

Homework 2

$$\textcircled{1} \quad \frac{\delta C}{\delta t} = \frac{\delta^2 C}{\delta x^2} \quad 0 < x < 20 \quad C(x, t=0) = \delta(x-10)$$

$$\frac{\delta C}{\delta x} \Big|_{x=0} = \frac{\delta C}{\delta x} \Big|_{x=20} = 0$$

Polygonia tells us the solution for this is

$$\int_0^{20} \delta(\xi-10) G(x, \xi, t) d\xi \quad G(x, \xi, t) = \frac{1}{20} + \frac{2}{20} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{20}\right) \cos\left(\frac{n\pi \xi}{20}\right) e^{-\frac{n^2 \pi^2 t}{20}}$$

$$\left. \begin{array}{l} \text{(i) } [L] = \text{length} \\ [D] = \text{length}^2 \text{ Time}^{-1} \end{array} \right\} \text{Combine to get } \tau = \frac{L^2}{D}$$

↓
only natural
timescale for parameters

(ii) See figures + code

$$C(x, t) = \frac{1}{20} + \frac{1}{10} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{20}\right) \cos\left(\frac{n\pi 10}{20}\right) e^{-\frac{n^2 \pi^2 t}{20}}$$

When $C(t=0) = \delta(x-15)$

$$C(x, t) = \frac{1}{20} + \frac{1}{10} \sum_{n=1}^{\infty} \cos\left(\frac{n\pi x}{20}\right) \cos\left(\frac{n\pi 15}{20}\right) e^{-\frac{n^2 \pi^2 t}{20}}$$

$$(2) \quad \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad 0 < x < \infty$$

$$C(x, t=0) = 0 \quad C(x=0, t) = C_0$$

From Polgarin

$$(i) \quad C(x, t) = \int_0^t C_0 H(x, t-\tau) d\tau \quad H(x, t) = \frac{x}{2\sqrt{\pi D}} t^{-3/2} e^{-x^2/4Dt}$$

Evaluate this integral with Mathematica for example

$$C(x, t) = C_0 \left(1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right)$$

or

$$= C_0 \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right)$$

$$(ii) \quad M(t) = \int_0^{\infty} C(x, t) dx = \frac{2}{\sqrt{\pi}} \sqrt{Dt}$$

$$(iii) \quad M \propto \sqrt{D} \Rightarrow \text{double } D \text{ means } \sqrt{2} \text{ more mass}$$

%Problem1.m

```
clear
clc
close all
```

```
x=linspace(0,20,1000);
```

```
D=1;
L=20;
```

```
tau=L^2/D;
```

```
%for C(t=0)=delta(x-10)
```

```
for t=[0.001 0.01 0.1 1 10]*tau;
    for ll=1:length(x)
```

```
        n=1:100;
        sm=cos(n*pi*x(ll)/L).*cos(n*pi*10/L).*exp(-D*n.^2*pi^2*t/L^2);
```

```
        w(ll)=1/L+2/L*sum(sm);
```

```
    end
    figure(1)
    hold on
    plot(x,w)
end
```

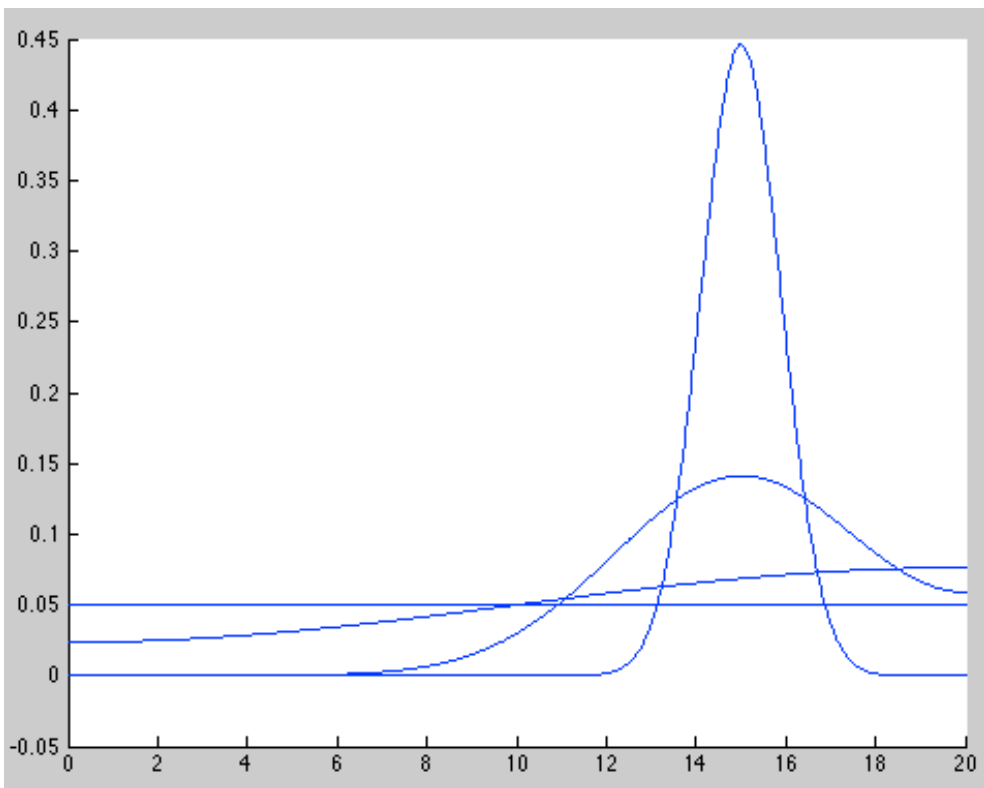
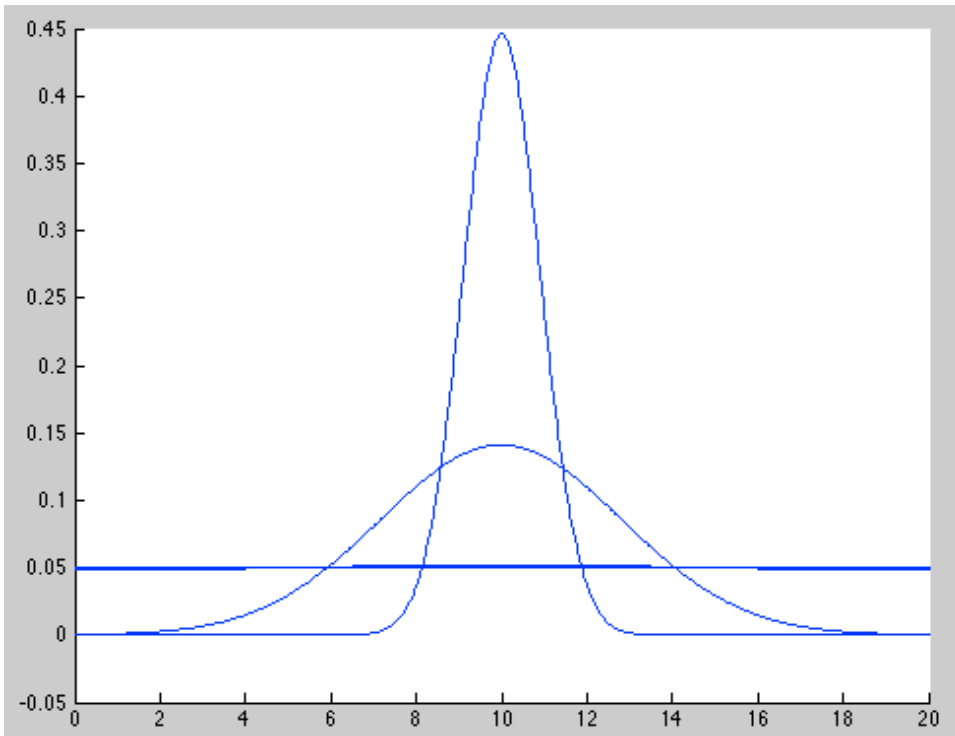
```
%for C(t=0)=delta(x-15)
```

```
for t=[0.001 0.01 0.1 1 10]*tau;
    for ll=1:length(x)
```

```
        n=1:101;
        sm=cos(n*pi*x(ll)/L).*cos(n*pi*15/L).*exp(-D*n.^2*pi^2*t/L^2);
```

```
        w(ll)=1/L+2/L*sum(sm);
```

```
    end
    figure(2)
    hold on
    plot(x,w)
end
```



%Problem_3.m

```
clear
clc
close all
```

```
x=0:0.1:15; %Define your spatial domain
dx=x(2)-x(1); %spatial discretization;
dt=0.001; %time step
Nsteps=100000; %Number of Timesteps
D=1; %Diffusion Coefficient
```

```
C=zeros(size(x)); %Our Initial Concentration
C(1)=1; %The Boundary Condition
```

```
for j=1:Nsteps
```

```
    %update concentration based on finite differences. We only update
    %locations 2 through N-1 as the end are determined from the boundary
    %conditions.
```

```
    Cnew(2:length(x)-1)=C(2:length(x)-1)+D*dt/dx^2*(C(1:length(x)-2)-
    2*C(2:length(x)-1)+C(3:length(x))));
```

```
    %Boundary Conditions
    Cnew(1)=1;
    Cnew(length(x))=Cnew(length(x)-1);
```

```
    %Update concentration field
    C=Cnew;
```

```
end
```

```
plot(x,C,'.')
hold on
%Greens function - finite domain.
```

```
n=0:1000; %number of terms in expansion
```

```
t=Nsteps*dt;
l=max(x);
```

```
for kk=1:length(x)
```

```
sm=4*(1-exp(-  
D.*pi^2.*(1+2*n).^2/4/l^2*t))./pi./((1+2*n).*sin((1+2*n)*pi*x(kk)/2/l));
```

```
Cg(kk)=sum(sm);
```

```
end
```

```
Cg(1)=1;
```

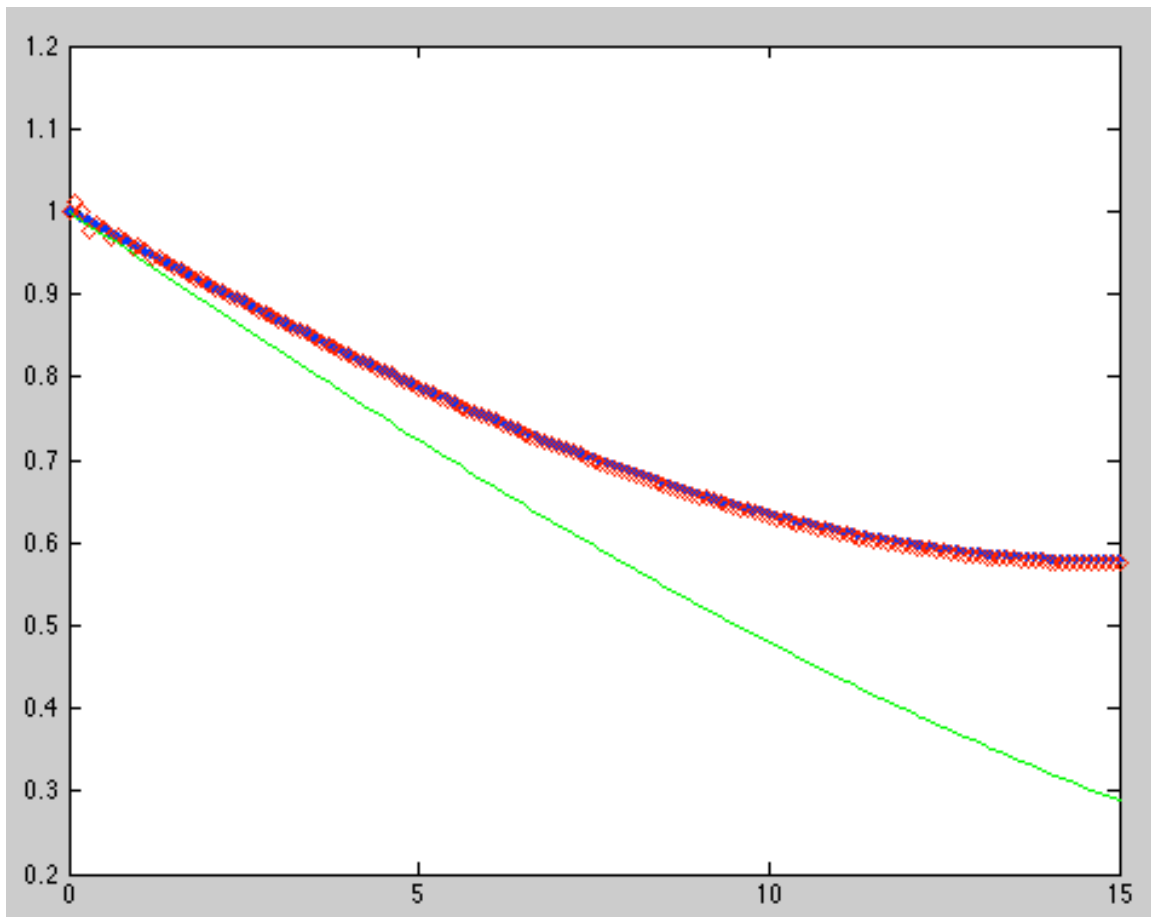
```
hold on
```

```
plot(x,Cg,'rd')
```

```
%seminfite domain
```

```
Csm=erfc(x/sqrt(4*D*t));
```

```
plot(x,Csm,'g')
```



%Problem 4

tic

clear

clc

%close all

%define your boundaries

xlow=0;

xup=20;

dt=.01; %timestep

D=1; %diffusion coefficient

N=1e6; % number of particles

xinit=10; %initial location of all the particles

x=xinit*ones(1,N); %initial condition4

Nsteps=1e3;

for kk=1:Nsteps

kk

x=x+sqrt(2*D*dt)*randn(size(x));

%reflect

apple=find(x<xlow);

x(apple)=-x(apple);

apple=find(x>xup);

x(apple)=2*xup-x(apple);

end

[c,x]=hist(x,100);

dx=x(2)-x(1);

plot(x,c/sum(c)/dx,'k')

toc

The following subplot shows concentrations for various numbers of particles with the above code. Notice as how particle numbers increase solution becomes smoother and looks much more like that in Problem 1.

