Homework 3

① (i) Calculate the first three temporal moments

$$M_0 = \text{Sum}\,(C\,\Delta t) = 100$$
$$M_1 = \text{Sum}\,(t\,C\,\Delta t) = 1.0002 \times 10^{6}$$
$$M_2 = \text{Sum}\,(t^2 C\,\Delta t) = 1.0006 \times 10^{10}$$

Now recall $M_0 = M/v$

$$M_1 = \frac{2D + vx}{v^3} M$$

We have 3 eqns
3 unknowns (M, v, D)

$$M_2 = \frac{12D^2 + 6Dvx + v^2x^2}{v^5} M$$

$x = 1000$

You can solve this by hand or by asking Mathematica

2 solution sets exist

$$\{M, D, v\} = \{5, \underset{\text{unphysical}}{-12.5}, 0.05\} \text{ OR } \{10, 0.03, 0.1\}$$

$\therefore$ $M = 10$ kg
$D = 0.03$ m^2/s
$v = 0.1$ m/s

At $x = 10000$m

$$C(x,t) = \frac{10}{\sqrt{4\pi D t}}\, e^{-\frac{(10000 - 0.1t)^2}{4(0.03)t}}$$

$$C_{max} \simeq \frac{10}{\sqrt{4\pi(0.03)(10^5)}} = 5 \times 10^{-2}\ \text{kg/m}$$

less than threshold

Problem 2

$$\frac{\delta c}{\delta t} + v(y)\frac{\delta c}{\delta x} = D\frac{\delta^2 c}{\delta x^2} + D\frac{\delta^2 c}{\delta y^2} \qquad (1)$$

Let $c = \bar{c} + c'$ $\qquad v = \bar{v} + v'$ $\qquad \bar{c}(x)\ ;\ c'(x,y)\ ;\ \bar{v}\ ;\ v'(y)$

$$\Rightarrow \frac{\delta c'}{\delta t} + \frac{\delta \bar{c}}{\delta t} + \bar{v}\frac{\delta \bar{c}}{\delta x} + v'\frac{\delta \bar{c}}{\delta x} + \bar{v}\frac{\delta c'}{\delta x} + v'\frac{\delta c'}{\delta x} = D\frac{\delta^2 \bar{c}}{\delta x^2} + D\frac{\delta^2 c'}{\delta y^2} + D\frac{\delta^2 c'}{\delta y^2} \ (2)$$

Average (2)

$$\frac{\delta \bar{c}}{\delta t} + \bar{v}\frac{\delta \bar{c}}{\delta x} = D\frac{\delta^2 \bar{c}}{\delta x^2} - \frac{\delta}{\delta x}\left(\overline{v'c'}\right) \qquad (3)$$

Subtract (3) from (2)

$$\frac{\delta c'}{\delta t} + v'\frac{\delta \bar{c}}{\delta x} + \bar{v}\frac{\delta c'}{\delta x} + v'\frac{\delta c'}{\delta x} = D\frac{\delta^2 c'}{\delta x^2} + D\frac{\delta^2 c'}{\delta y^2} + \frac{\delta}{\delta x}\left(\overline{v'c'}\right) \ (4)$$

Now, following Taylor's argument when $t > \tau = \frac{(2h)^2}{D}$ we expect several terms to be negligible and

$$v'\frac{\delta \bar{c}}{\delta x} = D\frac{\delta^2 c'}{\delta y^2}$$

Integrating once $\qquad D\frac{\delta c'}{\delta y^2} = \frac{\delta \bar{c}}{\delta x}\int v'(y)\,dy$

Again $\qquad c' = \frac{1}{D}\frac{\delta \bar{c}}{\delta x}\iint v'(y')\,dy'\,dy$

$$v'(y) = \frac{3}{2}\bar{v}\left(1 - \frac{y^2}{h^2}\right) - \bar{v} = \frac{1}{2}\bar{v} - \frac{3}{2}\bar{v}\frac{y^2}{h^2}$$

$$\int v'(y) = \frac{1}{2}\bar{v}y - \frac{1}{2}\bar{v}\,{}^{y^3}\!/_{h^2} + C_1$$

$$\iint v'(y')dy'dy = \frac{1}{4}\bar{v}y^2 - \frac{1}{8}\bar{v}\frac{y^4}{h^2} + C_1 y + C_2$$

C_1 and C_2 are constant of integration

$c'(y) = c'(-y)$ by symmetry $\Rightarrow C_1 = 0$

$$\frac{1}{2h}\int_{-h}^{h} c'(y)\,dy = 0$$ as average $c' = 0$ by definition

$$\therefore \int_{-h}^{h} \frac{1}{4}\bar{v}y^2 - \frac{1}{8}\bar{v}\frac{y^4}{h^2} + C_2 \; dy = 0$$

$$\frac{7}{60}\bar{v}h^3 + 2C_2 h = 0$$

$$C_2 = -\frac{7}{120}\bar{v}h^2$$

$$\therefore c'(y) = \frac{\bar{v}}{D}\frac{\delta\bar{c}}{\delta x}\left(\frac{1}{4}y^2 - \frac{1}{8}\frac{y^4}{h^2} - \frac{7}{120}h^2\right)$$

Now we want $\overline{v'c'}$ for (4)

$$\Rightarrow \frac{1}{2h}\int_{-h}^{h}\left(\frac{1}{2}\bar{v} - \frac{3}{2}\bar{v}\frac{y^2}{h^2}\right)\left(\frac{\bar{v}}{D}\frac{\delta\bar{c}}{\delta x}\left(\frac{1}{4}y^2 - \frac{1}{8}\frac{y^4}{h^2} - \frac{7}{120}h^2\right)\right)dy$$

$$= -\frac{2}{105}h^2\frac{\bar{v}^2}{D}\frac{\delta\bar{c}}{\delta x}$$

$\therefore$ (4) can be written as

$$\frac{\delta\bar{c}}{\delta t} + \bar{v}\frac{\delta\bar{c}}{\delta x} = \underbrace{\left(D + \frac{2}{105}\frac{h^2\bar{v}^2}{D}\right)}_{D_{Taylor}}\frac{\delta^2\bar{c}}{\delta x^2}$$

Problem 1

Part 2

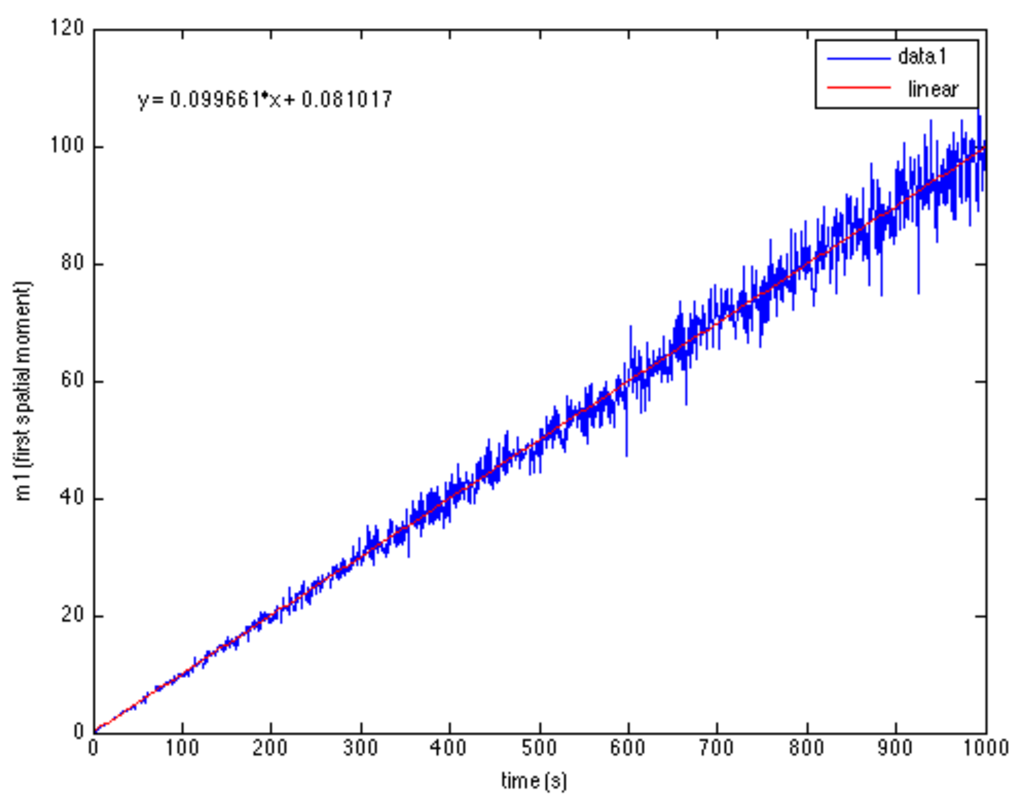
Below are plots of time against, first moment and linear fit, second moment and a quadratic fit and second centered moment with a linear fit.

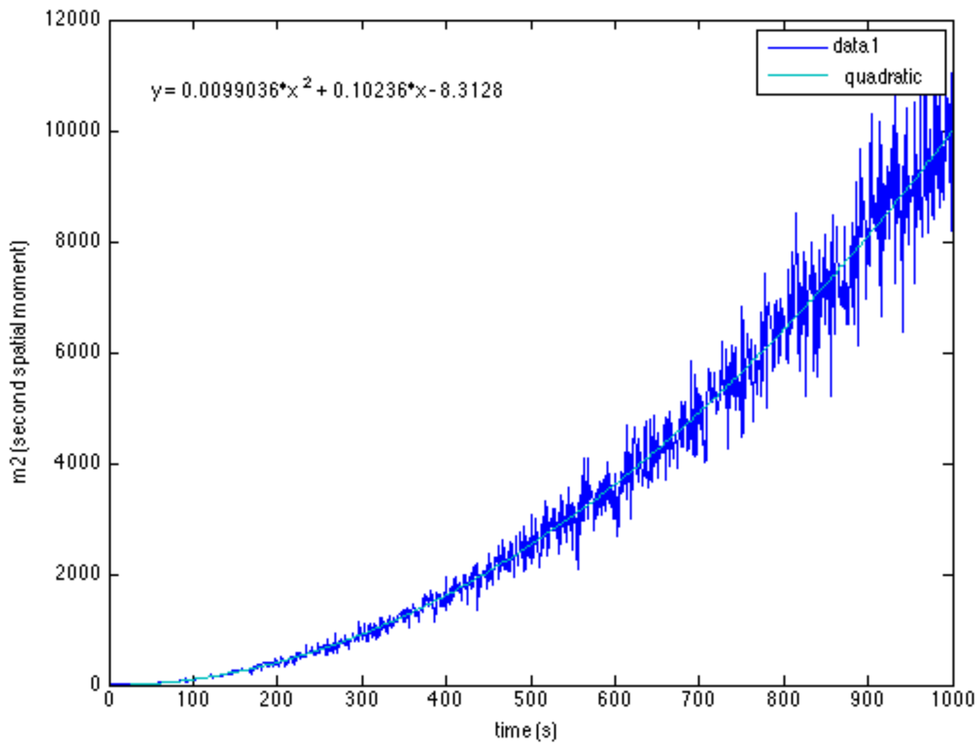
While the fit for mu1 gives us a good measure or the velocity – i.e. the slope is approximately 0.1 m/s, which matches well, the fit for kappa11 gives us a slope of 0.036 m^2/s and thus a diffusion coefficient of 0.018, which is bigger than estimated by temporal moments (but will still ensure a concentration that does not violate the threshold).

Part of the issue is that the data is so noisy and so we must be careful in dealing with this.

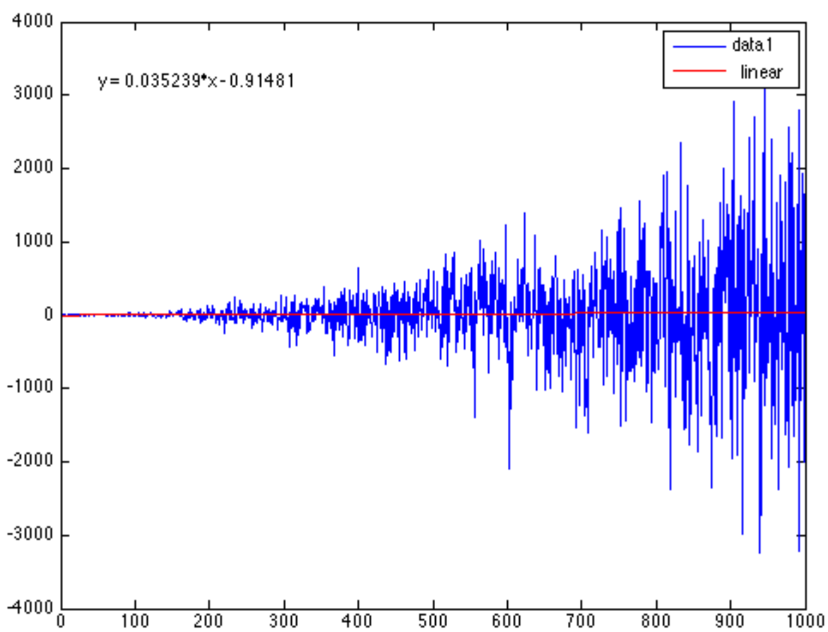
If we perform a quadratic fit of the second moment and recognize

m2=v^2t+2Dt, we again get a good measure of v, but D is even bigger. This highlights that this method works well for estimating v, but can be troublesome for D and noise propagates into each higher order moment and can amplify.





data1
quadratic
y = 0.0099036*x^2 + 0.10236*x - 8.3128
m2 (second spatial moment)
time (s)
12000
10000
8000
6000
4000
2000
0
0
100
200
300
400
500
600
700
800
900
1000

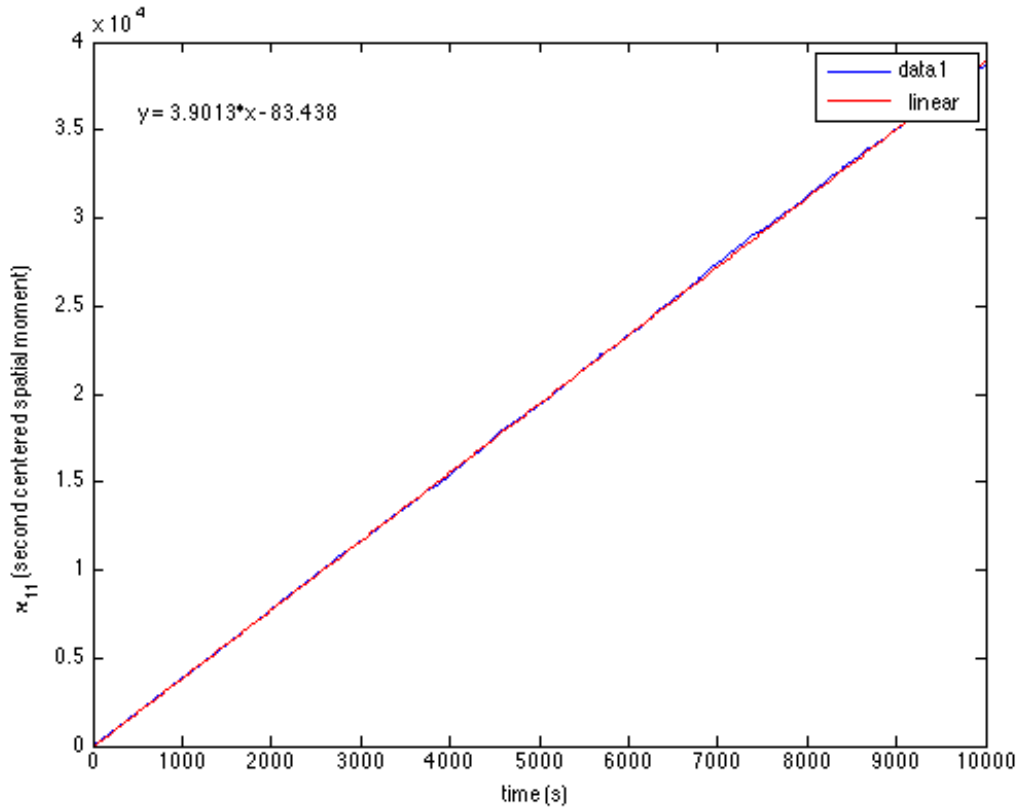


data1
linear
y = 0.035239*x - 0.91481
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
0
100
200
300
400
500
600
700
800
900
1000

Problem 3

Code

```
%rw_taylor

clear
clc
close all

D=0.01;
dt=0.1;

N=1e4;

x=zeros(1,N);
y=linspace(-1,1,N);

Nsteps=1e5;

time=[];
for jj=1:Nsteps
  jj
  x=x+3/2*(1-y.^2)*dt+sqrt(2*D*dt)*randn(size(x));
  y=y+sqrt(2*D*dt)*randn(size(x));

  %reflect particles
  apple=find(y>1);
  y(apple)=2-y(apple);
  apple=find(y<-1);
  y(apple)=-2-y(apple);

  if mod(jj,1)==0
    plot(x,y,'.')
    pause(0.1)
  end

  m1(jj)=1/N*sum(x);
  m2(jj)=1/N*sum(x.^2);
  time(jj)=jj*dt;
end

kappa=m2-m1.^2;
plot(time,kappa)
```



The above curve is the second centered moment against time with a linear fit, whose slope is 3.9, which means that the dispersion coefficient is 3.9/2=1.95.

From our calculation in Problem 2 we would get

D_{Taylor}=0.01+2/105*1/0.01=1.92 , very close to what we measure