Microelectronics Simulation Lab

Some Examples and Report Format

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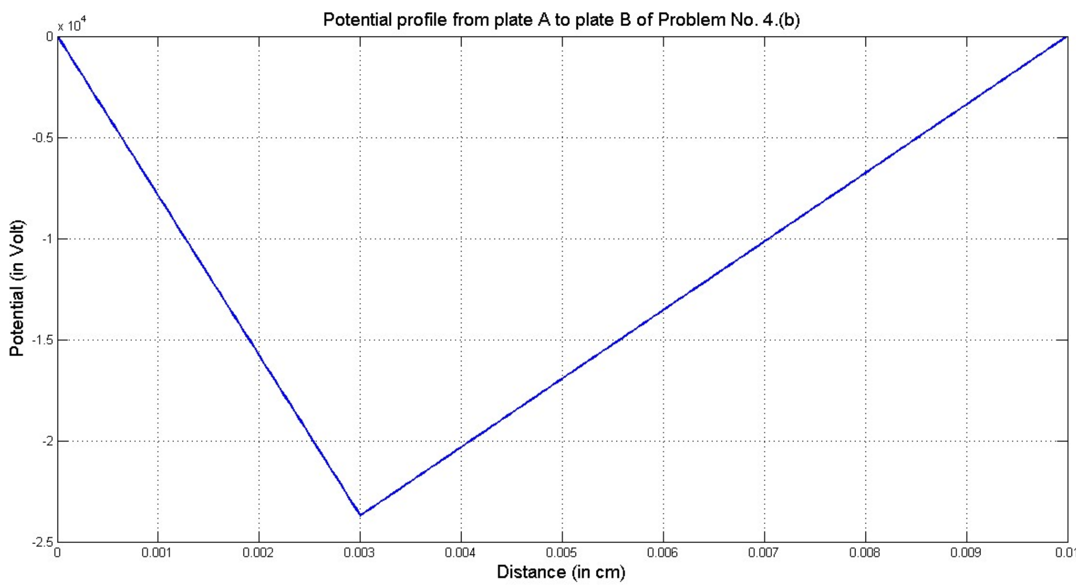
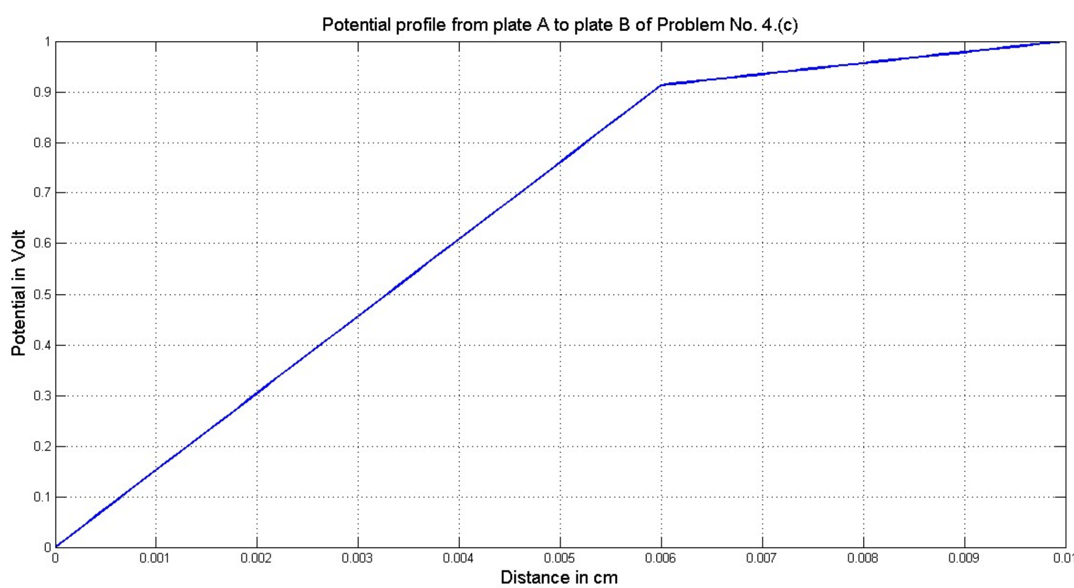
```matlab
% Problem: Assume two metal plates A and B are kept at a separation of
%100um in free space. Both plates are grounded, and a charge sheet of zero
% thickness but with charge of -10^6 C/cm^2 is placed at a distance of 30um
% from plate A towards plate B. Find the potential profile from plate A to
% plate B.

clear;
clc;
nx=201;                 % Number of grid points %
M=sparse(nx,nx);        % Creates nx*nx zero sparse matrix %
d=100e-4;               % Distance between two plates in cm %
nx1=((nx-1)*30e-4/d)+1;
eps_0=8.85418e-14;      % Permitivity of air vacuum or air %
Q=-1e-6;
delx=d/(nx-1);

% Finite difference method to solve 2nd derivative in Poisson's equation %
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-2;
end
M(1,1)=1;               % Setting boundary conditions %
M(nx,nx)=1;
N=zeros(nx,1);          % Setting N matrix of MX=N linear equation %
N(nx1)=-(Q*delx)/eps_0;
X=M\N;                  % Finding solutions %
Nx=linspace(0,d,nx);
plot(Nx,X,'linewidth',2);
grid on;
temp2=['Potential profile from plate A to plate B of Problem No. 4.(b)'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Potential (in Volt)','fontsize',14);
```



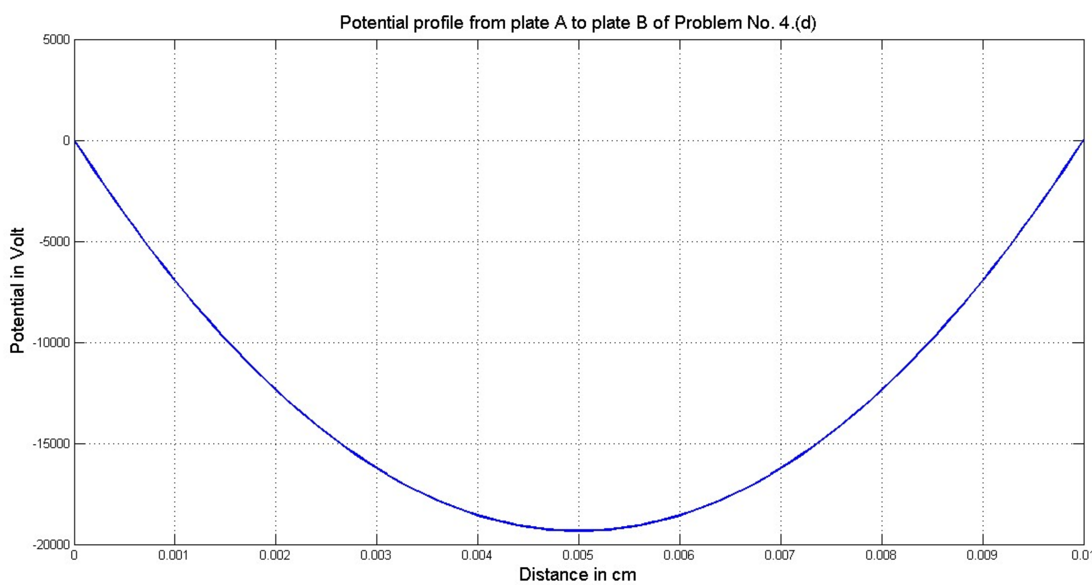
```matlab
% Problem: For the same problem in the previous section, assume that the
%dielectric constant varies as a function of spatial co-ordinate as follows
% er1=1, 0<x<60um
% er2=7, 60um<x<100um
% Find the potential profile from Plate A to Plate B.

clear;
clc;
nx=101;                 % Number of grid points %
M=sparse(nx,nx);        % Creates nx*nx zero sparse matrix %
d=100e-4;               % Distance between two plates in cm %
nx1=((nx-1)*60e-4/d)+1;
eps_0=8.85418e-14;      % Permitivity of air vacuum or air %
eps_r1=1*eps_0;
eps_r2=7*eps_0;

% Finite difference method to solve 2nd derivative in Poisson's equation %
% For eps_r1=1, 0<x<60um
for i=2:nx1-1
M(i,i-1)=eps_r1; M(i,i+1)=eps_r1; M(i,i)=-2*eps_r1;
end
% For eps_r2=7, 60um<x<100um
for i=nx1+1:nx-1
M(i,i-1)=eps_r2; M(i,i+1)=eps_r2; M(i,i)=-2*eps_r2;
end
M(1,1)=1;               % Setting boundary conditions %
M(nx,nx)=1;
M(nx1,nx1-1)=eps_r1;
M(nx1,nx1+1)=eps_r2;
M(nx1,nx1)=-(eps_r1+eps_r2);
```



```
% Problem: Assuming the conditions in the first problem, assume that the
% region between A and B has a charge density of q×10^16 cm-3, where q is
% the electronic charge. Find the potential profile between the plates.
% Here I have assumed that the relative permittivity is 11.68 (Si)
clear;
clc;
nx=101;                    % Number of grid points %
rho=-1.6*10^-19*10^16;     % Charge density %
M=sparse(nx,nx);           % Creates nx*nx zero sparse matrix %
d=100e-4;                  % Distance between two plates in cm %
eps_0=8.85418e-14;         % Permitivity of air vacuum or air %
delx=d/(nx-1);
epsilon=11.68*eps_0;
% Finite difference method to solve 2nd derivative in Poisson's equation %
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-2;
end
M(1,1)=1;                  % Setting boundary conditions %
M(nx,nx)=1;
N=zeros(nx,1);             % Setting N matrix of MX=N linear equation %
N(nx)=1;
for j=2:nx-1
N(j,1)=-(rho*delx^2)/epsilon;
end
X=M\N;                     % Finding solutions %
Nx=linspace(0,d,nx);
plot(Nx,X,'linewidth',2);
grid on;
temp2=['Potential profile from plate A to plate B of Problem No. 4.(d)'];
title(temp2,'fontsize',14);
xlabel('Distance in cm','fontsize',14);
ylabel('Potential in Volt','fontsize',14);
```



Newton's method to solve a system of non-linear equations:

Usually one can find the solution of a system of equation if the number of unknown matches with the number of equations. So the system of "n" variables can be expressed as:

$$\begin{gathered}
f_1(x_1, x_2, x_3, \dots\dots\dots\dots.., x_n) = 0 \\
f_2(x_1, x_2, x_3, \dots\dots\dots\dots.., x_n) = 0 \\
f_3(x_1, x_2, x_3, \dots\dots\dots\dots.., x_n) = 0 \\
\vdots \\
f_n(x_1, x_2, x_3, \dots\dots\dots\dots.., x_n) = 0
\end{gathered}$$

For single valued case the Newton's method can be derived by considering linear approximation of the function "f" at the initial guess x_0. From Calculus, the following is the linear approximation of function "f" at x_0, for vector and vector-valued functions

$$f(x) = f(x_0) + Df(x_0)(x - x_0) + \cdots$$

Here, $Df(x_0)$ is a N*N matrix which is formed by taking partial derivative of components of $f(x_0)$

$$Df(x_0) = \begin{pmatrix}
\frac{\partial f_1}{\partial x_1}(x_0) & \frac{\partial f_1}{\partial x_2}(x_0) & \frac{\partial f_1}{\partial x_3}(x_0) & \dots\dots\dots\dots\dots & \frac{\partial f_1}{\partial x_n}(x_0) \\
\frac{\partial f_2}{\partial x_1}(x_0) & \frac{\partial f_2}{\partial x_2}(x_0) & \frac{\partial f_2}{\partial x_3}(x_0) & \dots\dots\dots\dots\dots & \frac{\partial f_2}{\partial x_n}(x_0) \\
\frac{\partial f_3}{\partial x_1}(x_0) & \frac{\partial f_3}{\partial x_2}(x_0) & \frac{\partial f_3}{\partial x_3}(x_0) & \dots\dots\dots\dots\dots & \frac{\partial f_3}{\partial x_n}(x_0) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{\partial f_n}{\partial x_1}(x_0) & \frac{\partial f_n}{\partial x_2}(x_0) & \frac{\partial f_n}{\partial x_3}(x_0) & \dots\dots\dots\dots\dots & \frac{\partial f_n}{\partial x_n}(x_0)
\end{pmatrix}$$

To find out the value of x which makes the value of f(x) equal to zero vectors. Let choose x_1 so that

$$\begin{gathered}
f(x_0) + Df(x_0)(x_1 - x_0) = 0 \\
x_1 = x_0 - (Df(x_0))^{-1} f(x_0)
\end{gathered}$$

Provided that the inverse matrix does exists. To find out the solution this above method can be run iteratively and at each iteration the value of $f(x_1)$ will be compared to the tolerance error limit.

The Poisson equation for any semiconductors can be written as:

$$\nabla^2\varphi = -\frac{\rho}{\epsilon}$$

Where φ is the potential, ρ is charge density and ϵ is the permittivity of the semiconductor.

For one dimensional case the Poisson equation can be written as:

$$\frac{\partial^2\varphi(x)}{\partial x^2} = -\frac{\rho}{\epsilon}$$

If a semiconductor is doped then the net amount of charge that is present inside the semiconductor is:

$$\rho = q(p - n + N_D - N_A)$$

where p and n denote the hole and electron concentration respectively, whereas, N_D and N_A denote the donor and acceptor concentration. Hence the Poisson equation becomes

$$\frac{\partial^2\varphi(x)}{\partial x^2} = -\frac{q}{\epsilon}(p - n + N_D - N_A)$$

But here in this given problem the semiconductor is intrinsic and we are asked to consider only the electrons as the carriers. So the above equation reduced to a form like:

$$\frac{\partial^2\varphi(x)}{\partial x^2} = \frac{q}{\epsilon}n$$

Here we are also asked to consider Maxwell-Boltzmann distribution for carriers. Hence the carrier concentration will be a function like:

$$n(x) = n_i e^{(E_F - E_i(x))/kT} = n_i e^{q\varphi(x)/kT}$$

where n_i is the intrinsic carrier concentration of silicon at room temperature. So, the expression becomes

$$\frac{\partial^2\varphi(x)}{\partial x^2} = \frac{q}{\epsilon}n_i e^{(E_F - E_i(x))/kT} = \frac{q}{\epsilon}\, n_i e^{q\varphi(x)/kT}$$

But as the semiconductor is not biased, if it is intrinsic (i.e $E_F = E_i$) and it is in thermal equilibrium also (as we have used Maxwell-Boltzmann distribution), so the exact expression for this particular problem becomes:

$$\frac{\partial^2\varphi(x)}{\partial x^2} = \frac{q}{\epsilon}n_i$$

The equation $\frac{\partial^2\varphi(x)}{\partial x^2} = \frac{q}{\epsilon}n_i e^{q\varphi(x)/kT}$ is not a linear one, it is a non-linear transcendental (a transcendental equation is an analytic function that does not satisfy a polynomial equation) equation and cannot be solved directly. Different types of analytical and numerical methods can be used to solve this type of equations. Here we are asked to discretise the equation in such a way so that the ‘Finite Difference Method’ can solve the equation. The method has been employed to solve the equation numerically considering a certain minimum error tolerance. We know how to represent the second derivative using FDM:

$$\frac{\varphi_{i-1} - 2\varphi_i + \varphi_{i+1}}{\Delta x^2} = \frac{q}{\epsilon} n_i e^{q\varphi_i/kT}$$

$$\varphi_{i-1} - 2\varphi_i - \frac{q}{\epsilon} n_i \Delta x^2 e^{\frac{q\varphi_i}{kT}} + \varphi_{i+1} = 0$$

Now if we divide the entire length of the semiconductor in to N points, we will get N number of non-linear equation of potential which will look like the above equation. In Newton's method we can write those equation in a general form like:

$$f_i(\varphi) = f(\varphi_1, \varphi_2, \varphi_3, \varphi_4, \dots \dots \dots, \varphi_N) = 0 \quad where\ i = 1,2,3, \dots \dots \dots, N$$

The above function at i^{th} point only depends upon the potential of $(i\text{-}1)^{th}$, i^{th} and $(i+1)^{th}$ points except for the two boundary (the 1^{st} point and the N^{th} point). So if the boundary potential conditions are provided as A and B respectively then the general form will look like:

$$f_i(\varphi) = f(\varphi_{i-1}, \varphi_i, \varphi_{i+1}) = 0 \quad for\ i = 2,3, \dots \dots \dots, (N-1)$$

$$\varphi_i = A \qquad for\ i = 1$$

$$\varphi_i = B \qquad for\ i = N$$

To solve the non-linear equations we have seen in the previous section we must construct the 1^{st} order Jacobian Matrix. The Jacobian Matrix is ideally an NxN matrix which can be described as:

$$J = \frac{\partial f_i}{\partial x_j} \quad where\ i = 1, 2, \dots \dots \dots, N \ \ and \ \ j = 1, 2, \dots \dots \dots, N$$

For the given case the Jacobian matrix can be written as:

$$J = \frac{\partial f_i}{\partial x_j} \quad where\ i = 2, 3, 4, \dots \dots \dots, (N-1) \ \ and \ \ j = (i-1), i, (i+1)$$

From the equation

$$\varphi_{i-1} - 2\varphi_i - \frac{q}{\epsilon} n_i \Delta x^2 e^{\frac{q\varphi_i}{kT}} + \varphi_{i+1} = 0$$

We can write as:

$$\frac{\partial f_i}{\partial x_{i-1}} = 1, \ \ \frac{\partial f_i}{\partial x_{i+1}} = 1, \ \ \frac{\partial f_i}{\partial x_i} = -2 - \frac{q}{\epsilon} n_i \Delta x^2 \left(\frac{q}{kT}\right) e^{\frac{q\varphi_i}{kT}} \ \ for\ i = 2, 3, 4, \dots \dots, (N-1)$$

$$\frac{\partial f_i}{\partial x_i} = 1 \ \ for\ i = 1\ and\ N$$

Now assume that $\frac{q}{\epsilon} n_i \Delta x^2 \left(\frac{q}{kT}\right) = C$, then the Jacobian matrix will look like:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & \dots\dots\dots & 0 \\ 1 & -2-Ce^{\frac{q\varphi_i}{kT}} & 1 & 0 & 0 & \dots\dots\dots & 0 \\ 0 & 1 & -2-Ce^{\frac{q\varphi_i}{kT}} & 1 & 0 & \dots\dots\dots & 0 \\ 0 & 0 & 1 & -2-Ce^{\frac{q\varphi_i}{kT}} & 1 & \dots\dots\dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots\dots\dots & 1 \end{bmatrix}$$

Report Format

I have provided an example of the report format according to the provided question. For your case you should answer according to the task given to you. You have to make a proper report and also have to submit the code.

Question:

Numerical solution of steady state continuity equation: For each of the cases listed below, provide analytical solutions and compare with numerical results. Assume D=30 cm^2/s, unless otherwise stated ($Equation$: $D\nabla^2 n = n/\tau$):

a. Consider diffusive transport of particles from point A to point B and the separation between these points being 100um. The concentration of particles at A is n=10^12 cm^-3, and at B is n=0 cm^-3. Assume $\tau = \infty$. Find the particle profile from A to B. What is the particle flux from A to B?

b. Solve (a) with τ = 10^$-7s$ and other conditions remaining the same. Compare with the solution obtained in part (a).

c. For the configuration in part (a), assume that the boundary condition at B is such that $J = kn$, where J is the particle flux (outgoing), k = 10^3 cm/s, and n is the particle density. Assume $\tau = \infty$. Find the particle profile from A to B and the particle flux at B. Explore the implications of the change in boundary conditions at B.

d. Solve (c) with τ = 10^$-7s$ and other conditions remaining the same. Can you comment on the conservation of particles for the whole system?

e. For the configuration in part (b), assume that a particle flux is introduced at x=30um at the rate of 10^12 cm^-2/s. Assume that the particle density at A and B are held constant at n=0 and τ = 10^$-7\ s$. Find the particle profile from A to B, and the flux at A and B.

f. Solve (e) with the boundary condition at A and B being $J = kn$, where J is the particle flux (outgoing), k = 10^3 cm/s, and n is the particle density.

Solution:

a)

Analytical Solution:

Given $D = 30\ cm^2/s$,

$\tau = \infty$,

Hence,

$$D\frac{d^2n(x)}{dx^2} = 0$$
$$\frac{d^2n(x)}{dx^2} = 0$$
$$\frac{dn(x)}{dx} = C_1$$
$$n(x) = C_1x + C_2$$

Apply boundary conditions:

$$at\ x = 0,\ \ n(x) = 10^{12}\ cm^{-3}\ and\ at\ x = 100 \times 10^{-4}\ cm,\ \ n(x) = 0$$

Applying these boundary conditions we can find out the constants

$$C_2 = 10^{12}\ \ and\ \ C_1 = -10^{14}$$

So the solution is:

$$n(x) = -10^{14}x + 10^{12}$$

For numerical solution:

$$\frac{d^2n(x)}{dx^2} = 0 \qquad as\ \tau = \infty$$
$$n_{i-1} - 2n_i + n_{i+1} = 0$$

$$MX = N, \qquad where\ \ M\ matrix\ is\ related\ to\ n_i$$

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$N = \begin{bmatrix} 10^{12} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
$$X = (M^{-1}) * N$$

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% Problem No. 2_a) Consider diffusive transport of particles from point A
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% to point B and the separation between these points being 100?m. The
% concentration of particles at A is n=10^12 cm^-3, and at B is n=0 cm^-3.
% Assume T = infinite. Find the particle profile from A to B.
% What is the particle flux from A to B?

clear;
clc;
nx=201;              % Number of grid points %
M=zeros(nx);         % Creates nx*nx zero sparse matrix %
d=100e-4;            % Distance between A and B point %
deltax=d/(nx-1)
D=30;                % in cm^2/s
flux=zeros(nx,1);

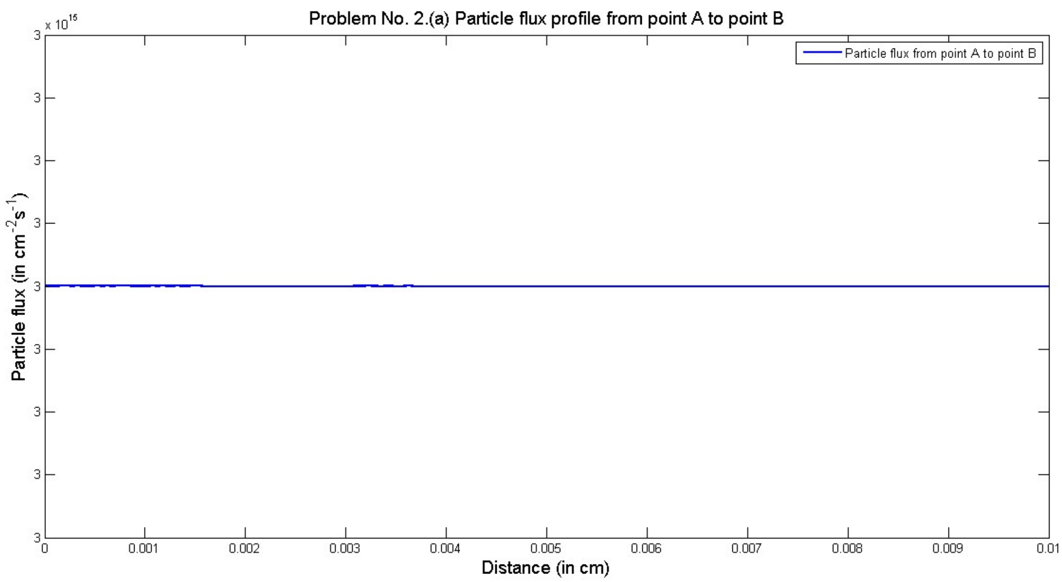
% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-2;
end
M(1,1) = 1;          % Setting boundary conditions for M matrix %
M(nx,nx) = 1;        % Setting boundary conditions for M matrix %
N=zeros(nx,1);       % Initialize N matrix of MX=N linear equation %
N(1)=1e12;           % Setting N matrix value for point A %
X=M\N;               % Finding numerical solutions %
NX=linspace(0,d,nx);
flux(1,1)=D*((X(1)-X(2))/deltax);
for i=2:nx
    flux(i)=-D*((X(i)-X(i-1))/deltax);
end

% Analytical Solution %
X1=-(1e14.*NX)+1e12 ;

figure(1)
plot(NX,X,'b',NX,X1,'g','linewidth',2);
grid on;
temp2=['Problem No. 2.(a) Particle profile from point A to point B,    Flux
= ',num2str(flux(nx)*1e-15),'x10^1^5 cm ^-^2s^-^1'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');

figure(2)
plot(NX,flux,'linewidth',2)
temp2=['Problem No. 2.(a) Particle flux profile from point A to point B'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle flux (in cm ^-^2s^-^1)','fontsize',14);
legend('Particle flux from point A to point B');
```

Here I have plotted both the solutions (Numerical and Analytical) and they are perfectly matched with each other. The flux profile from A to B is plotted bellow:



b)

Analytical Solution:

Given $D = 30\ cm^2/s,$
$\tau = 10^{-7} sec,$
$\sqrt{D\tau} = 1.732 \times 10^{-3}\ cm,$

Hence,

$$D\frac{d^2n(x)}{dx^2} = \frac{n(x)}{\tau}$$
$$\frac{d^2n(x)}{dx^2} - \frac{n(x)}{D\tau} = 0$$

The general solution of the above equation is:

$$n(x) = Ae^{\frac{-x}{\sqrt{D\tau}}} + Be^{\frac{x}{\sqrt{D\tau}}}$$

Apply boundary conditions:

$$at\ x = 0,\ \ n(x) = 10^{12}\ cm^{-3}\ and\ at\ x = 100 \times 10^{-4}\ cm,\ \ n(x) = 0$$

Applying these boundary conditions we can find out the constants A and B

$$A = 9.99985 \times 10^{11}\ \ and\ \ B = 9.660573 \times 10^{6}$$

So the solution is:

$$n(x) = 9.99985 \times 10^{11} \times e^{\frac{-x}{\sqrt{D\tau}}} + 9.660573 \times 10^{6} \times e^{\frac{x}{\sqrt{D\tau}}}$$

For numerical solution:

$$\frac{n_{i-1} - 2n_i + n_{i+1}}{\Delta x^2} = \frac{n_i}{D\tau}$$
$$n_{i-1} - \left(2 + \frac{\Delta x^2}{D\tau}\right)n_i + n_{i+1} = 0$$

$$MX = N, \qquad where\ \ M\ matrix\ is\ related\ to\ n_i$$

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$N = \begin{bmatrix} 10^{12} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$X = (M^{-1}) * N$$

For flux calculation:

$$J = -D \frac{n_{i+1} - n_i}{\Delta x}$$

```
% Problem No. 2_b) Solve (a) with T = 10^-7 sec and other conditions
% remaining the same. Compare with the solution obtained in part (a).

clear;
clc;
nx=201;                 % Number of grid points %
MM=zeros(nx);           % Creates nx*nx zero sparse matrix %
d=100e-4;               % Distance between A and B point %
D=30;                   % in cm^2/s
T=1e-7;                 % Lifetime %
deltax=d/(nx-1);
L=sqrt(D*T);            % Diffusion length %

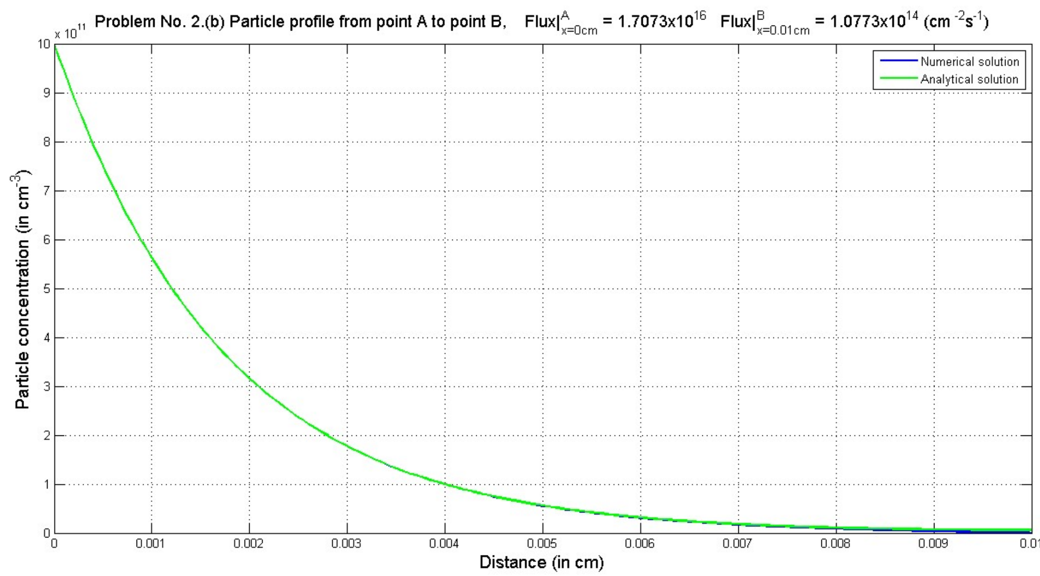
% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
MM(i,i-1)=1; MM(i,i+1)=1; MM(i,i)=-(2+(deltax/L)^2);
end
MM(1,1) = 1;             % Initialize M matrix %
MM(nx,nx) = 1;           % Setting boundary conditions for M matrix %
NN=zeros(nx,1);          % Initialize N matrix of MX=N linear equation %
NN(1)=1e12;              % Setting N matrix value for point A %
XX=MM\NN;                % Finding numerical solutions %
NX=linspace(0,d,nx);
fluxA=-D*((XX(2)-XX(1))/deltax);       %Flux at point A %
fluxB=-D*((XX(nx)-XX(nx-1))/deltax);   %Flux at point B %

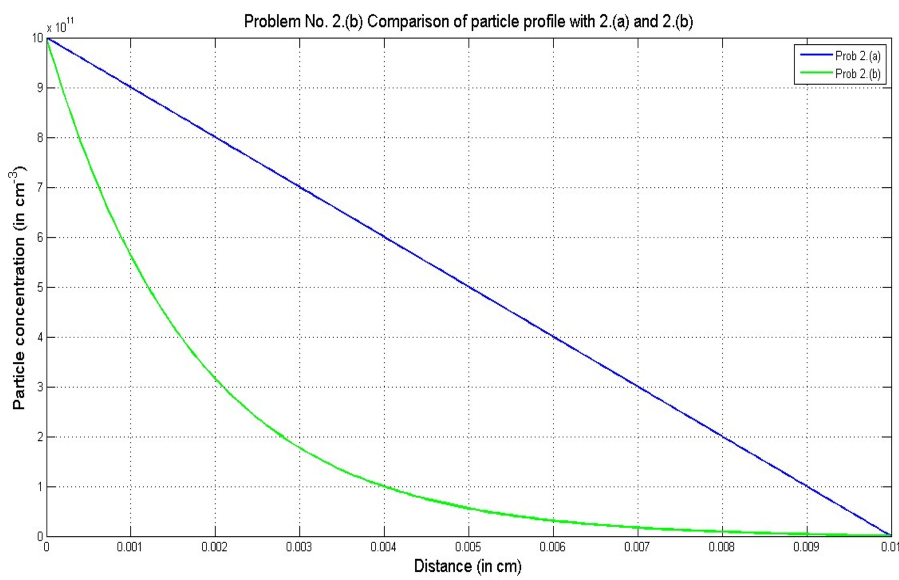
% Analytical Solution %
A=9.99985e11;
B=9.660573e6;
X1=A*exp(-NX./L)+B*exp(NX./L);

figure(1)
plot(NX,XX,'b',NX,X1,'g','linewidth',2);
grid on;
temp2=['Problem No. 2.(b) Particle profile from point A to point B,
Flux|^A_x_=_0_c_m = ',num2str(fluxA*1e-16),'x10^1^6', '
Flux|^B_x_=_0_._0_1_c_m = ',num2str(fluxB*1e-14),'x10^1^4 (cm ^-^2s^-^1)'];
title(temp2,'fontsize',13);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');

% Comparison with part (a) %
M=zeros(nx);            % Creates nx*nx zero sparse matrix %
% Finite difference method to solve 2nd derivative in Diffusion  equation %
```

```
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-2;
end
M(1,1) = 1;          % Initialize M matrix %
M(nx,nx) = 1;        % Setting boundary conditions for M matrix %
N=zeros(nx,1);       % Initialize N matrix of MX=N linear equation %
N(1)=1e12;           % Setting N matrix value for point A %
X=M\N;               % Finding numerical solutions %
figure(2)
plot(NX,X,'b',NX,XX,'g','linewidth',2);
grid on;
temp2=['Problem No. 2.(b) Comparison of particle profile with 2.(a) and 
2.(b)'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Prob 2.(a)','Prob 2.(b)');
```





c)

Analytical Solution:

Given $D = 30\ cm^2/s,$

$\tau = \infty\ sec,\ \ k = 10^3\ cm/s$

$at\ x = 0.01\ cm,\ J = kn(x),$

$$J = -D\frac{dn(x)}{dx}$$
$$-\frac{J}{D} = \frac{dn(x)}{dx}$$
$$n(x) = -\frac{J}{D}x + C$$

Apply boundary condition

$$at\ x = 0,\ \ n(x) = 10^{12}\ cm^{-3}$$
$$hence\ the\ constant\ C = 10^{12}$$
$$this\ gives\ us\quad n(x) = -\frac{J}{D}x + 10^{12}$$

Now use the condition (<u>implications of the change in boundary conditions at B</u>)

$$at\ x = 0.01\ cm,\qquad J = kn(x)$$
$$n(x) = \frac{J}{k}$$

Hence,

$$\frac{J}{k} = -\frac{J}{D}0.01 + 10^{12}$$
$$J = \frac{10^{12}}{\left(\frac{1}{k} + \frac{0.01}{D}\right)} = \frac{10^{12}}{\left(\frac{1}{10^3} + \frac{0.01}{30}\right)} = 7.5 \times 10^{14}\ \ cm^{-2}s^{-1}$$

So the solution is:

$$n(x) = -2.5 \times 10^{13}x + 10^{12}$$

Numerical Solution:

The M matrix will look like as the case of part (a) except at the last row where the boundary condition ($at\ x = 0.01\ cm,\ J = kn(x)$) will be applied:

Hence,

$$-D\frac{dn(x)}{dx} = kn(x)$$

This can be written as:

$$-D\frac{n_i - n_{i-1}}{\Delta x} = kn_i$$
$$\left(1 + \frac{\Delta x k}{D}\right)n_i - n_{i-1} = 0$$

Hence the M matrix will look like:

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & \left(1+\frac{\Delta x k}{D}\right) \end{bmatrix}$$

N matrix will be the same as it is written earlier.

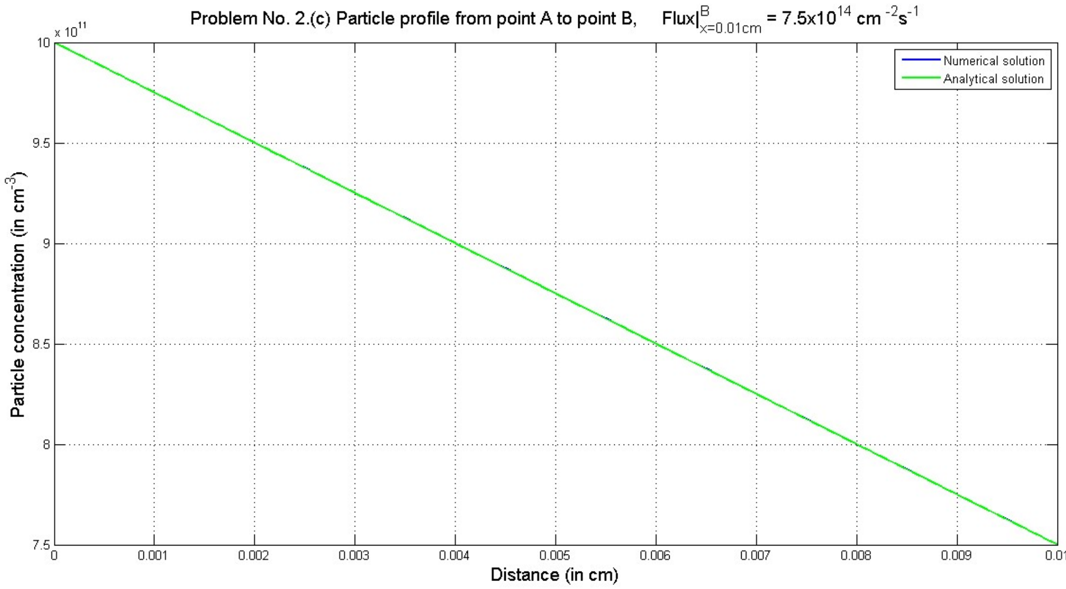
```
% Problem No. 2_c) For the configuration in part (a), assume that the
% boundary condition at B is such that J = kn, where J is the particle
% flux (outgoing), k = 10^3 cm/s, and n is the particle density. Assume
% T = ?. Find the particle profile from A to B and the particle flux at B.
% Explore the implications of the change in boundary conditions at B.

clear;
clc;
nx=201;                % Number of grid points %
M=zeros(nx);           % Creates nx*nx zero sparse matrix %
d=100e-4;              % Distance between A and B point %
D=30;                  % in cm^2/s
k=1e3;                 % in cm/s
deltax=d/(nx-1);


% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-2;
end
M(1,1) = 1;                    % Setting boundary conditions for M matrix %
M(nx,nx) = (1+k*deltax/D);     % Setting boundary conditions for M matrix %
M(nx,nx-1)=-1;         % Setting boundary conditions for M matrix %
N=zeros(nx,1);         % Initialize N matrix of MX=N linear equation %
N(1)=1e12;             % Setting N matrix value for point A %
X=M\N;                 % Finding numerical solutions %
NX=linspace(0,d,nx);
flux=-D*((X(nx)-X(nx-1))/deltax); % From Fick's first law %


% % Analytical Solution %
X1=-(2.5e13.*NX)+1e12;

figure(1)
plot(NX,X,'b',NX,X1,'g','linewidth',2);
grid on;
temp2=['Problem No. 2.(c) Particle profile from point A to point B,
Flux|^B_x_=_0_._0_1_c_m = ',num2str(flux*1e-14),'x10^1^4 cm ^-^2s^-^1'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');
```



Here I have plotted both the solutions (Numerical and Analytical) and they are perfectly matched with each other.

d)

Analytical Solution:

Given $D = 30\ cm^2/s,$
$\tau = 10^{-7} sec,$
$\sqrt{D\tau} = 1.732 \times 10^{-3}\ cm,$

Hence,

$$D\frac{d^2n(x)}{dx^2} = \frac{n(x)}{\tau}$$
$$\frac{d^2n(x)}{dx^2} - \frac{n(x)}{D\tau} = 0$$

The general solution of the above equation is:

$$n(x) = Ae^{\frac{-x}{\sqrt{D\tau}}} + Be^{\frac{x}{\sqrt{D\tau}}}$$

Apply boundary condition $at\ x = 0,\ \ n(x) = 10^{12}\ cm^{-3}$ we can get

$$10^{12} = A + B \text{..(1)}$$

Another boundary condition is $at\ x = 0.01\ cm,\ J = kn(x)$

$$J = -D\frac{dn(x)}{dx} = -D\frac{d}{dx}\left\{Ae^{\frac{-x}{\sqrt{D\tau}}} + Be^{\frac{x}{\sqrt{D\tau}}}\right\}$$
$$k\left\{Ae^{\frac{-0.01}{1.732\times10^{-3}}} + Be^{\frac{0.01}{1.732\times10^{-3}}}\right\} = \frac{-3}{1.732\times10^{-3}}\left\{-Ae^{\frac{-0.01}{1.732\times10^{-3}}} + Be^{\frac{0.01}{1.732\times10^{-3}}}\right\}\text{...(2)}$$

From the equation (1) and (2) we can solve for constants A and B.

$$A = 1.000107 \times 10^{12}\ \ and\ \ B = 8.54 \times 10^{6}$$

So the equation is:

$$n(x) = 1.000107 \times 10^{12} \times e^{\frac{-x}{\sqrt{D\tau}}} - 1.07 \times 10^{8} \times e^{\frac{x}{\sqrt{D\tau}}}$$

For numerical solution:

$$\frac{n_{i-1} - 2n_i + n_{i+1}}{\Delta x^2} = \frac{n_i}{D\tau}$$
$$n_{i-1} - \left(2 + \frac{\Delta x^2}{D\tau}\right)n_i + n_{i+1} = 0$$

$$MX = N, \qquad where\ \ M\ matrix\ is\ related\ to\ n_i$$

And $at\ x = 0.01\ cm,\ J = kn(x)$ so we can write

$$-D\frac{n_i - n_{i-1}}{\Delta x} = kn_i$$
$$\left(1 + \frac{\Delta xk}{D}\right)n_i - n_{i-1} = 0$$

So the M matrix will look like:

$$
M = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 \\
0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 \\
0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 \\
0 & 0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 \\
0 & 0 & 0 & 0 & -1 & \left(1+\frac{\Delta x k}{D}\right)
\end{bmatrix}
$$

N matrix will be the same as it is written earlier.

```
% Problem No. 2_d) Solve (c) with T = 10^-7 s and other conditions
% remaining the same. Can you comment on the conservation of
% particles for the whole system ?

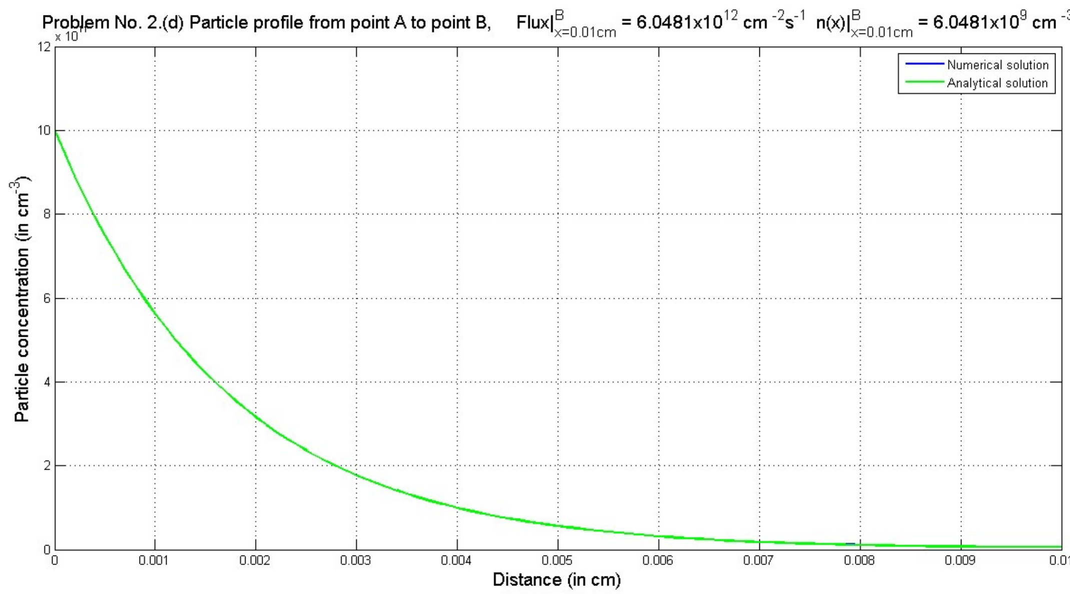
clear;
clc;
nx=201;                 % Number of grid points %
M=zeros(nx);            % Creates nx*nx zero sparse matrix %
d=100e-4;               % Distance between A and B point %
D=30;                   % in cm^2/s
T=1e-7;                 % Lifetime %
k=1e3;                  % in cm/s
L=sqrt(D*T);            % Diffusion length %
deltax=d/(nx-1);


% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
M(i,i-1)=1; M(i,i+1)=1; M(i,i)=-(2+(deltax/L)^2);
end
M(1,1) = 1;                 % Setting boundary conditions for M matrix %
M(nx,nx) = (1+k*deltax/D);  % Setting boundary conditions for M matrix %
M(nx,nx-1)=-1;          % Setting boundary conditions for M matrix %
N=zeros(nx,1);          % Initialize N matrix of MX=N linear equation %
N(1)=1e12;              % Setting N matrix value for point A %
X=M\N;                  % Finding numerical solutions %
NX=linspace(0,d,nx);
flux=-D*((X(nx)-X(nx-1))/deltax); % From Fick's first law %


% % Analytical Solution %
A=1.000107e12;
B=8.54e6;
X1=A*exp(-NX./L)+B*exp(NX./L);

figure(1)
plot(NX,X,'b',NX,X1,'g','linewidth',2);
grid on;
```

```
temp2=['Problem No. 2.(d) Particle profile from point A to point B,
Flux|^B_x_=_0_._0_1_c_m = ',num2str(flux*1e-12),'x10^1^2 cm ^-^2s^-^1'];
title(temp2,'fontsize',14);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');
```



Conservation of particle:

The particle concentration build-up at any point must satisfy the continuity equation

$$\frac{\partial n(x)}{\partial t} = \lim_{\Delta x \to 0} \frac{J(x) - J(x+\Delta x)}{\Delta x} - \frac{n(x)}{\tau}$$

At steady state:

$$0 = \lim_{\Delta x \to 0} \frac{J(x) - J(x+\Delta x)}{\Delta x} - \frac{n(x)}{\tau}$$

$$\lim_{\Delta x \to 0} \frac{J(x) - J(x+\Delta x)}{\Delta x} = \frac{n(x)}{\tau}$$

$$J(x = 0.01) = \frac{n(x = 0.01)\Delta x}{\tau}$$

Now we have the particle concentration at x=0.01 cm n(x)=6.0481x10^9 cm^{-3}

$$\Delta x = 10^{-4} \;\; and \;\; \tau = 10^{-7}$$

Hence

$$J(x = 0.01) = \frac{6.0481 \times 10^9 \times 10^{-4}}{10^{-7}} = 6.0481 \times 10^{12}$$

Which matches with the calculated flux value at B point. Similarly for every point it is valid.

e)

Analytical Solution:

Given $D = 30\ cm^2/s,$
$\tau = 10^{-7} sec,$
$\sqrt{D\tau} = 1.732 \times 10^{-3}\ cm,$

$$at\ x = 0.003\ cm,\ \ J = 10^{12}\ cm^{-2}s^{-1}$$

Hence,

$$D\frac{d^2n(x)}{dx^2} = \frac{n(x)}{\tau}$$

$$\frac{d^2n(x)}{dx^2} - \frac{n(x)}{D\tau} = 0$$

The general solution of the above equation is:

$$n(x) = Ae^{\frac{-x}{\sqrt{D\tau}}} + Be^{\frac{x}{\sqrt{D\tau}}}$$

Apply boundary condition $at\ x = 0,\ \ n(x) = 0$, we can get

$$A + B = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

$$for\quad 0 < x < 0.003\quad cm$$

$$\left[-D\frac{dn(x)}{dx}\right]_{x=0.003} = -10^{12}$$

$$\frac{D}{\sqrt{D\tau}}\left[Ae^{\frac{-0.003}{\sqrt{D\tau}}} - Be^{\frac{0.003}{\sqrt{D\tau}}}\right] = -10^{12}$$

$$\frac{30}{1.732\times10^{-3}}\left[Ae^{\frac{-0.003}{1.732\times10^{-3}}} - Be^{\frac{0.003}{1.732\times10^{-3}}}\right] = -10^{12} \ldots\ldots\ldots (2)$$

From equation (1) and (2) we can solve for constants A and B

$$A = -9.904527861 \times 10^6$$

$$B = 9.904527861 \times 10^6$$

Apply boundary condition $at\ x = 0.01\ cm,\ \ n(x) = 0$, we can get

$$Ae^{\frac{-0.01}{1.732\times10^{-3}}} + Be^{\frac{0.01}{1.732\times10^{-3}}} = 0 \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

$$for\quad 0.003 > x > 0.01\ \ cm$$

$$\left[-D\frac{dn(x)}{dx}\right]_{x=0.003} = 10^{12}$$

$$\frac{D}{\sqrt{D\tau}}\left[Ae^{\frac{-0.003}{\sqrt{D\tau}}} - Be^{\frac{0.003}{\sqrt{D\tau}}}\right] = 10^{12}$$

$$\frac{30}{1.732\times10^{-3}}\left[Ae^{\frac{-0.003}{1.732\times10^{-3}}} - Be^{\frac{0.003}{1.732\times10^{-3}}}\right] = 10^{12} \ldots\ldots\ldots\ldots (4)$$

From equation (3) and (4) we can solve for constants A and B

$$A = 3.262311319 \times 10^8$$

$$B = -3.153005 \times 10^3$$

So the analytical solution is:

$$for\ 0 < x < 0.003 \quad cm$$

$$n(x) = -9.904527861 \times 10^6 \times e^{\frac{-x}{\sqrt{D\tau}}} + 9.904527861 \times 10^6 \times e^{\frac{x}{\sqrt{D\tau}}}$$

And $for \quad 0.003 > x > 0.01 \ \ cm$

$$n(x) = 3.262311319 \times 10^8 \times e^{\frac{-x}{\sqrt{D\tau}}} - 3.153005 \times 10^3 \times e^{\frac{x}{\sqrt{D\tau}}}$$

For numerical solution:

$$for\ 0 < x < 0.003\ cm \ \ and \ \ 0.003 > x > 0.01\ cm$$

$$\frac{n_{i-1} - 2n_i + n_{i+1}}{\Delta x^2} = \frac{n_i}{D\tau}$$

$$n_{i-1} - \left(2 + \frac{\Delta x^2}{D\tau}\right) n_i + n_{i+1} = 0$$

$$for\ x = 0.003$$

$$-D\frac{dn(x)}{dx} = 10^{12}$$

$$\frac{dn(x)}{dx} = -\frac{10^{12}}{D}$$

$$\frac{[n(x+\Delta x) - n(x)] - [n(x) - n(x-\Delta x)]}{2\Delta x} = -\frac{10^{12}}{D}$$

$$\frac{[n(x+\Delta x) - 2n(x) - n(x-\Delta x)]}{2\Delta x} = -\frac{10^{12}}{D}$$

$$n_{i-1} - 2n_i + n_{i+1} = -\frac{2 \times 10^{12} \times \Delta x}{D}$$

Hence the M matrix will look like:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -\left(2+\frac{\Delta x^2}{D\tau}\right) & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

And N matrix will look like

$$N = \begin{bmatrix} 0 \\ 0 \\ -\frac{2 \times 10^{12} \times \Delta x}{D} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

```
% Problem No. 2_e) For the configuration in part (b), assume that a
% particle flux is introduced at x=30um at the rate of 10^12cm^-2/s. Assume
% that the particle density at A and B are held constant at n=0 and
% T=10^-7s. Find the particle profile from A to B, and the flux at A and B.

clear;
clc;
nx=101;              % Number of grid points %
MM=zeros(nx);        % Creates nx*nx zero sparse matrix %
d=100e-4;            % Distance between A and B point %
d1=30e-4;            % Flux at x=30um %
Flux=1e12;           % Flux value %
D=30;                % in cm^2/s
T=1e-7;              % Lifetime %
L=sqrt(D*T);         % Diffusion length %
deltax=d/(nx-1);

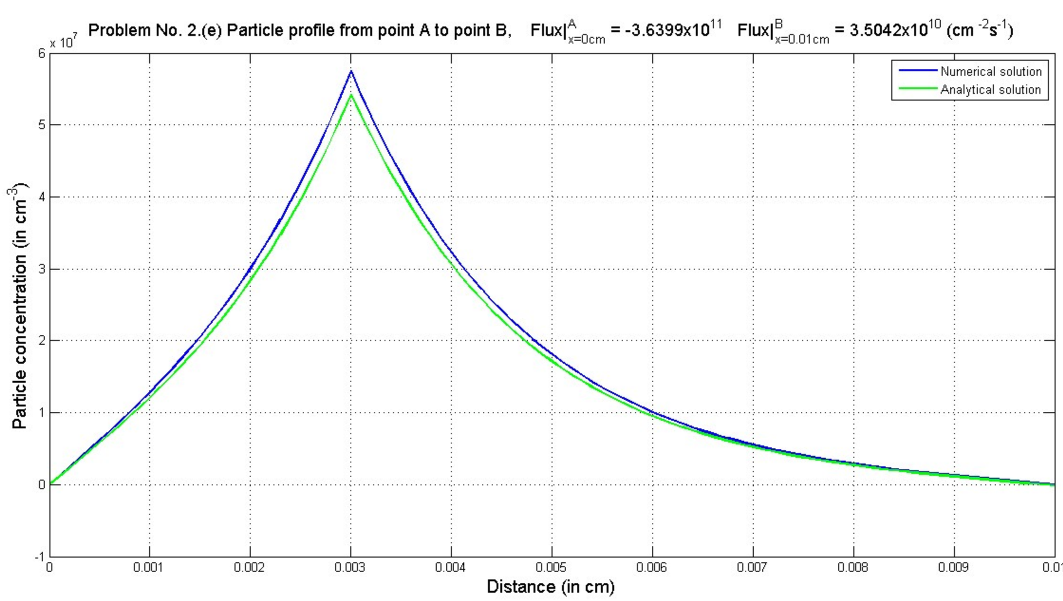
% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
    if i==(d1/deltax)+1
        MM(i,i-1)=1; MM(i,i+1)=1; MM(i,i)=-2;
    else
        MM(i,i-1)=1; MM(i,i+1)=1; MM(i,i)=-(2+(deltax/L)^2);
    end
end
```

```
MM(1,1) = 1;          % Initialize M matrix %
MM(nx,nx) = 1;        % Setting boundary conditions for M matrix %
NN=zeros(nx,1);       % Initialize N matrix of MX=N linear equation %
NN((d1/deltax)+1)=-2*1e12*deltax/D; % Setting N matrix value for point
x=30um %
XX=MM\NN;             % Finding numerical solutions %
NX=linspace(0,d,nx);
fluxA=-D*((XX(2)-XX(1))/deltax);       %Flux at point A %
fluxB=-D*((XX(nx)-XX(nx-1))/deltax);   %Flux at point B %

% Analytical Solution %
X1=zeros(1,nx);

for i=1:nx;
    if i<=(d1/deltax)+1
        A=-9.904527861e6;
        B=9.904527861e6;
        X1(i)=A*exp(-(i-1)*deltax/L)+B*exp((i-1)*deltax/L);
    else
        A=3.262311319e8;
        B=-3.153005e3;
        X1(i)=A*exp(-i*deltax/L)+B*exp(i*deltax/L);
    end
end

figure(1)
%plot(NX,X1,'b','linewidth',2);
plot(NX,XX,'b',NX,X1,'g','linewidth',2);
grid on;
temp2=['Problem No. 2.(e) Particle profile from point A to point B,
Flux|^A_x_=_0_c_m = ',num2str(fluxA*1e-11),'x10^1^1', '
Flux|^B_x_=_0_._0_1_c_m = ',num2str(fluxB*1e-10),'x10^1^0 (cm ^-^2s^-^1)'];
title(temp2,'fontsize',13);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');
```



f)

Analytical Solution:

Given $D = 30\ cm^2/s$,

$\tau = 10^{-7}$ sec, $k = 10^3\ cm/s$

$\sqrt{D\tau} = 1.732 \times 10^{-3}\ cm$,

$$at\ x = 0.003\ cm,\ \ J = 10^{12}\ cm^{-2}s^{-1}$$

Hence,

$$D\frac{d^2n(x)}{dx^2} = \frac{n(x)}{\tau}$$

$$\frac{d^2n(x)}{dx^2} - \frac{n(x)}{D\tau} = 0$$

The general solution of the above equation is:

$$n(x) = Ae^{\frac{-x}{\sqrt{D\tau}}} + Be^{\frac{x}{\sqrt{D\tau}}}$$

$$at\ x = 0,\ \ J = kn(x)$$

Hence,

$$-D\frac{dn(x)}{dx} = kn(x)$$

$$n(x) = e^{\frac{-kx}{D}}$$

$$n(x = 0) = 1$$

And

$$-D\frac{dn(x=0)}{dx} = \frac{D}{\sqrt{D\tau}}(Ae^0 - Be^0)$$

$$kn(x = 0) = \frac{D}{\sqrt{D\tau}}(Ae^0 - Be^0)$$

$$A - B = \frac{\sqrt{D\tau}}{D}k \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$at\ x = 0.003_+,\ \ J = 10^{12}\ \ \ and\ \ \ at\ x = 0.003_-,\ \ J = -10^{12}$$

$$\frac{D}{\sqrt{D\tau}}\left[Ae^{\frac{-0.003}{\sqrt{D\tau}}} - Be^{\frac{0.003}{\sqrt{D\tau}}}\right] = 10^{12} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

And

$$\frac{D}{\sqrt{D\tau}}\left[Ae^{\frac{-0.003}{\sqrt{D\tau}}} - Be^{\frac{0.003}{\sqrt{D\tau}}}\right] = -10^{12} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

$at\ x = 0.01\ cm,\ \ J = kn(x)$,

$$-D\frac{dn(x)}{dx} = kn(x)$$

$$n(x) = e^{\frac{-kx}{D}}$$
$$n(x = 0.01) = e^{\frac{-k\times 0.01}{D}}$$

And

$$-D\frac{dn(x = 0.01)}{dx} = \frac{D}{\sqrt{D\tau}}\left(Ae^{\frac{-0.01}{\sqrt{D\tau}}} - Be^{\frac{0.01}{\sqrt{D\tau}}}\right)$$
$$kn(x = 00.01) = \frac{D}{\sqrt{D\tau}}\left(Ae^{\frac{-0.01}{\sqrt{D\tau}}} - Be^{\frac{0.01}{\sqrt{D\tau}}}\right)$$
$$\frac{D}{\sqrt{D\tau}}\left(Ae^{-\frac{0.01}{\sqrt{D\tau}}} - Be^{\frac{0.01}{\sqrt{D\tau}}}\right) = ke^{\frac{-k\times 0.01}{D}} \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

$for\ 0 < x < 0.003\ cm$,
From equation (1) and (3) we can get the value of constants (for 0<x<0.003):

$$A = 1.0544608658 \times 10^7 \ \ and\ \ B = 1.05446085 \times 10^7$$
$$n(x) = 1.0544608658 \times 10^7 \times e^{\frac{-x}{\sqrt{D\tau}}} + 1.05446085 \times 10^7 \times e^{\frac{x}{\sqrt{D\tau}}}$$

$for\ 0.003 < x < 0.01\ cm$,
From equation (2) and (4) we can get the value of constants (for 0.003<x<0.01):

$$A = 3.264477661 \times 10^8 \ \ and\ \ B = 3.62788 \times 10^3$$
$$n(x) = 3.264477661 \times 10^8 \times e^{\frac{-x}{\sqrt{D\tau}}} + 3.62788 \times 10^3 \times e^{\frac{x}{\sqrt{D\tau}}}$$

For numerical solution:

$$for\ 0 < x < 0.003\ cm\ \ and\ \ 0.003 > x > 0.01\ cm$$

$$\frac{n_{i-1} - 2n_i + n_{i+1}}{\Delta x^2} = \frac{n_i}{D\tau}$$
$$n_{i-1} - \left(2 + \frac{\Delta x^2}{D\tau}\right)n_i + n_{i+1} = 0$$

$$for\ \ x = 0.003$$
$$-D\frac{dn(x)}{dx} = 10^{12}$$
$$\frac{dn(x)}{dx} = -\frac{10^{12}}{D}$$
$$\frac{[n(x + \Delta x) - n(x)] - [n(x) - n(x - \Delta x)]}{2\Delta x} = -\frac{10^{12}}{D}$$
$$\frac{[n(x + \Delta x) - 2n(x) - n(x - \Delta x)]}{2\Delta x} = -\frac{10^{12}}{D}$$

$$n_{i-1} - 2n_i + n_{i+1} = -\frac{2 \times 10^{12} \times \Delta x}{D}$$

$at\ x = 0.01\ cm,\ J = kn(x)$ so we can write

$$-D\frac{n_i - n_{i-1}}{\Delta x} = kn_i$$
$$\left(1 + \frac{\Delta xk}{D}\right)n_i - n_{i-1} = 0$$

And $at\ x = 0\ cm,\ J = kn(x)$ so we can write

$$-D\frac{n_{i+1} - n_i}{\Delta x} = kn_i$$
$$\left(1 - \frac{\Delta xk}{D}\right)n_i - n_{i+1} = 0$$

Hence the M matrix will look like:

$$\begin{bmatrix} \left(1 - \frac{\Delta xk}{D}\right) & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\left(2 + \frac{\Delta x^2}{D\tau}\right) & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & \left(1 - \frac{\Delta xk}{D}\right) \end{bmatrix}$$

And N matrix will look like

$$N = \begin{bmatrix} 0 \\ 0 \\ -\frac{2 \times 10^{12} \times \Delta x}{D} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

```
% Problem No. 2_f) For the configuration in part (b), assume that a
% particle flux is introduced at x=30um at the rate of 10^12cm^-2/s. Assume
% that the particle density at A and B are held constant at n=0 and
% T=10^-7s. Find the particle profile from A to B, and the flux at A and B.

clear;
clc;
nx=101;              % Number of grid points %
MM=zeros(nx);        % Creates nx*nx zero sparse matrix %
d=100e-4;            % Distance between A and B point %
d1=30e-4;            % Flux at x=30um %
Flux=1e12;           % Flux value %
D=30;                % in cm^2/s
T=1e-7;              % Lifetime %
k=1e3;               % in cm/s
L=sqrt(D*T);         % Diffusion length %
deltax=d/(nx-1);

% Finite difference method to solve 2nd derivative in Diffusion  equation %
for i=2:nx-1
    if i==(d1/deltax)+1
        MM(i,i-1)=1; MM(i,i+1)=1; MM(i,i)=-2;
    else
        MM(i,i-1)=1; MM(i,i+1)=1; MM(i,i)=-(2+(deltax/L)^2);
    end
end
MM(1,1) = (1-k*deltax/D);    % Setting boundary conditions for M matrix %
MM(1,2)=-1;
MM(nx,nx) = (1+k*deltax/D); % Setting boundary conditions for M matrix %
MM(nx,nx-1)=-1;             % Setting boundary conditions for M matrix %

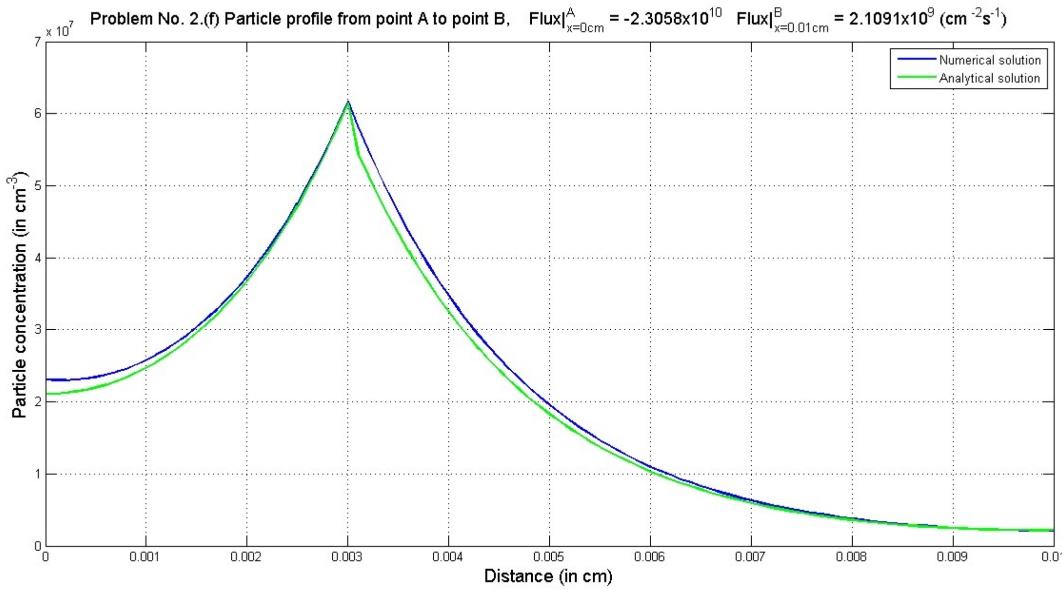

NN=zeros(nx,1);      % Initialize N matrix of MX=N linear equation %
NN((d1/deltax)+1)=-2*1e12*deltax/D; % Setting N matrix value for point
x=30um %
XX=MM\NN;            % Finding numerical solutions %
NX=linspace(0,d,nx);
fluxA=-D*((XX(2)-XX(1))/deltax);      %Flux at point A %
fluxB=-D*((XX(nx)-XX(nx-1))/deltax);  %Flux at point B %

% Analytical Solution %
X1=zeros(1,nx);

for i=1:nx;
    if i<=(d1/deltax)+1
        A=1.05446086e7;
        B=1.05446086e7;
        X1(i)=A*exp(-(i-1)*deltax/L)+B*exp((i-1)*deltax/L);
    else
        A=3.264877661e8;
        B=3.62788e3;
        X1(i)=A*exp(-(i-1)*deltax/L)+B*exp((i-1)*deltax/L);
    end
end

figure(1)
plot(NX,XX,'b',NX,X1,'g','linewidth',2);
grid on;
```

```
temp2=['Problem No. 2.(f) Particle profile from point A to point B,
Flux|^A_x_=_0_c_m = ',num2str(-fluxA*1e-10),'x10^1^0', '
Flux|^B_x_=_0_._0_1_c_m = ',num2str(fluxB*1e-9),'x10^9 (cm ^-^2s^-^1)'];
title(temp2,'fontsize',13);
xlabel('Distance (in cm)','fontsize',14);
ylabel('Particle concentration (in cm ^-^3)','fontsize',14);
legend('Numerical solution','Analytical solution');
```



PN Junction Solver (1D)

- Poisson's Equation

$$\frac{d^2\phi}{dx^2} = -\frac{\rho(x)}{\varepsilon}$$

- Current Equation

$$J_n = qn\mu_n\xi + qD_n\frac{dn}{dx}$$

$$J_p = qp\mu_p\xi - qD_p\frac{dp}{dx}$$

- Continuity Equations

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} + G_p - R_p$$

Solution Approach to Poisson's Equation

$$\frac{d^2\phi}{dx^2} = -\frac{q}{\varepsilon} n_{\text{int}} \left(e^{-\frac{\phi}{V_T}} - e^{\frac{\phi}{V_T}} + \frac{N_D - N_A}{n_{\text{int}}} \right) \qquad \rho = p - n + N_D - N_A$$

Now Suppose $\phi_{new} \geq \phi_{old} + \delta$

$$\frac{d^2\phi_{new}}{dx^2} = -\frac{q}{\varepsilon} n_{\text{int}} \left(e^{-\frac{\phi_{old}+\delta}{V_T}} - e^{\frac{\phi_{old}+\delta}{V_T}} + \frac{N_D - N_A}{n_{\text{int}}} \right)$$

$$e^{\pm\frac{\delta}{V_T}} = 1 \pm \frac{\delta}{V_T} + \frac{\delta^2}{2!V_T^2} \pm \frac{\delta^3}{3!V_T^3} + \ldots\ldots$$

Which gives us

$$\frac{d^2\phi_{new}}{dx^2} = -\frac{q}{\varepsilon} n_{\text{int}} \left(e^{-\frac{\phi_{old}}{V_T}} - e^{\frac{\phi_{old}}{V_T}} + \frac{N_D - N_A}{n_{\text{int}}} \right) + \frac{q}{\varepsilon} n_{\text{int}} \frac{\delta}{V_T} \left(e^{-\frac{\phi_{old}}{V_T}} + e^{\frac{\phi_{old}}{V_T}} \right)$$

Now put $\delta = \phi_{new} - \phi_{old}$ which will give us the 'Linearized Poisson's Equation'

$$\frac{d^2\phi_{new}}{dx^2} - \frac{q}{\varepsilon}\frac{n_{\text{int}}}{V_T}\phi_{new} \left(e^{-\frac{\phi_{old}}{V_T}} + e^{\frac{\phi_{old}}{V_T}} \right) = -\frac{q}{\varepsilon} n_{\text{int}} \left(e^{-\frac{\phi_{old}}{V_T}} - e^{\frac{\phi_{old}}{V_T}} + \frac{N_D - N_A}{n_{\text{int}}} \right) - \frac{q}{\varepsilon}\frac{n_{\text{int}}}{V_T}\phi_{old} \left(e^{-\frac{\phi_{old}}{V_T}} + e^{\frac{\phi_{old}}{V_T}} \right)$$

Linearized Poisson's Equation with Finite Difference Scheme

Using 'Finite Difference' scheme we can write

$$\frac{d^2\phi_j^{new}}{dx^2} = \frac{\phi_{j-1}^{new} - 2\phi_j^{new} + \phi_{j+1}^{new}}{(\Delta x)^2}$$

This will give us

$$\frac{\phi_{j-1}^{new}}{(\Delta x)^2} - \phi_j^{new}\left[\frac{2}{(\Delta x)^2} + \frac{q}{\varepsilon}\frac{n_{\text{int}}}{V_T}\left(e^{-\frac{\phi_j^{old}}{V_T}} + e^{\frac{\phi_j^{old}}{V_T}}\right)\right] + \frac{\phi_{j+1}^{new}}{(\Delta x)^2}$$

$$= -\frac{q}{\varepsilon} n_{\text{int}}\left(e^{-\frac{\phi_j^{old}}{V_T}} - e^{\frac{\phi_j^{old}}{V_T}} + \frac{N_D - N_A}{n_{\text{int}}}\right) - \frac{q}{\varepsilon}\frac{n_{\text{int}}}{V_T}\phi_j^{old}\left(e^{-\frac{\phi_j^{old}}{V_T}} + e^{\frac{\phi_j^{old}}{V_T}}\right)$$

We can write the above equation like a set of linear equation based on the position of the node

$$b_j\phi_{j-1}^{new} + a_j\phi_j^{new} + c_j\phi_{j+1}^{new} = f(\phi_j^{old})$$

Solution to the Linearized Poisson's Equation

The set of linear equation we got in the last slide can be written in matrix form as

$$\underbrace{\begin{bmatrix} a_1 & c_1 & 0 & 0 & 0 & 0 & .... & 0 & 0 & 0 \\ b_2 & a_2 & c_2 & 0 & 0 & 0 & .... & 0 & 0 & 0 \\ 0 & b_3 & a_3 & c_3 & 0 & 0 & .... & 0 & 0 & 0 \\ 0 & 0 & b_4 & a_4 & c_4 & 0 & .... & 0 & 0 & 0 \\ 0 & 0 & 0 & b_5 & a_5 & c_5 & .... & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & 0 & 0 & .... & b_{N-1} & a_{N-1} & c_{N-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_N & a_N \end{bmatrix}}_{[M_{a,b,c}]} \times \underbrace{\begin{bmatrix} \phi_1^{new} \\ \phi_2^{new} \\ \phi_3^{new} \\ \phi_4^{new} \\ \phi_5^{new} \\ . \\ . \\ . \\ \phi_{N-1}^{new} \\ \phi_N^{new} \end{bmatrix}}_{[\phi]} = \underbrace{\begin{bmatrix} f(\phi_1^{old}) \\ f(\phi_2^{old}) \\ f(\phi_3^{old}) \\ f(\phi_4^{old}) \\ f(\phi_5^{old}) \\ . \\ . \\ . \\ f(\phi_{N-1}^{old}) \\ f(\phi_N^{old}) \end{bmatrix}}_{[f]}$$

Doing lower upper decomposition

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & ...... & 0 & 0 \\ \beta_2 & 1 & 0 & 0 & ...... & 0 & 0 \\ 0 & \beta_3 & 1 & 0 & ...... & 0 & 0 \\ 0 & 0 & \beta_4 & 1 & ...... & 0 & 0 \\ . & . & . & . & . & 0 & 0 \\ . & . & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & ...... & \beta_N & 1 \end{bmatrix}}_{[L]} \times \underbrace{\begin{bmatrix} \alpha_1 & c_1 & 0 & 0 & ...... & 0 & 0 \\ 0 & \alpha_2 & c_2 & 0 & ...... & 0 & 0 \\ 0 & 0 & \alpha_3 & c_3 & ...... & 0 & 0 \\ 0 & 0 & 0 & \alpha_4 & ...... & 0 & 0 \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & ...... & \alpha_{N-1} & c_{N-1} \\ 0 & 0 & 0 & 0 & ...... & 0 & \alpha_N \end{bmatrix}}_{[U]} = [M_{a,b,c}]$$

Solution to the Linearized Poisson's Equation Using LU Decomposition

As

$$[L]\times[U]=[M_{a,b,c}]$$

So, we can get

$$\alpha_1 = a_1$$

$$\beta_k = \frac{b_k}{\alpha_{k-1}} \qquad and \qquad \alpha_k = a_k - \beta_k c_{k-1}$$

Now we can write

$$[L]\times[U]\times[\phi]=[f]$$

Suppose

$$[L]\times[G]=[f] \qquad where \qquad [G]=\begin{bmatrix} g_1 \\ g_2 \\ . \\ . \\ g_N \end{bmatrix}$$

Then we get

$$g_k = f\left(\phi_1^{old}\right) = f_1 \qquad and \qquad g_k = f_k - \beta_k g_{k-1}$$

Hence $[L]\times[U]\times[\phi]=[f]$ so, $[G]=[U]\times[\phi]$

This will give us the solution in the form

$$\phi_N^{new}=\frac{g_N}{\alpha_N}; \qquad \phi_k^{new}=(N-1),(N-2),\ldots\ldots 3,2,1$$

Algorithm for Equilibrium Solution to the Linearized Poisson's Equation