Scharfetter-Gummel Discretization Scheme for Drift-Diffusion Equations

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The Scharfetter-Gummel scheme provides an optimum way to discretize the drift-diffusion equation for particle transport. (Drift is also known as advection or streaming in different disciplines.) For the purpose of developing the key relations, let us just consider a one-dimensional transport problem in the spatial variable x. Let $n(x, t)$ be the density of transporting particles. Then the key transport equations are the continuity equation:

$$\frac{\partial n}{\partial t} = -\frac{\partial j}{\partial x}, \tag{1}$$

and the drift-diffusion equation:

$$j = -D\frac{\partial n}{\partial x} + v(x, t)n. \tag{2}$$

Here j is the particle current density (flux), D is the diffusivity, and $v(x, t)$ is the drift (or advection or streaming) velocity. We assume that v depends upon n only indirectly, such as through a self-consistent potential which is computed in a loop that lies outside of the present transport calculation. While v is usually taken to obey some simple relationship such as $v = -\mu\, d\phi/dx$, where μ is a mobility and ϕ the electrostatic potential, we will here leave the dependence unspecified, to achieve greater generality.

On a uniform mesh, the continuity equation (1) can be discretized by assuming that the densities are associated with the meshpoints i and the currents are associated with the intervals between meshpoints. Thus, if the mesh spacing is Δ, we can write the discrete continuity equation as:

$$\frac{\partial n_i}{\partial t} = -\frac{j_{i+½} - j_{i-½}}{\Delta} = \frac{j_{i-½} - j_{i+½}}{\Delta}. \tag{3}$$

Now, the thrust of the Scharfetter-Gummel scheme is to find the optimum approximation for $j_{i+½}$ in the interval $[x_i, x_{i+1}]$.

What we will assume is that $j_{i+½}$ is constant over the interval $[x_i, x_{i+1}]$, and moreover that v and D are also constant over this interval. What is *not* constant is the density n, but we assume that we do know the boundary values of n:

$$\begin{aligned} n_i &= n(x_i), \\ n_{i+1} &= n(x_{i+1}). \end{aligned}$$

We thus have a boundary-value problem for the equation

$$j_{i+½} = -D\frac{\partial n}{\partial x} + v n(x). \tag{4}$$

How can we have a boundary value problem with two boudnary values but only a first-order equation? Because we only know $j_{i+½}$ is constant, not that it has a particular value. This gives the second degree of freedom in the problem.

Now, we know that any first-order equation can be integrated with the proper integrating factor. In this case it is an exponential, and we can write

$$\begin{aligned} j_{i+½}e^{-v(x-x_i)/D} &= \left(-D\frac{\partial n}{\partial x} + v n\right) e^{-v(x-x_i)/D}, \\ &= -D\frac{\partial}{\partial x}\left(ne^{-v(x-x_i)/D}\right). \end{aligned}$$

Integrating both sides of this equation:

$$\begin{aligned} \int_{x_i}^{x_i+\Delta} j_{i+½}e^{-v(x-x_i)/D}\,dx &= -D\int_{x_i}^{x_{i+1}} \frac{\partial}{\partial x}\left(ne^{-v(x-x_i)/D}\right)\,dx, \\ j_{i+½}\int_0^{\Delta} e^{-vx'/D}\,dx' &= -D\left(ne^{-v(x-x_i)/D}\right)\Big|_{x_i}^{x_{i+1}}, \\ j_{i+½}\frac{D}{v}\left(e^{-v\Delta/D} - 1\right) &= D\left(n_i - n_{i+1}e^{-v\Delta/D}\right). \end{aligned}$$

Thus, we have

$$j_{i+½} = v\frac{n_i - e^{-v\Delta/D}n_{i+1}}{1 - e^{-v\Delta/D}}. \tag{5}$$

This is the generalized Scharfetter-Gummel expression for the current density. [If you prefer, it can be written in a more symmetric form by multiplying numerator and denominator by $\exp(v\Delta/2D)$.]

Since (5) gives $j_{i+½}$ as a linear combination of n_i and n_{i+1}, we will get a three-point fininte-difference scheme when we insert (5) into (3).

But the three coefficients will now vary with v/D. Examining the limiting cases, we see

$$\lim_{v\to 0} j_{i+½} = D\frac{n_i - n_{i+1}}{\Delta},$$

which just gives the usual three-point approximation for $-D\partial^2 n/\partial x^2$ when inserted into (3). On the other hand, when the drift current is large compared to the diffusion current ($|v|\Delta \gg D$),

$$j_{i+½} \to \begin{cases} v n_i & \text{if } v > 0, \\ v n_{i+1} & \text{if } v < 0. \end{cases}$$

This produces precisely the upwind-difference form in this limit.