A Boltzmann Transport Simulation using Open Source Physics

by

J. E. Hasbun

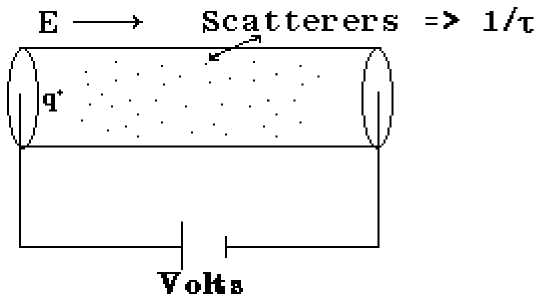
State University of West Georgia

Acknowledgements:

Paul Drallos (Plasma Dynamics Corporation)
J. M. Wadehra - (Wayne State U)

2003 Summer OSP Workshop - Davidson College
- Wolfgang Christian and Mario Belloni
- Harvey Gould
- Jan Tobochnik

- Start with a charged particle in an electric field in a substance



- The particle is accelerated by

$$F_E = qE$$

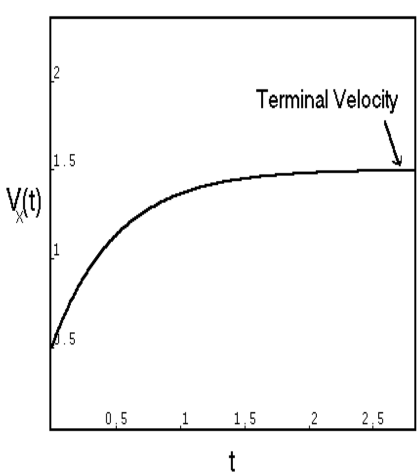
and decelerated by

$$R_F = -m\frac{v}{\tau}$$

Newton's 2nd Law gives

$$m\frac{dv}{dt} = qE - m\frac{v}{\tau} \quad \Rightarrow \quad \int \frac{dv}{v - \frac{qE\tau}{m}} = -\frac{1}{\tau}\int dt$$

with the solution: $$v(t) = \frac{qE\tau}{m}(1 - e^{-t/\tau}) + v_0 e^{-t/\tau}$$



if $\tau \to \infty$, $v \to \frac{qE\tau}{m} \to \infty$

if τ is finite,

as $t \to \infty$, $v \to \frac{qE\tau}{m}$ }drift velocity $\to v_t$

at t=0, $v = v_0$

-Motivation → to simulate the Boltzmann transport equation (BTE) and to see how it's possible to reproduce the above result

- The BTE has the form:

$$\frac{\partial f}{dt} + \vec{v} \cdot \vec{\nabla}_r f + \vec{F} \cdot \vec{\nabla}_p f = \frac{\partial f}{\partial t}\Big|_{G-R}$$

A partial d.e. for $f = f(\vec{r}, \vec{p}, t)$

- Making use of the relaxation time approximation with τ as the scattering time, we write

$$\frac{\partial f}{\partial t}\Big|_{G-R} \sim \frac{\partial f}{\partial t}\Big|_{coll} = -\frac{f_A}{\tau}$$

where $f_A = f - f_0$ } a deviation from equilibrium

and neglecting the 2nd term; i.e., taking $f = f(\vec{p}, t)$ where $\vec{p} = m\vec{v}$

get

$$\frac{\partial f}{dt} + \frac{F}{m}\frac{\partial f}{\partial v} = -\frac{f - f_0}{\tau}$$

First numerical way

$$\frac{\partial f}{\partial t} = \frac{f(v,t+\Delta t) - f(v,t)}{\Delta t} \quad , \quad \frac{\partial f}{\partial v} = \frac{f(v+\Delta v,t) - f(v,t)}{\Delta v}$$

define (discretize)

$v_i = (i-1)dv$, $t_j = (j-1)dt$, $i = 1..N$, $j = 1...M$, then

$$\frac{f(v_i,t_{j+1}) - f(v_i,t_j)}{dt} + c\frac{f(v_{i+1},t_j) - f(v_i,t_j)}{dv} = -\frac{f(v_i,t_j) - f_0(v_i,\infty)}{\tau}$$

or

$$f_{i,j+1} = f_{i,j}(1 - \frac{dt}{\tau} + c\frac{dt}{dv}) - c\frac{dt}{dv} f_{i+1,j} + \frac{dt}{\tau} f_{0i}$$

- We work with the following units (typical)

mean free path: $a_b \sim 10^{-7} m$

rms speed: $v_b \sim 500 m/s$

time: $t_b = \frac{a_b}{v_b} = 2x10^{-10}\sec$, $m \sim 10u = 10.6x10^{-27} kg$

energy: $\varepsilon_b = mv_b^2 = 2.65x10^{-21} J = 16.5meV$

temperature: $T_b = \frac{\varepsilon_b}{k} \sim 192K$

force: $F_b = \frac{\varepsilon_b}{a_b} = 2.65x10^{-14} N$, thus $qE = cF_b$, and for $E \sim 10^5 V/m$

then: $0 < c < 0.6$ (a measure of the E field)

□ However, this method breaks down.

- The Drallos and Wadehra Method - a different approach

They noticed that the form of the BTE

$$\frac{\partial f(\vec{v},t)}{dt} + \vec{a}\cdot\vec{\nabla}_v f(\vec{v},t) = R(\vec{v},t)$$

Or, multiplying by Δt and adding $f(\vec{v},t)$, to both sides, using $\Delta\vec{v} = \vec{a}\Delta t$,

$$f(\vec{v},t) + (\Delta t\frac{\partial}{\partial t} + \Delta\vec{v}\cdot\vec{\nabla}_v) f(\vec{v},t) = f(\vec{v},t) + R(\vec{v},t)\Delta t$$

<u>can also be obtained</u> if one expands a function of two variables $f(\vec{v},t)$ to first order; i.e., in the form

$$f(t+\Delta t,\vec{v}+\Delta\vec{v}) = f(t,\vec{v}) + f_t(t,\vec{v})\Delta t + f_{v_x}(t,\vec{v})\Delta v_x + f_{v_y}(t,\vec{v})\Delta v_y$$

$$= f(t,\vec{v}) + \Delta t\frac{\partial}{\partial t} f(t,\vec{v}) + \Delta\vec{v}_x\frac{\partial}{\partial v_x} f(t,\vec{v}) + \Delta\vec{v}_{yx}\frac{\partial}{\partial v_y} f(t,\vec{v})$$

or

$$f(t+\Delta t,\vec{v}+\Delta\vec{v}) = f(t,\vec{v}) + \Delta t\frac{\partial}{\partial t} f(t,\vec{v}) + \Delta\vec{v}\cdot\vec{\nabla}_v f(t,\vec{v})$$

and noticing that this means that,

$$\frac{f(t+\Delta t,\vec{v}+\Delta\vec{v}) - f(t,\vec{v})}{\Delta t} = \frac{\partial}{\partial t} f(t,\vec{v}) + \frac{\Delta\vec{v}}{\Delta t}\cdot\vec{\nabla}_v f(t,\vec{v})$$

so that in the limit as $\Delta t \to 0$, with $\vec{a} = \frac{d\vec{v}}{dt}$, we get

$$\frac{\partial}{\partial t} f(t,\vec{v}) + \vec{a}\cdot\vec{\nabla}_v f(t,\vec{v}) = R(t,\vec{v})$$

with

$$R(t,\vec{v}) = \lim_{\Delta t\to 0}\frac{f(t+\Delta t,\vec{v}+\Delta\vec{v}) - f(t,\vec{v})}{\Delta t} \equiv \left(\frac{\partial f}{\partial t}\right)_{coll}$$ $\leftarrow$ our collision term!

- Application of the Drallos and Wadehra (DW) Method

Solving the BTE then is equivalent to solving

$$f(t+\Delta t,\vec{v}+\Delta\vec{v}) = f(t,\vec{v}) + R(t,\vec{v})\Delta t$$

In our case, we write

$f_{i+1,j} = f_{i,j} + R_{i,j}\Delta t$, with $R_{i,j} \equiv -(f_{i,j} - f_{-\infty,j})/\tau$

with arrays (with M and N suitable integers):

$0 < t < t$, with $dt = \frac{t_f - 0}{M}$, and $-v_{\min} < v < v_{\max}$, with $dv = \frac{v_{\max} - v_{\min}}{N}$

for later times shift v according to

$v_{i+1,j} = v_{i,j} + \Delta v$, where $\Delta v = \frac{qE}{m}\Delta t$

so that for every $f_{i+1,j}$ there is a $v_{i+1,j}$ which corresponds to obtaining $f(t+\Delta t, v+\Delta v)$ which is plotted versus v for every t

<u>BC's</u>

At t=0 (initial), $f(t=0,v) = \frac{1}{\sqrt{2\pi T_0}} e^{-\left(\frac{mv^2}{2} - eE\langle z\rangle_0\right)/kT_0}$

At t=∞, (final), $f(t=\infty,v) = \frac{1}{\sqrt{2\pi T_\infty}} e^{-\left(\frac{m(v-v_d)^2}{2} - eE\langle z\rangle_\infty\right)/kT_\infty}$

Where,

v_d = drift speed (input), $\langle Z\rangle_0 \equiv 0$, $\langle Z\rangle \equiv L$, T_0=50K, T_∞=800K

Finally, after obtaining $f(v,t)$, the average velocity as a function of time is

$$\langle v(t)\rangle = \int_{-\infty}^{\infty} f(v,t)v\,dv \Big/ \int_{-\infty}^{\infty} f(v,t)\,dv \equiv v(t)$$

which is compared to

$$v(t) = \frac{qE\tau}{m}(1 - e^{-t/\tau}) + v_0 e^{-t/\tau}$$

Simulation #1 - First method (Not so good)
Boltzm_applet_App.htm

Simulation #2 - 2nd Method (DW - better)
Boltzmn_applet_App.htm

These and other java applications are found at:
http://www.westga.edu/~jhasbun/osp/osp.htm

Conclusion

- The OSP library has been beneficial in both teaching and research

- The Java programming environment has been found to be versatile in many applications. The present is only one example of its power.

- It is expected that the OSP project will become even more friendly as contributors improve the currently available library and more applications are made available to the scientific community.