-bh_i}{(e^{bh_i}-1)}C_{i+1}+\frac{-bh_i}{(e^{-bh_i}-1)}C_i\right]\\
&= \frac{D}{h_i}\left[-B(-t_i)C_{i+1}+B(t_i)C_i\right]
\end{aligned}
\tag{6}
$$

where

$$
\begin{aligned}
b &= \frac{\mu E}{D} = -\beta\frac{d\phi}{dx} = -\beta\frac{\phi_{i+1}-\phi_i}{h_i}, \quad \beta = \frac{q}{k_B T}\\
t_i &= \beta\Delta\phi_i,\ \Delta\phi_i = \phi_{i+1}-\phi_i\\
B(t) &= \frac{t}{e^t-1} \quad \text{is the Bernoulli function.}
\end{aligned}
\tag{7}
$$

For uniform mesh, i.e., $h_{i-1} = h_i$, the Scharfetter-Gummel method for (1) at x_i is thus

$$
\frac{d}{dx}J(x_i) \approx \frac{1}{\frac{h_{i-1}+h_i}{2}}\left(J_{i+\frac{1}{2}}-J_{i-\frac{1}{2}}\right) = 0 \Rightarrow a_{i-1}C_{i-1}+a_iC_i+a_{i+1}C_{i+1} = 0 \tag{8}
$$

$$
\begin{aligned}
J_{i+\frac{1}{2}} &= D\left[-B(-t_i)C_{i+1}+B(t_i)C_i\right], \quad J_{i-\frac{1}{2}} = D\left[-B(-t_{i-1})C_i+B(t_{i-1})C_{i-1}\right]\\
a_{i-1} &= -B(t_{i-1}), \quad a_i = B(-t_{i-1})+B(t_i), \quad a_{i+1} = -B(-t_i).
\end{aligned}
$$