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(MTech VLSI Sem 1, EE22M302)

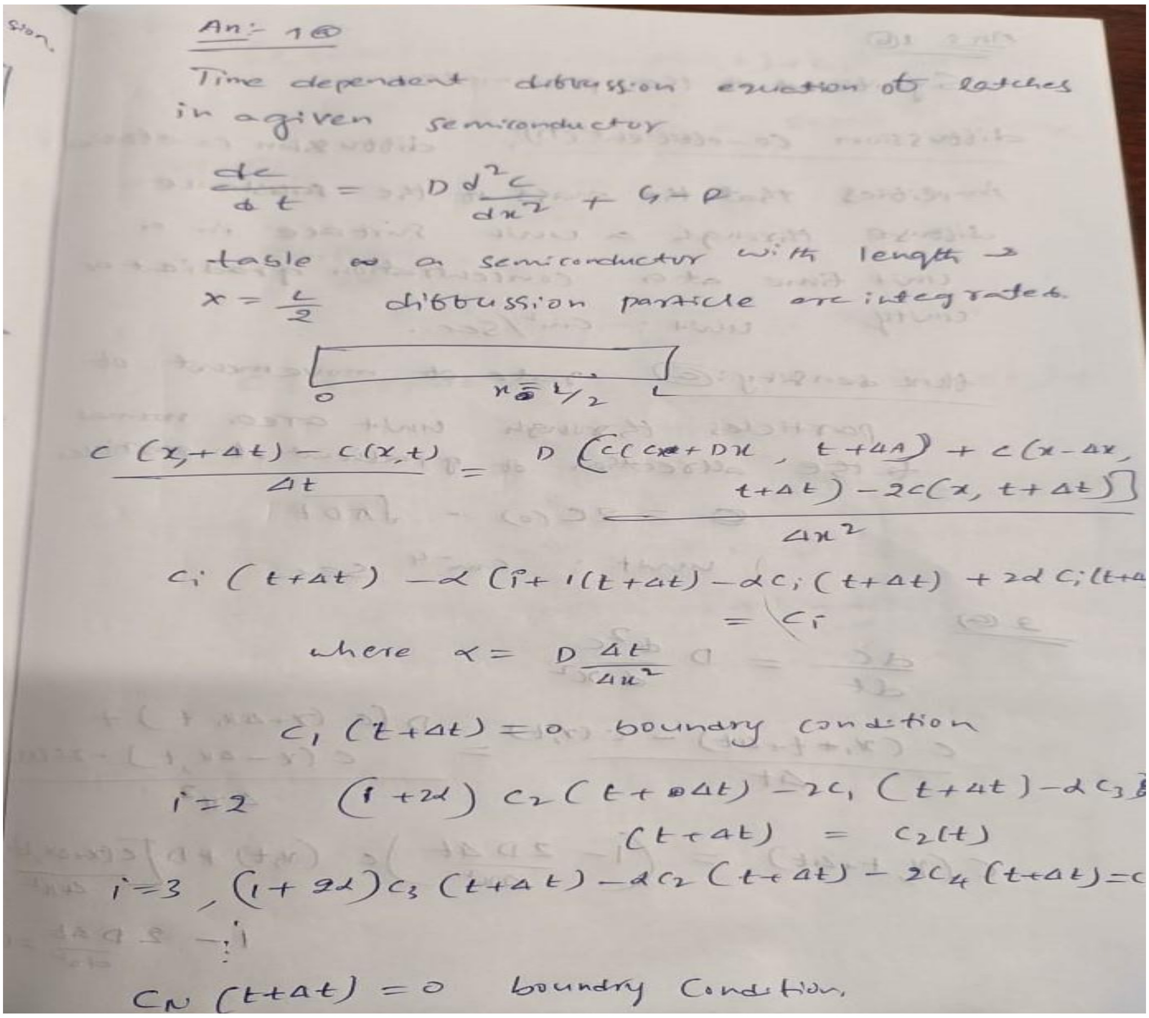
Lab no. : 7

Used version: Matlab 2022

Q.1: Numerical solution of Time dependent Diffusion equation

(a) Describe the formalism to solve time dependent diffusion equation using backward Euler scheme.

Ans:



An:- 1(a)

Time dependent diffussion equation of latches in a given semiconductor

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2} + G - R$$

table as a semiconductor with length → $x = \frac{L}{2}$ diffussion particle are integrated.

$0 \qquad x = L/2 \qquad L$

$$\frac{c(x, t+\Delta t) - c(x,t)}{\Delta t} = D\frac{\left[c(x+\Delta x, t+\Delta t) + c(x-\Delta x, t+\Delta t) - 2c(x, t+\Delta t)\right]}{\Delta x^2}$$

$c_i(t+\Delta t) - \alpha\,(c_{i+1}(t+\Delta t) - \alpha c_i(t+\Delta t) + 2\alpha\, c_i(t+\Delta t) = c_i$

where $\alpha = D\frac{\Delta t}{\Delta x^2}$

$c_1(t+\Delta t) = 0$ boundry condition

$i=2 \quad (1+2\alpha)\, c_2(t+\Delta t) - \alpha c_1(t+\Delta t) - \alpha c_3(t+\Delta t) = c_2(t)$

$i=3, \ (1+2\alpha) c_3(t+\Delta t) - \alpha c_2(t+\Delta t) - \alpha c_4(t+\Delta t) = c$

$\vdots$

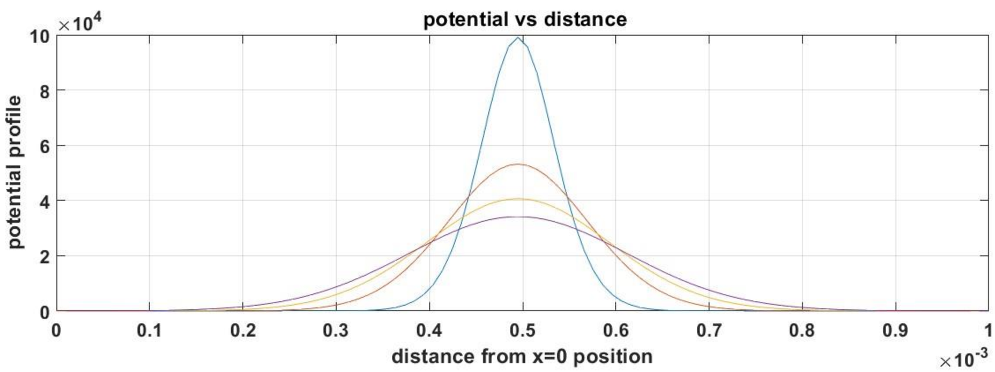
$c_N(t+\Delta t) = 0$ boundry Condition.

(b) Consider a region of length 10 µm. Assume perfectly absorbing boundary conditions at x=0 and at x=10 µm. At time t=0, assume that particles are injected at x=5 µm is such that the density is 10^6cm-3 (i.e., the injection is a delta function in both space and time). Using the formalism described in (a) explore the evolution of particle density over the specified domain (use D=10-4 cm2/s). Compare with analytical results. Explore the significance of the parameter.

Ans :

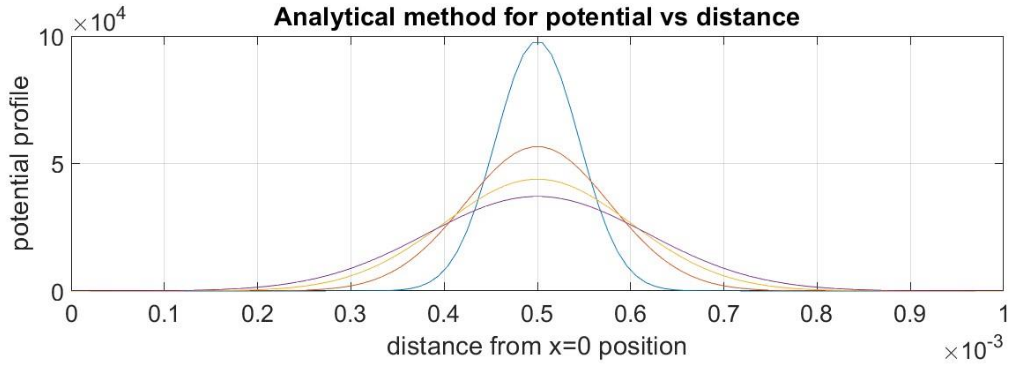
Numerical method:

```
clc;
clear all;
len=100*10^-6;
n=linspace(0,10^-5,1000);
a=1;
q=zeros(1000,1);
q(500,1)=100;
e=[];
hyp=eye(1000);
for i=1:100
h=zeros(1000);
    for i=2:999
        h(i,i-1)=0.5;
        h(i,i+1)=0.5;
    end
f=hyp*(h*q);
e=[e,q];
q=f;
end
hold on
plot(n,e(:,1),n,e(:,30),n,e(:,50),n,e(:,70));
grid on
xlabel('Numerical method : Distance in meters')
ylabel('density of particles')
title('numerical method for random walk for N=100 particles')
```




```
Analytical method:
clear all;
clc;
D=10^-4; % take D in cm^2/sec
l=10^-3; % take length in cm
t1=10*10^-6; %take time 100 micro sec
```

```
t2=30*10^-6;
t3=50*10^-6;
t4=70*10^-6;
% m=linspace(0,time,100); % take 100 spacing between time
M=linspace(0,l,100) ; % take 100 spacing between length
t=10^-6; % small portion of time
h=10^-5; % small portion of distance
Q=1.1*10^1;
q=[];
a1=2*((pi*D*t1)^0.5);
a2=2*((pi*D*t2)^0.5);
a3=2*((pi*D*t3)^0.5);
a4=2*((pi*D*t4)^0.5);
C1=((Q/a1)*exp(-((M-(0.5*l)).^2)/(4*D*t1)));

C2=((Q/a2)*exp(-((M-(0.5*l)).^2)/(4*D*t2)));

C3=((Q/a3)*exp(-((M-(0.5*l)).^2)/(4*D*t3)));

C4=((Q/a4)*exp(-((M-(0.5*l)).^2)/(4*D*t4)));

plot(M,C1,M,C2,M,C3,M,C4);
grid on
xlabel('distance from x=0 position');
ylabel('potential profile');
title('Analytical method for potential vs distance');
```



Ans 1(b)

Significant of the parameter

diffussion co-efficient (D): diffussion co-effi

implicities that the mass of the substence
difouse through a unit surface in a
unit time at a concentration gradient
unity, unit : cm^2/Sec..

flux density: (Q) rate of movement of
particles through unit area normal
to the direction of gradient of particle

$$Q = 2C(0) \cdot \sqrt{\pi D t}$$

unit : cm^{-4} sec,

Q.2: Random Walk simulations:

(a) Discretize the time dependent diffusion equation and arrive at a scheme for solving the time dependent diffusion equation through random walk simulations. For D=10-4 cm2/s and Δx=10 nm, what should be the Δt, the time step in such simulations?

Ans:

2(a)

$$\frac{dC}{dt} = D\frac{\partial^2 C}{\partial x^2}$$

$$\frac{C(x, t+\Delta t) - C(x,t)}{\Delta t} = \frac{D\left(C(x+\Delta x, t) + C(x-\Delta x, t) - 2C\right.}{\Delta x^2}$$

$$C(x, t+\Delta t) = \left(1 - \frac{2D\Delta t}{\Delta x^2}\right) C(x,t) + D\left[\frac{C(x+\Delta}{\Delta}\right]$$

then

$$C(x, t+\Delta t) = \frac{1}{2}\left[C(x+\Delta x, t) + C(x-\Delta x, t)\right]$$

$$D = \frac{1}{2} \times \frac{100\times 10^{-18}}{1\times 10^{-6}} = 50\times 10^{-12}\ m^2/sec$$

case (2):

$$1 - \frac{2D\Delta t}{dx^2} = \frac{1}{2}$$

$$\text{then } \frac{D\Delta t}{\Delta x^2} = \frac{1}{4}$$

$$D = \frac{1}{4} \times \frac{100\times 10^{-18}}{1\times 10^{-6}} = 25\times 10^{-12}$$

$$C(x, t+\Delta t) = \frac{1}{2}C(x,t) + \frac{1}{4}C(x+\Delta x, t) + C(x-\Delta x, t)$$

$$\begin{bmatrix} 1+2\alpha & -\alpha & 0 & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ 0 & -\alpha & 1+\alpha & -\alpha \\ \vdots & & & \end{bmatrix} \begin{bmatrix} c_2(t+\Delta t) \\ c_3(t+\Delta t) \\ c_4(t+\Delta t) \\ \vdots \end{bmatrix} = \begin{bmatrix} c_2(t) \\ c_3(t) \\ c_4(t) \\ \vdots \end{bmatrix}$$

$$C(t+\Delta t) = H^{-1} C(t)$$

(b) Assume that N=100 particles are released at x=5 µm at t=0. Explore the evolution of particle density profile as a function of time using random walk simulations. Compare with analytical results. Explore the density function for N=1000, and N=10000 particles.

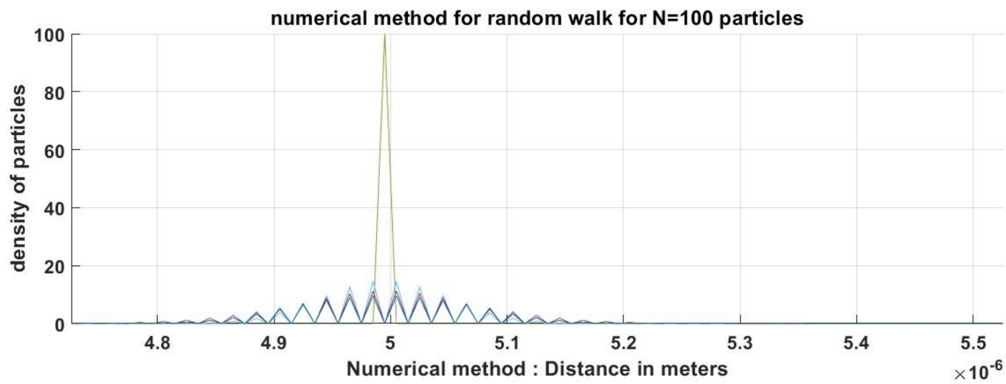
Ans

Code:

For N=100

Numerical:

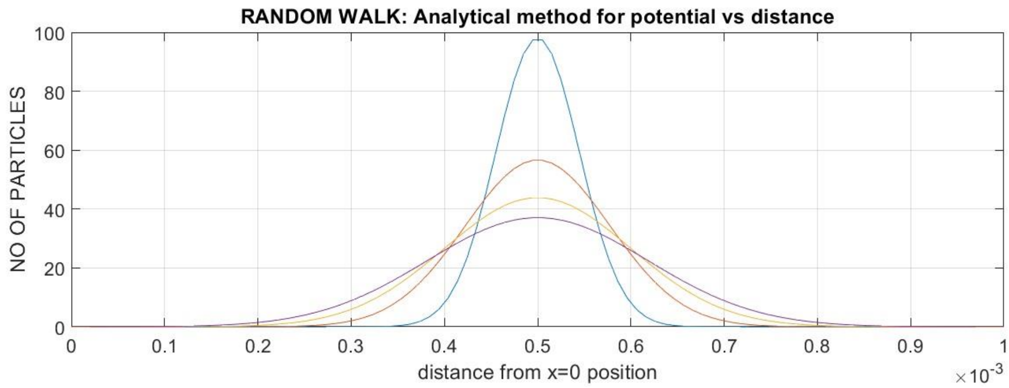
```
clc;
clear all;
len=100*10^-6;
n=linspace(0,10^-5,1000);
a=1;
q=zeros(1000,1);
q(500,1)=100;
e=[];
hyp=eye(1000);
for i=1:100
h=zeros(1000);
    for i=2:999
        h(i,i-1)=0.5;
        h(i,i+1)=0.5;
    end
f=hyp*(h*q);
e=[e,q];
q=f;
end
hold on
plot(n,e(:,1),n,e(:,30),n,e(:,50),n,e(:,70));
grid on
xlabel('Numerical method : Distance in meters')
ylabel('density of particles')
title('numerical method for random walk for N=100 particles')
```



ANALYTICAL:

```
clear all;
clc;
D=10^-4;
l=10^-3;
t1=10*10^-6;
t2=30*10^-6;
t3=50*10^-6;
```

```
t4=70*10^-6;
M=linspace(0,l,100) ;
t=10^-6;
h=10^-5;
Q=0.011;
q=[];
a1=2*((pi*D*t1)^0.5);
a2=2*((pi*D*t2)^0.5);
a3=2*((pi*D*t3)^0.5);
a4=2*((pi*D*t4)^0.5);
C1=((Q/a1)*exp(-((M-(0.5*l)).^2)/(4*D*t1)));
C2=((Q/a2)*exp(-((M-(0.5*l)).^2)/(4*D*t2)));

C3=((Q/a3)*exp(-((M-(0.5*l)).^2)/(4*D*t3)));

C4=((Q/a4)*exp(-((M-(0.5*l)).^2)/(4*D*t4)));

plot(M,C1,M,C2,M,C3,M,C4);
grid on
xlabel('distance from x=0 position');
ylabel('NO OF PARTICLES');
title('RANDOM WALK: Analytical method for potential vs distance');
```

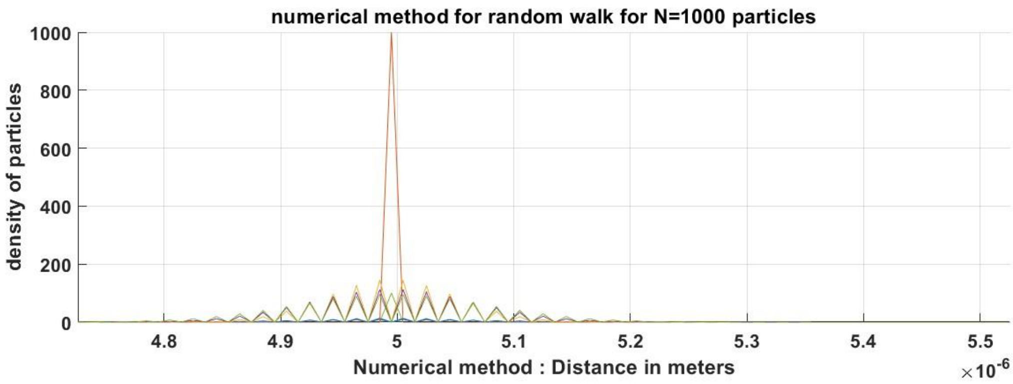


FOR N=1000

NUMERICAL:

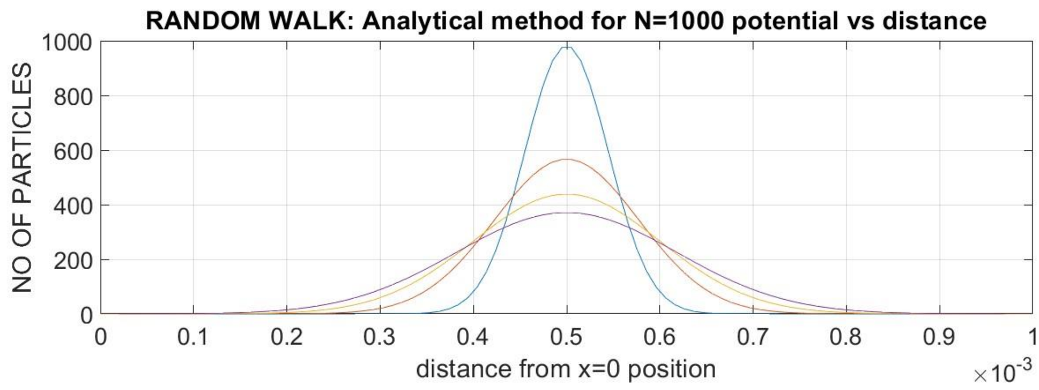
```
clc;
clear all;
len=100*10^-6;
n=linspace(0,10^-5,1000);
a=1;
q=zeros(1000,1);
q(500,1)=1000;
e=[];
hyp=eye(1000);
for i=1:100
h=zeros(1000);
    for i=2:999
        h(i,i-1)=0.5;
        h(i,i+1)=0.5;
    end
```

```
f=hyp*(h*q);
e=[e,q];
q=f;
end
hold on
plot(n,e(:,1),n,e(:,30),n,e(:,50),n,e(:,70));
grid on
xlabel('Numerical method : Distance in meters')
ylabel('density of particles')
title('numerical method for random walk for N=1000 particles')
```



ANALYTICAL:

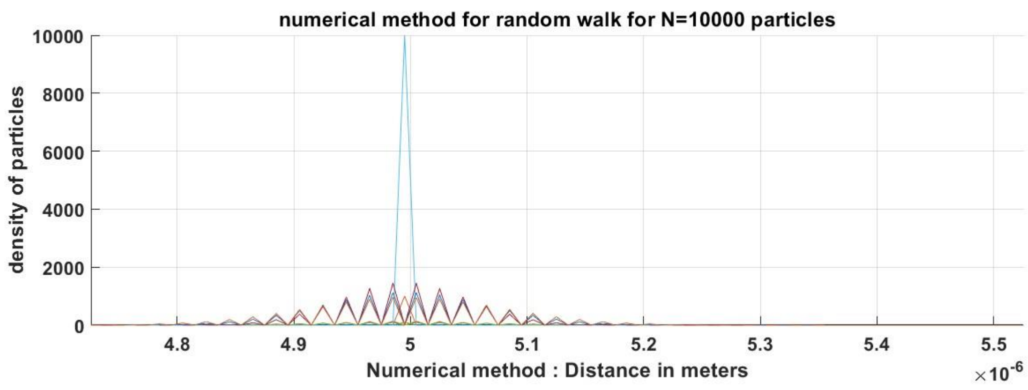
```
clear all;
clc;
D=10^-4;
l=10^-3;
t1=10*10^-6;
t2=30*10^-6;
t3=50*10^-6;
t4=70*10^-6;
M=linspace(0,l,100) ;
t=10^-6;
h=10^-5;
Q=0.11;
q=[];
a1=2*((pi*D*t1)^0.5);
a2=2*((pi*D*t2)^0.5);
a3=2*((pi*D*t3)^0.5);
a4=2*((pi*D*t4)^0.5);
C1=((Q/a1)*exp(-((M-(0.5*l)).^2)/(4*D*t1)));
C2=((Q/a2)*exp(-((M-(0.5*l)).^2)/(4*D*t2)));

C3=((Q/a3)*exp(-((M-(0.5*l)).^2)/(4*D*t3)));

C4=((Q/a4)*exp(-((M-(0.5*l)).^2)/(4*D*t4)));

plot(M,C1,M,C2,M,C3,M,C4);
grid on
xlabel('distance from x=0 position');
ylabel('NO OF PARTICLES');
title('RANDOM WALK: Analytical method for N=1000 potential vs distance');
```



FOR N=10000

NUMERICAL:

```
clc;
clear all;
len=100*10^-6;
n=linspace(0,10^-5,1000);
a=1;
q=zeros(1000,1);
q(500,1)=10000;
e=[];
hyp=eye(1000);
for i=1:100
h=zeros(1000);
    for i=2:999
        h(i,i-1)=0.5;
        h(i,i+1)=0.5;
    end
f=hyp*(h*q);
e=[e,q];
q=f;
end
hold on
plot(n,e(:,1),n,e(:,30),n,e(:,50),n,e(:,70));
grid on
xlabel('Numerical method : Distance in meters')
ylabel('density of particles')
title('numerical method for random walk for N=10000 particles')
```



ANALYTICAL:

```
clear all;
clc;
D=10^-4;
l=10^-3;
t1=10*10^-6;
t2=30*10^-6;
t3=50*10^-6;
t4=70*10^-6;
M=linspace(0,l,100) ;
t=10^-6;
h=10^-5;
Q=1.1;
q=[];
a1=2*((pi*D*t1)^0.5);
a2=2*((pi*D*t2)^0.5);
a3=2*((pi*D*t3)^0.5);
a4=2*((pi*D*t4)^0.5);
C1=((Q/a1)*exp(-((M-(0.5*l)).^2)/(4*D*t1)));
C2=((Q/a2)*exp(-((M-(0.5*l)).^2)/(4*D*t2)));

C3=((Q/a3)*exp(-((M-(0.5*l)).^2)/(4*D*t3)));

C4=((Q/a4)*exp(-((M-(0.5*l)).^2)/(4*D*t4)));

plot(M,C1,M,C2,M,C3,M,C4);
grid on
xlabel('distance from x=0 position');
ylabel('NO OF PARTICLES');
title('RANDOM WALK: Analytical method for N=10000 potential vs distance');
```