Resistivity

This exercise modifies the previous exercise on random walks and diffusion by adding an electric field that accelerates particles between collisions. Momentum is added by the electric field and is taken away by the collisions. On average, the momentum lost per unit time in collisions is -mu / τ where u is the average drift velocity and τ is the mean time between collisions.
The momentum gained per unit time is m du/dt = q E. If we balance the gain and loss we find u = q E τ / m. The current is J = n q u = (n q^2 τ / m) E which tells us that the conductivity is σ = (n q^2 τ / m) and the resistivity is η = (m / n q^2 τ).

Below we will follow a group of particles that is accelerating AND having collisions. We will find the average drift velocity and verify that the conductivity is what we expect.

Let $q := 1$ $m := 1$ $E := 1$ $a := \frac{q \cdot E}{m}$ then

$a = 1$ is the acceleration.

The distance travelled between collisions is $v_x \cdot \Delta t + \frac{a \cdot \Delta t^2}{2}$

$imax := 250$ number of particles followed

$\tau := 1$ the time step $jmax := 1000$ the number of time steps

The program loop below adds a constant acceleration along the x axis to the random walk.
It calculates and stores the X positions of the particles.

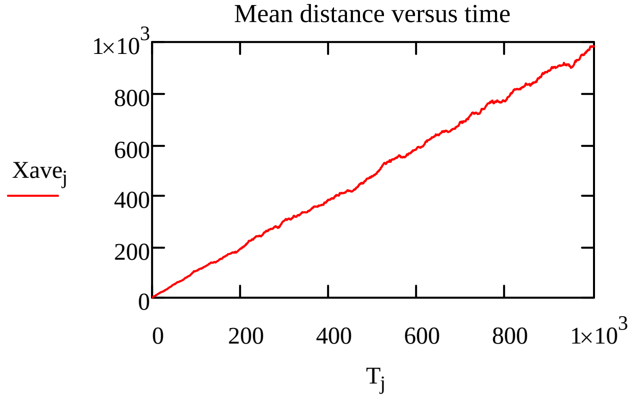
```
X := | X[imax,jmax] ← 0                         Initialize X. Start the particles at x = 0.
     | for i ∈ 0 .. imax                        Do for each particle i:
     |   v ← 0                                  The starting v is zero for each particle
     |   for j ∈ 1 .. jmax                      Follow that particles' motion for j time steps
     |     θ ← 2·π rnd(1)                       Select a random starting angle for v
     |     v_x ← v·cos(θ)                       and project v onto the x direction.
     |     Δt ← −τ·ln(rnd(1))                   Select a time interval to the next collision.
     |     v_y ← v·sin(θ)
     |     X[i,j] ← X[i,j−1] + v_x·Δt + a·Δt^2/2    Find the change in the X position between
     |                                              collisions and the change in the x velocity.
     |     v_xnew ← v_x + a·Δt
     |     v ← sqrt(v_xnew^2 + v_y^2)           Store the new value of the speed v
     | X
```

$j := 0 .. jmax$ $\qquad$ $i := 0 .. imax$

$T_j := j \cdot \tau$ $\qquad$ Approximate time of the jth time step.

Let's find the average location at the jth time step

$$Xave_j := \sum_{i=0}^{imax} \frac{X_{i,j}}{imax + 1}$$



The slope of x(t) gives us the mean velocity of the drift:

$v_d := \text{slope}(T, Xave)$

$v_d = 0.978$

Thus with an electric field E of 1, and a mean collision time of 1, the mean drift velocity is one.

Mobility:
The mobility is defined by $\quad \mu := \frac{E}{|v_d|}$ $\quad$ where v_d is the drift velocity

From momentum balance we find that $\quad \mu := \frac{|q|}{m\nu}$ $\quad$ where $\nu = 1/\tau$ is the collision frequency.

For our example above, $\mu = 1$.

Resistivity:
The resistivity is defined by $\quad \eta := \frac{m}{n \cdot q^2 \cdot \tau}$ $\quad$ where n is the number density of the current-carrying particles.

In this exercise we will not calculate a final value for the reisistivity or conductivity because the number density has not been specified. The mobility is independent of density and is $\mu = 1$ for the example above.

Resistive heating

This program loop records both the velocity AND the location. How can we save two matrices if the program loop only returns one thing? We can use the stack command to create one longer matrix by combining the matrices for the x locations and for the velocities.

$$
XV := \left|
\begin{array}{l}
X_{imax,jmax} \leftarrow 0 \\
V_{imax,jmax} \leftarrow 0 \\
\text{for } i \in 0..imax-1 \\
\quad \left| \begin{array}{l}
v \leftarrow 0 \\
\text{for } j \in 1..jmax \\
\quad \left| \begin{array}{l}
\theta \leftarrow 2\cdot\pi\, rnd(1) \\
\Delta t \leftarrow -\tau\cdot \ln(rnd(1)) \\
v_x \leftarrow v\cdot\cos(\theta) \\
v_{xnew} \leftarrow v_x + a\cdot\Delta t \\
v_y \leftarrow v\cdot\sin(\theta) \\
X_{i,j} \leftarrow X_{i,j-1} + v_x\cdot\Delta t + \dfrac{a\cdot\Delta t^2}{2} \\
v \leftarrow \sqrt{v_{xnew}^2 + v_y^2} \\
V_{i,j} \leftarrow v
\end{array} \right.
\end{array} \right. \\
XV \leftarrow stack(X,V)
\end{array}
\right.
$$

We will use the -1 after imax so that the number of entries in the matrix is imax rows and jmax+1 columns.

X is location and V is velocity.
i is the particle number.
j is the time step number.

These lines advance the velocity values in time.

This line finds and stores the current X location.

This line stores the current speed.
The last line stacks these into one matrix which we call XV.

The submatrix command allows us to recover X and V from XV

$$X := submatrix(XV, 0, imax-1, 0, jmax)$$

$$V := submatrix(XV, imax, 2\cdot imax-1, 0, jmax)$$

Let's check on the size of of the matrices using the *rows* and *cols* functions to be sure we did the stacking and unstacking correctly

$cols(V) = 1001$ $\quad rows(V) = 250$

$cols(X) = 1001$ $\quad rows(X) = 250$

$cols(XV) = 1001$ $\quad rows(XV) = 502$

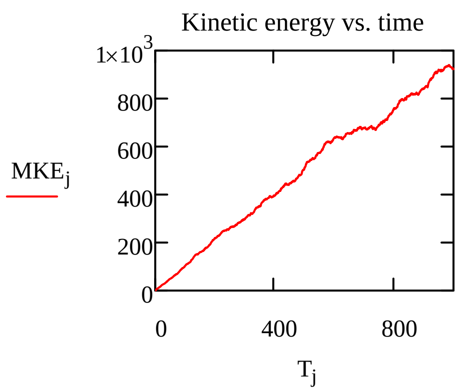
We will average the square of the velocity over all i particles and find the mean squared velocity V2ave for the group at each time j. Define the mean kinetic energy at time j:

$$V2ave_j := \frac{1}{imax} \cdot \sum_{i=0}^{imax-1} \left(V_{i,j}\right)^2$$

$$MKE_j := \frac{1}{2} \cdot m \cdot V2ave_j$$

$$T_j := j$$

The mean time at the jth time step



The mean kinetic energy increases linearly with time because the electric field causes the particles to be heated. The velocity vector increases between collisions and the elastic collisions only reorient the vector, they do not change the length.

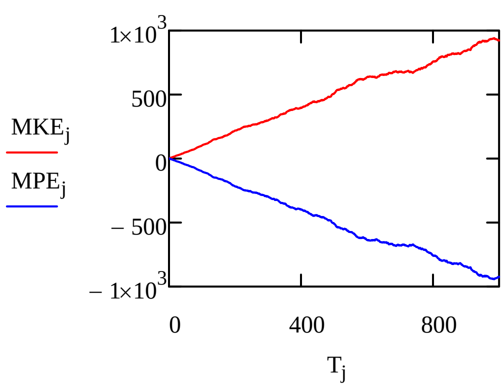
$$\text{slope}(T, MKE) = 0.936$$

Try it: If we change from a = qE/m = 1 to a = 2 the slope increases by a factor 4. Why?

Is energy conserved?

The energy gained by the particle is determined by the potential through which it has dropped. We can plot on one axis the average change in potential energy -x q E. Recall that the product of x and -qE gives the potential energy qϕ. On the other axis we plot the mean kinetic energy. Let's define the mean potential energy change from the mean value of X:

$$Xave_j := \frac{1}{imax} \cdot \sum_{i=0}^{imax-1} X_{i,j} \qquad MPE_j := -q \cdot E \cdot Xave_j$$



The mean potential energy has gone down by the same amount that the mean kinetic energy has gone up!

Try it: What would a plot of the sum of the potential and kinetic energies, MPE+MKE, look like? Are there any bumps in the plot or is it smooth? In other words, is energy conserved precisely, or is it conserved only after averaging over events?