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# Phase field modeling; the materials science, mathematics and computational aspects

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**Module No.9**
**Lecture No.36**
**Diffusion equation: zero flux BC & explicit method**

Welcome we are looking at solution to the diffusion and we derived the expression using explicit and implicit discretization schemes. We have not talked about exactly how the boundary conditions are implemented, we will look into the details today. And we also want to write scripts in octave to solve for these equations. So the equation that we are trying to solve is the diffusion equation.

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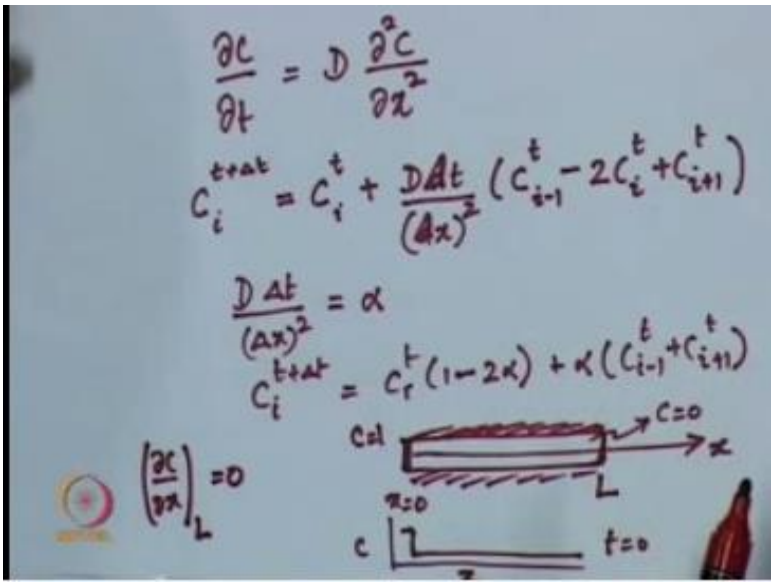


So it is $\partial C/\partial t = D\partial^2 C/\partial x^2$ this is the equation that we are trying to solve. And the discretized version looks like this $C_i^t + \Delta t = C_i^t + Ddt/dx^2$ I probably use $\Delta t$ and $\Delta x$, so let me use $\Delta t$, $\Delta x$ and then $C_{i-1}^t - 2C_i^t + C_{i+1}^t$. So I am going to call this $D\Delta t/\Delta x^2$ as some $\alpha$ so it becomes $C_i^{t+\Delta t} = C_i^t(1-s\alpha) + \alpha(C_{i-1}^t + C_{i+1})$. Now let me consider a scenario in which, of course it is one dimensional diffusion which means there is diffusion barrier on this side. So diffusion can take place only along the X direction.

Let me assume that at this point where X=0 the composition takes a value of 1 okay, so this is all normalized, so this is going to take a value of 1. Everywhere else at the beginning the composition is going to be 0, and as time proceeds what happens is the thing that we are looking at, so initial profile is very clear, it is 1 and then it goes to 0 everywhere. This is the at time T=0, this is C as the function of X right.

So this is the initial condition and we have one boundary condition this end is always kept at 1, the other end we need to decide what is the boundary condition going to be. So I am going to keep the boundary condition, that there is no flux at this boundary. In other words I am going to consider the boundary condition as follows $\partial C/\partial x$ at this point L is equal to 0. What is the

implication of this for our discretization scheme is what we need to look at and what is the implication of this for our scheme is something that we need to look at.

So let us take a closer look at the boundary condition, so I have this boundary condition at one end, at the left end where we are the first node point, the composition is always kept at 1 right.

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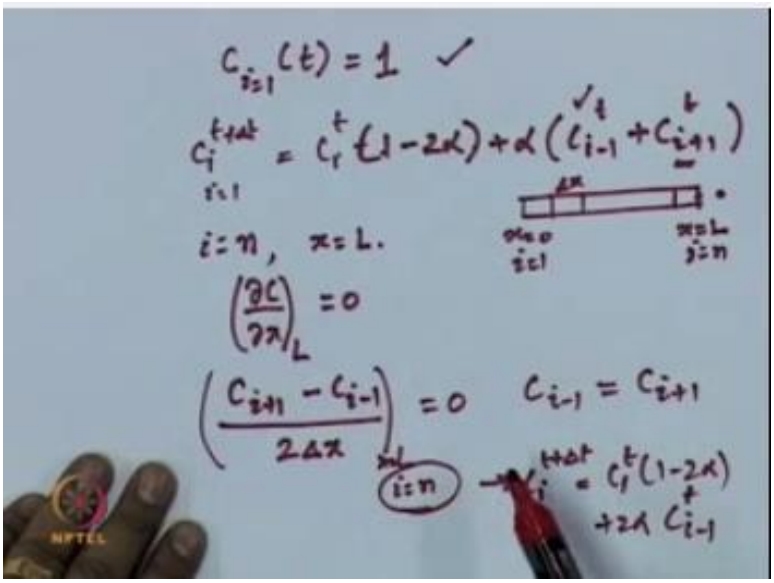


$C_{i=1}$ is for all times equal to 1 right, that means this is not changing with time, so I do not need to solve for this equation at all, the solution, this point when I have this expression which says $C_i^{t+\Delta t} = C_i^t$ + something, something I do not need to consider the case i=1, because i=1 there is nothing is happening, so it is always remains at 1. Now when i=n that is the point where x=L we are assuming that $\partial C/\partial x$ at this L=0 okay.

Now what does that imply in our case is what we want to know, because $C_i^{t+\Delta t}$ is $C_i^t(1-2\alpha)+\alpha(C_{i-1}^t + C_{i+1}t)$ right, this is the expression that we have. Now when I am at this point right, this is x=0, this is x=L and for this point when i becomes n so i=n here, i=1 here and then there are this $\Delta x$ changes. When I am at this point I know that for this i there is an i-1 point, so this is not a problem, but I need to know what i+1 is, that is a ghost point here.

A point which lies outside of our domain, the way to calculate that is that, there is also this discretization for $\partial C/\partial x$ which says that $C_{i+1} - C_{i-1}/2\Delta x$, this is also $\partial C/\partial x$ at the point i okay, so this discretization is also there, this is the central difference discretization. So discretization if I use and because at L this is = 0 that is L is i = n right that is a point this is a point this is x= 0 at this point this is 0 this condition is satisfied if I take $C_{i-1}$ to be equal to $C_{i+1}$ in another for the nth point this the last point I am assume that $C_{i-1}$ and $C_{1+1}$ are the same so that becomes $2\alpha\ C_{i-1}$ t so fro just for this point it becomes $C_i^{t+\Delta t}$ is nothing but $C_i^t$ 1-2α+ $2\alpha C^t_{i-1}$ because i-1 is something that is available i+1 I do not know I replace the i+1 in terns of i-1 using the given boundary condition so this is what I am going to do first and we are going to see how the solution involves.

It is possible to look at in this case also how the solution evolves interactive mode by writing the code but is for more easier if we do in script mode because later when we are going to change this boundary condition you can take the same script you can change only things corresponding to the boundary condition and you can save it as new script file and you can learn it so that is the reason why I am going to write as script in octave for solving using this explicit discretization scheme with the boundary condition that at one end the composition is always stays at one and at the other end the flux is zero.

Okay no atom when it reaches that end can escape so when it reaches that end it is just stuck there so that point the concentration as time goes is going to build up more and more atoms will come from one side and it will reach that point and so we cannot go beyond that point so it is going to increases the concentration at that point which the solution which we will see later which is what we expect to get and so let us write a script which will do this competition okay so this explicit method that is all the right hand side of the discretization we took at the same time t which is the current time using which we are getting the further time and we are having no flux boundary condition at their right hand left is a dire line right hand is okay so let us do that as usual go to the computer.

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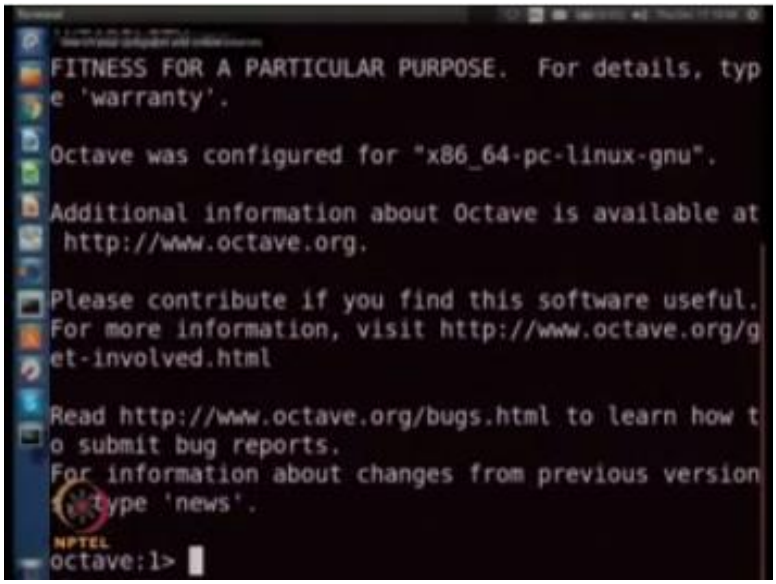


Open terminal okay and then I am going to the directory which I am going to write the script in and I am going to invoke octave from that okay so octave is there and if I now write the script I can come here and source the script I will get the solution now for writing the script.

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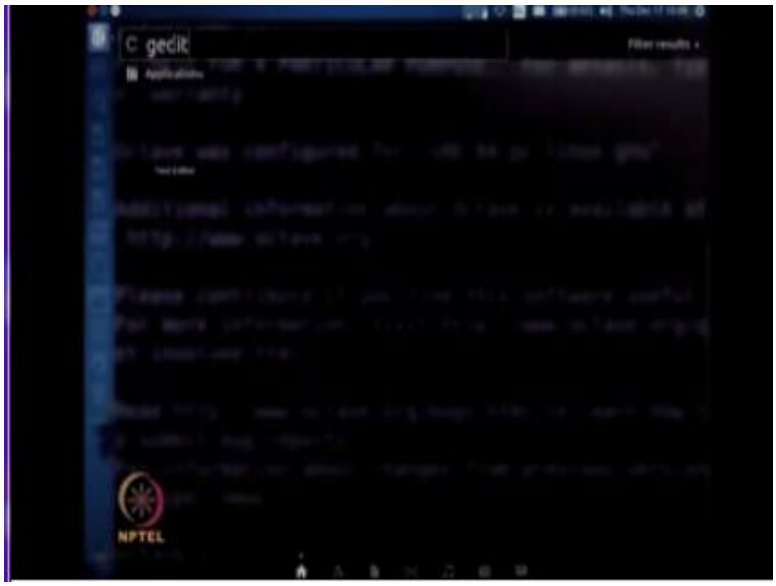


I am going to use this program call G edit you can use any text editor.

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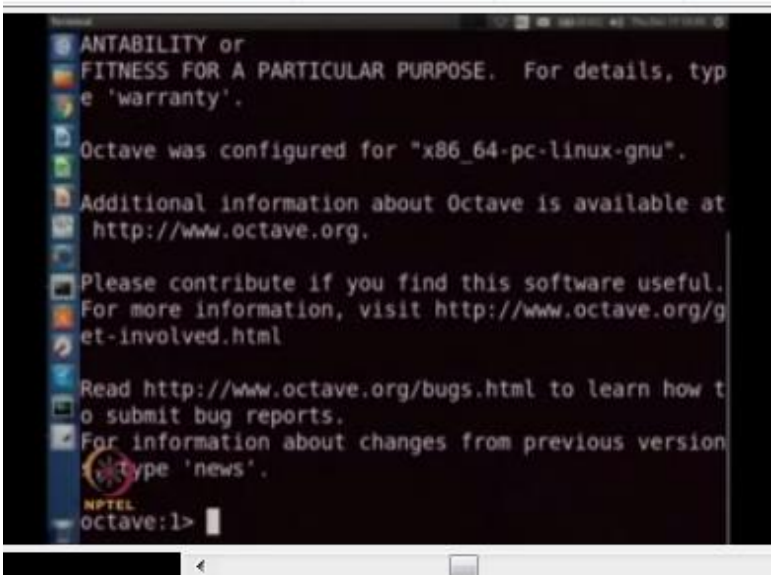


Simple text editor note pad kind of things okay.

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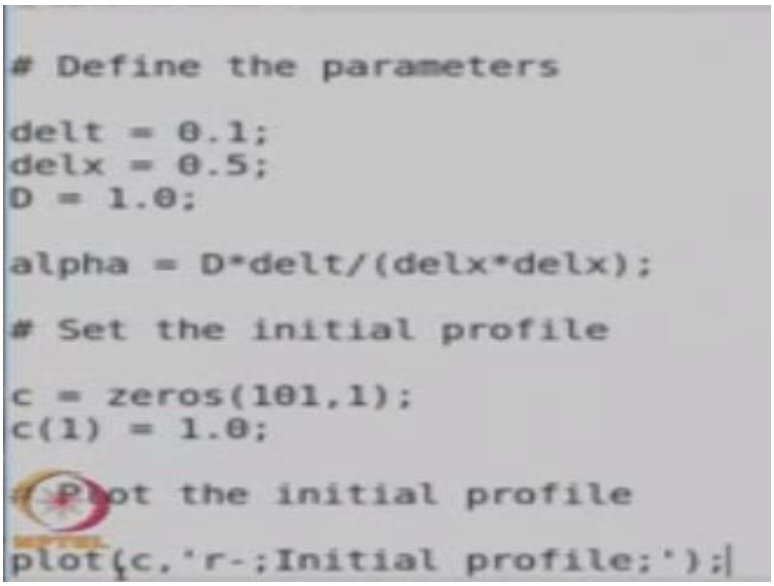


But you should not use word kind of editors because they put lots of hidden characters which interfere with your code so let save this file as I am going to save it in the same directory in which I have invoked octave that is phase we will move directory I am going to call this program as explicit no plugs 1D. oct okay so it is a good idea to name the files very clearly so that by look at the file name you know what the script is going to do so first thing we do it is always a good idea.

So let us put clear figure and clear all okay so we are cleared all the variables are parameters that octave might have in it is memory we have also cleared the figure window so it is a clean slate from which it is going to start the computations now let us defined this variable $\Delta t$ and $\Delta x$ so this is how we do so let me call it as $\Delta t$ is equal to some value some take a value of 0.1 please remember even though in the equation I call them as $\partial c/ \partial t$ and $\Delta^2 c/ \Delta x^2$ as I explained.

We assumed that all these quantizes are non dimensional okay so del t when I say 0.1 it sis in some non dimensional units it does not have any unit it is second it is not hour it is not minute it is not say it is non dimensional it is just the number okay so same is true for del x also del x is = to let me take n units are some 0.5 okay now I am define and D the diffusivity we need to know

let me defined the diffusivity as 1 because this is a non dimensional I have taken non dimensional deficit of 1 so we said that some quantity is α.

So let me call as α that was nothing but D*del t / del x * del x) right so this is Dt / del $x^2$ which we defined as α so I want to now defined the initial profile what was the initial profile so it is a good idea to put some commands and let me put the commands here so clean figure and clear all data that is I what is being done here then defined the parameters that is what we mean time here so we define the parameters, okay.

Now we are going to go and set the initial fine okay so initial profile requires so I am going to take some C and this is the way to define a vector so I am going to say zero's 101, 1 so what is this mean? This means that it is going to define a variable called a C.

And it is a vector it has 101 rows and 1 column that is what 101, 1 means and it is going to initialize this vector to have 0's in all the 101 rows is a column vector and is going to put 0's in all the rows of this column, okay. So 0's is a way of defining are initializing a vector to have 0 line but we know that C(1) is always 1, right. The rest of them remain at 0 but c(1) is 1 so this is the initial profile, okay.

Now it is a good idea once we have done that to plot the initial profile, okay. So let me plot the initial profile so I am going to plot I am going to plot it as C okay so I am going to plot it with a red color and with lines and then I am going to say that it should be labeled as initial profile, okay. So that is what this means, so I am plotting C so C is 101 points so those are our node pints the 101, I = 1, I = 2 etc equal to 101 that is what this means.

And at those values I have taken this C value to be something so this is a initial profile I want to distinguish the initial profile from the other profiles that we are going to plot as the composition involves, so I am going to plot the initial profile as a line that is what the dash indicates it is a red line so the other words will come in the color blue quite it called starts by plotting by blue color so red line will be the initial profile.

The blue color will be the actual profile after sometime is long and we are going to label the profile as initial profile so it will drop the red line and it will put a red line up there in the legend and say initial profile so people know which is the initial profile, okay. So that is what this one does and then there are things that you can go do to the plot.

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```
plot(c,'r-;Initial profile;');

# Get handle

ax = gca;

set(ax,"linewidth",2.0);
axis("square");

# Hold the plot for future

hold on

for k=1:20
for j=1:500
for i=2:100
```

Probably it is a good place to introduce some of them you get what is known as the handle okay, get handles so what is handle, so I am going to say ax = gca so this is getting handled for the access box, a box what is the purpose so if you say set ax, line width, 2.0 so what you would do is that it will make the box of the plot a little bit thicker, okay. You can also make this other one so generally I like my plots to be square instead of rectangle.

So access square will make the plot for as while, okay. So there are ways of changing things you can change the box the width of the line which makes up the plot box I made it thicker and I have made the plotted itself a square plot okay otherwise it is generally rectangular we width and the height are not the same in length so I have made it a square because I always feel that square plots look nice, okay.

So you can do this kind of changing the properties of the plot that you are going to get so this is just to introduce you, you can go to octave and look for help for getting handled on axis and are look at plot and then look at this sub-topics and so on and so forth, okay. Now I am going to say okay so this is just that and then hold the plot for future okay. So I am going to say hold on okay this plot will be kept.

Any other plot will be done on the same figure so we know what the initial profile looks like and what the profile looks like after sometime, now I am going to introduce three loops, okay. So what are they for so we will look at let me take for k = 1:20 this loop is for plotting, okay so there will be 20 figures that will be plotted this outer loop is for plotting. Then the inner loop so far j= 1:500.

So the plot will be dome once in every 500 steps right $\Delta t$ is 0.1 I think we took so a 0.1 x 500 is like 50 time units once the plot will be made and that is what will be plotted so that is why we have the other variable K, now of course for I = 2 to 100 because remember the first point we said is not in the equation at all because it always takes at one and we have taken it to be 1 so it will remain at 1 for all times because we are not going to change it at all. Now after 100 points because $101^{th}$ point expression is slightly different, okay so what we are going to do is that.

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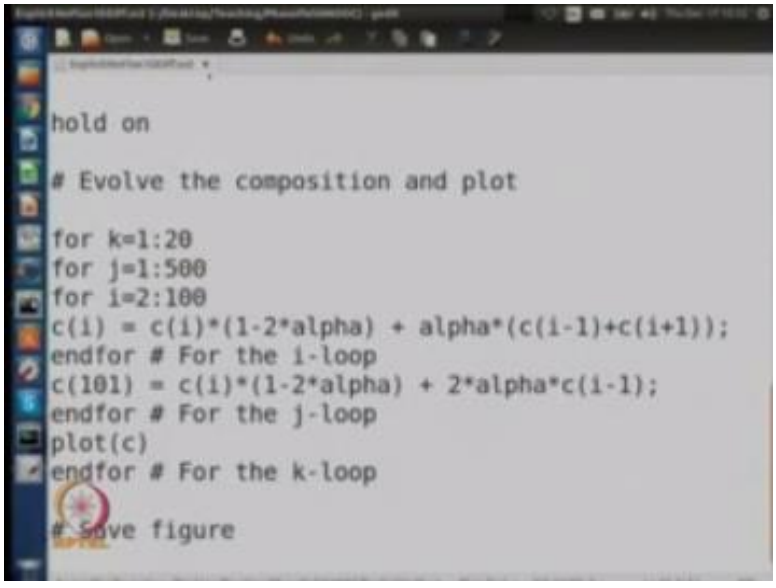

We are going have a inner loop which involves the composition values at points 2 to 100 1 always remains at the value 101 will be evolved outside of this loop and once 500 such steps are taken then the plot will be made and then it will go back and make another 500 steps and then plot will be make and so on and so forth, so that is why there are three loops, okay. So the outer most loop is just for plotting purposes, okay.

So now what do I say c(i)=c(i)*(1-2*alpha)+alpha*(c(i-1)+c(i+1)), okay so this is the expression I am going to end the for loop then I am going to say c(101) is equal the same expression except that want to copy paste this same expression and then I am going to say that it is 2*alpha (c-1) there is no (c+1) that is needed, right so this is what we said happens because of the boundary condition because of the no flux boundary conditions so that is what I have implemented.

So remember, what happens so it goes to this loop then it does this for each j so 500 times it has to do this, so let us end the j loop, right so this is for the i loop, so this is for the j loop and after the j loop I actually want to plot the function, okay and then I am going to end the k loop end for this is for the k loop, right. And then okay, so this is the, this part should be called evolve the composition and plot, okay so that is what we have done here of course it is always a good idea so save figure, okay if this I have not show you earlier so you make all this figures they look nice on screen and you might want to keep a copy of the figure so here is a way to say the figure in whatever format you want I am going to show you eps encapsulated post script format it is also possible to save it in j pack format, okay.

So I am going to say print, pint- device which device it should plot print to the encapsulated post script color, okay so I am going to save this figure as ExplicitNoFlux.eps, okay so let us save this script okay let us run through the script once more so we cleared everything we determine the parameters we decided what is alpha and we setup the initial profile we plotted the initial profile we made some small adjustments to be figured we made it look nice and then we said that every other figure now on should be plotted on the same plot because we have the initial profile and we want to see how the time evolution is.

And then we evolve the composition using this expression which is the explicit expression which is algebraic which is the simplest way you can do, and then once you evolve some number of steps you plotted and then you go back and evolve for some more time you plotted on and so on and so forth and then finally you save the figure that is generated, okay so we are going to that.

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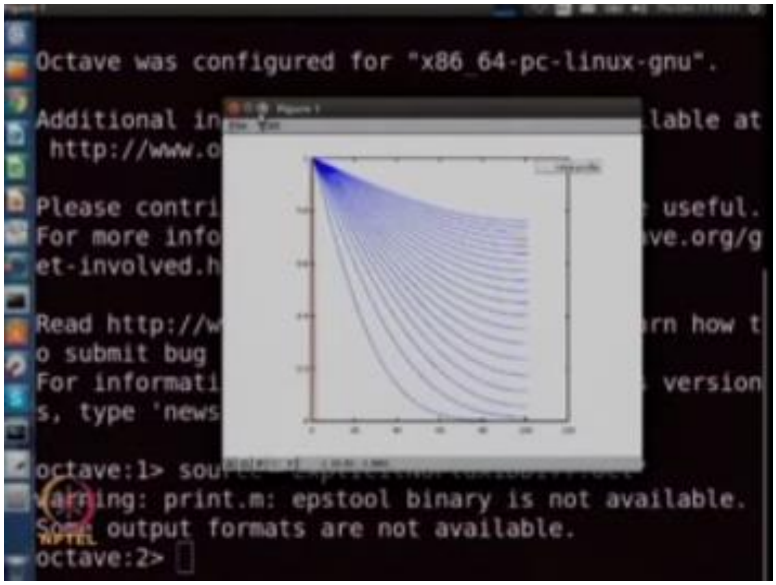


Now let us go here, and run the program so I have to say source explicit, okay so the way to not type the entire file name is to type the first two, three letters and then press the tab key and then octave will fill it for you because there are no other files which start with E and XP on Linux machines the capitals and small letters are distinguished so exp if it sees and then there is no other file with this name whatever is only file name that is available it will fill it for you.

So is a source file name.oct that is going to run the program , okay so you can see that it first command was clf so it first put the figure which is clean there is nothing there and now it is doing the computation as it is doing the computation and completes and it is going to come back and plot, back it completed and there is some warning message which I do not think is important.

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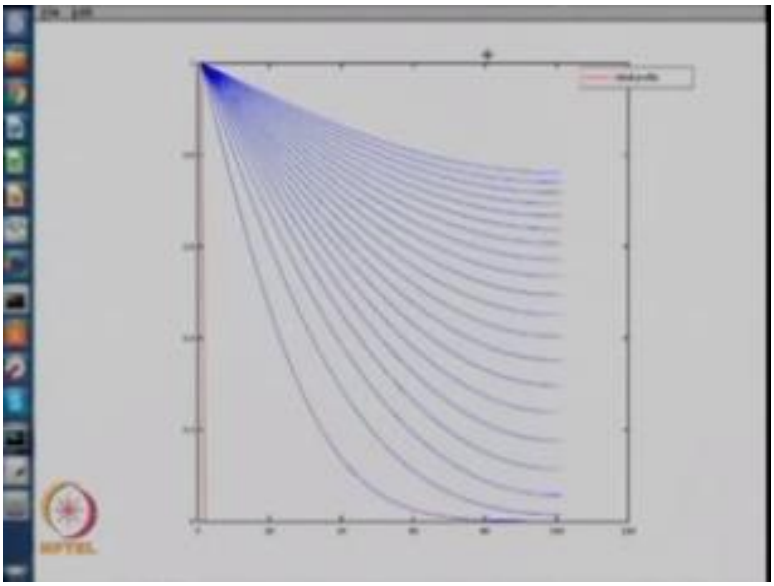

I do not know if you are able to see clearly so there is a red line so it is 1 and then it drops to 0 and it remains at 0 but this line is merged with the x axis that why you are not seeing and then you see the composition profile in all way so initially this profiles or there is some concentration that is coming in and it is going here it has not reached so this is quite close to your error function kind of solution the length is not reached probably much earlier than that it will actually be a much better fit with error function .

So we are going to do a tutorial to understand how the error function solution or where it is valid and things like that but as you can see I as I mention in the last lecture error function solution assumes that for a way from this region the composition always remain at Ci of the c initial that you started with, obviously in this case that is no long that true it is started with 0 and then this composition is building up.

Because of which these solution are deviating from the error function solution okay so we are getting numerically they are certainly deviating from the error function solution. But the deviation is because we said that atoms can reach this point but they are not suppose to escape here so the atoms come from all the way from here and then they get stuck here then what

happens at that point the composition key is increasing and you can also see another thing that the gap between the points here is much larger and then as time goes by it becomes smaller and smaller.

That is because if you look at the concentration gradient it goes from 1 to point some 7 and add here so overall concentration radiant which is driving the diffusion is lower as compare to here for example here to the composition gradient was like about one right it was one it was 0 sop the composition gradient is about 1-0/80 or much earlier it would have been some 20, 60, 80 whatever time pointy space points so that is the gradient.

So the gradient is very large here so there will be more flux because 6that is for what fix first class AC the flux is proportional to the radiant and as the gradient become smaller and smaller the flux is also going to become smaller and smaller so finally we expect that the composition becomes like 1 everywhere right that is the harmonization thing and you can see that it also says that this is the initial profile right it is a initial profile is noted here okay.

So that is the legend which says that the red line is basically the initial profile and as time increase you see that the composition keeps changing and finally we expected to become uniform single composition of 1 everywhere that what we expect and that where this system is involving okay so if you veal for few more like we plotted 20 times after every 500 steps maybe you can plot after every 1000 steps and go to much larger number of plots then you will see that these are all getting crowded and then it becomes self constant.

So this is at the one dimensional solution that we have obtain to using the explicit method now with one boundary condition being dwarfishly the other boundary condition being Nyman, the Nyman boundary condition said that the flux is actually 0 you can put some constant value for the flux so that is not what we did, we said that the flux is 0 and this is the solution so and we have written the script to obtain the solution so that brings us to be end of this part of the lecture explicit dissertation quant dimensional diffusion equation left boundary in Nyman the rashly boundary condition right boundary Nyman boundary condition we have solved.

And the solution has we can see is very, very simple and the advantage of using octave is that as you are getting the solution you can plot and you can look at the figures and you can actually understand what is happening because the computation and the visualization are happening together okay, of course you can also see that it takes some amount of time to do the computation because there are overheads that it is doing the repetition it is taking the value that is plotting them.

So all this takes some time so even though it is octave uses good for these kind of purposes if you want to write any proportional quality code using which you will generator results which are for example publishable some new research that you are doing the octave is not very efficient you can still do the job probably for you but it is not very efficient one d and about 100points and you can see the kind of resource it requires.

Whereas program which is written in C or for Tran will be much, much more efficient of course this disadvantage there is that you have to write the data to a file and you have to invoked this plotting as a separate exercise it is a post processing exercise that you need to do but here initialization running the pod post processing everything is done in one goal so it is great in terms of learning things but once you know probably for more involved computation you may have to go to a programming language like CRM photon okay.

So let us end this part of this lecture here we will come back and try it to look at solving the implicit scheme because that involves a matrix operation so we have to force the problem in terms of this matrix equation and we have to solve the result in set of matrix equation so we will do that in the next part of this lecture. Thank you.

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