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Phase field modelling; the materials science, mathematics and computational aspects

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Module No.1
Lecture No.39

Periodic boundary conditions (PBC)

Welcome we are looking at the solution for the diffusion equation, we are looking at you know equations of.

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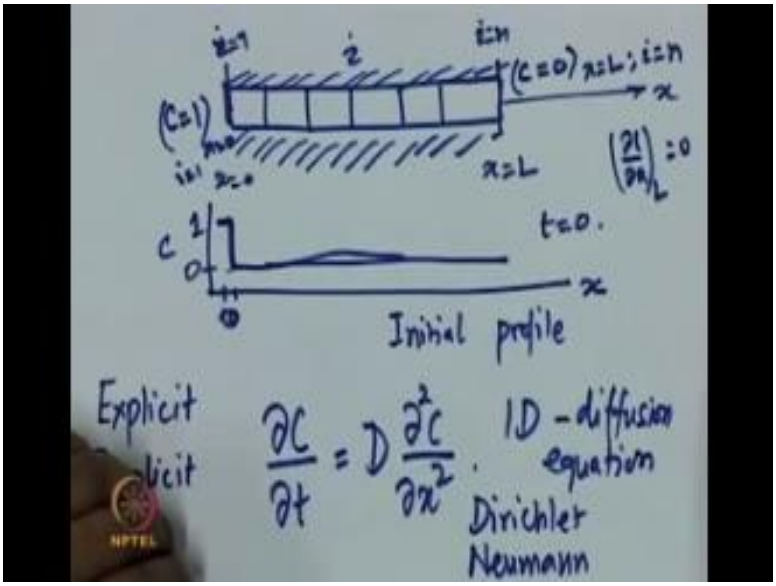

This type right this is 1D diffusion equation okay, so what we are trying to do is to solve this equation numerically, and we said that that there is explicit method, and there is implicit

method, you can use either of them and while doing that we said that there are different boundary conditions, one is deliciously the other one is normal.

So we have seen models scripts where you can implement these boundary conditions and solve this problem, now there is another kind of boundary condition which is slightly different from this which is sort of mathematical, I mean it does not follow from this or for it follow some physics but from a completely different type of argument, but with it is used for some purpose.

So I want to spend a couple of minutes discussing what this boundary condition is? and why it is there in the first place? And then we will go back to solving the diffusion equation using octave, with this particular boundary condition implemented, ok now this boundary condition is known as periodic boundary condition, okay.

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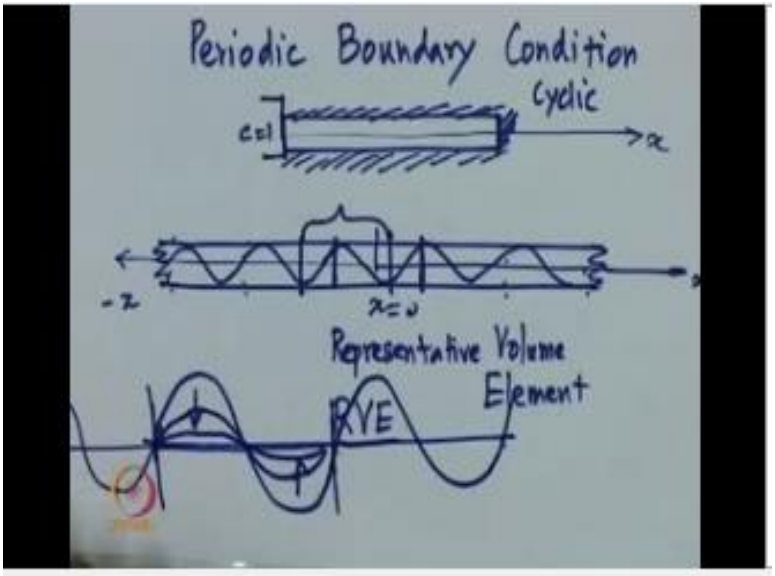

So periodic boundary condition, the origin of periodic boundary condition is slightly different see when we said the rich layer diamond, we took the actual system right I have this and it has some diffusion barrier, so the diffusion takes place along only x axis, so I am then and then I am considering cases where I put this end at some corpse concentration, and then keeping this end at some concentration, or making sure that I put a diffusion barrier here also, said that there is no flood.

So these are the type of boundary conditions when we talk about, then we get to directly and Neumann boundary condition, but think of a different case suppose I have a very long rod, okay right for all practical purposes it goes to ∞ on either side right, this is X let us say and the0 for X is somewhere here, and so this goes to so - x okay.

So these values are running from 1 ∞ to another ∞ for all practical purposes, because suppose I am interested in one part of this rod, and I am interested in what happens here? Because this is say representative volume element, so this is another terminology that is used, okay especially in finite element and solid mechanics context so this is sometimes known as RVE okay.

So I am going to consider a portion of this system, I am interested in what happens in this because I believe that this entire infinite the system is basically consisting of units like that, I mean this is say repeated infinitely, like this is repeated and that is repeated here on this side this is repeated, this is repeated, etcetera. Suppose I say that it is sufficient to look at what happens in this volume, because that is what is happening in every volume so this is sufficient to solve right.

Some of you who have looked at electronic properties will understand this because when we do band structure in such calculations, we do not do it for the entire crystal we do it for the unit cell, and say that because the crystal consists of repeating unit cells whatever is happening in one you'd cell is going to happen in all the other unit cells, and that is how we are getting the results that.

So in the condensed matter or solid-state physics, lots of times you use this boundary condition, this boundary condition is known as periodic boundary conditions, sometimes people also call it as cyclic boundary condition. You will see why an example of this is that, suppose I tell you that I have a composition profile which is sinusoidal, then it is sufficient for me to choose one wavelength, and the look at the domain for one wavelength because everything that is happening in the other boxes will be basically repetition of the same thing.

So it is sufficient for me to look at one wavelength, right in fact that is the case that we are going to solve, because remember we said that if you have a sinusoidal composition profile,

then classical diffusion equation predicts that this will come, down and this will go up this will not change, so that the composition becomes something like this after sometime, something like this after some time and then it becomes a constant, After a very long time.

So this is what we want to see, now if suppose I mean I have more than one wavelength in my system, it is not necessary for me to look at all wavelengths right, I can just restrict myself to one wavelength and suppose my system consists of a length which consists of two wavelengths, then whatever is happening in this wavelength is basically a repetition of this, or it could even have three wavelengths you know on this side.

So it does not matter I mean it is sufficient for me to look at only this side that is why it is called cyclic right, I mean what we what we are going to do is that this is going to get repeated. So how do we do that let us look at from the point view of Buford discretization what do I have when I discretize.

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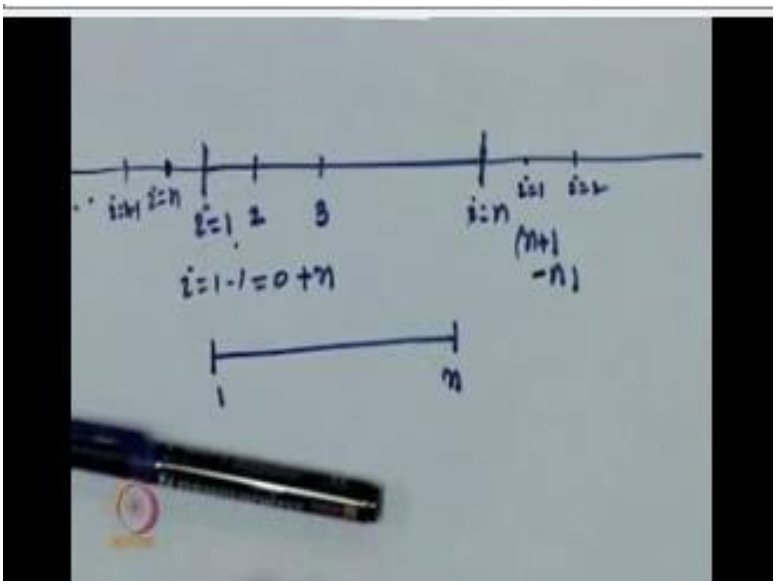

I have this domain I have I = 1, I have 2 I have 3etcetera I = n, here remember the boundary condition we needed because when I = 1 there is nothing to the left of this, when I = n there is nothing to the right of this, now when we say cyclic boundary condition I mean that this is the reason why it's called cyclic boundary condition, or periodic boundary condition because

we are assuming that whatever is there in this cell is getting periodically repeated and that is why it is periodic boundary condition.

What we tell is that let us assume for i = n, the point to the right is the same as I = 1, that is I am repeating this unit say again, what will happen this will become i = 1, this will become i = 2, etcetera right. So when I have i = n I can assume that the point to the right of n is nothing but the leftmost point, similarly when I have I = 1, because remember I mean if this is getting repeated on this side also, then this point will be actually i = n, because this will be i = n -1 and so on right.

So we are assuming that this is a representative volume, and the same thing is getting repeated on either side, which means for i = 1, i = n becomes the left neighbour and for i = n, i = 1becomes the right neighbour. So when we reach a point which is n + 1 basically what we are saying is subtract n from that right, when you have i +1 which becomes = n + 1 then just subtract here.

Similarly when you go to i = 1, when you are looking at i = 1 - 1 that is 0 we say just add an m to it in, other words your range is from someone to n, whenever you go about this you subtract n from it whenever you go below this add an end to it, and the map the points back to this domain, this is like I said done very extensively in condensed matter physics you might have seen band structures, you might have seen how the band structure is plotted, they have names like Wigner Seitz cell so everything folds back to the first Wigner Seitz cell or whatever okay.

So similar thing is what we are doing this is very important because we are going to do it in this context, but later we are going to use spectral methods and spectral methods always implicitly assume this kind of periodicity and periodic boundary condition okay, the implementation for spectral methods the periodic boundary condition is a little bit involved, but the idea is the same.

So I have one domain, I need points to the left of the domain and to the right of the domain, whenever I need them whenever I go outside of the domain depending on where whether I am going above n or below 1, I am going to either subtract or add n which is the size of the domain ok.

If I do that then the result is what is known as the periodic motion, so let us take the explicit method because that is very easy to implement, and let us implement periodic boundary condition for the explicit term implementation, and the solve the diffusion equation for an initial profile which is like, a one wavelength ok.

So that is the this is the at time T = 0, so this is the initial condition and because, I have periodic boundary condition I have gotten rid of the two boundary conditions, so instead I am going to impose the periodic boundary condition as you can see, in effect what the periodic boundary condition has done is that it has gotten rid of these two boundaries.

These two surfaces right, when I had a system like this was one surface this was one surface so I was implementing boundary conditions on these two surfaces, so I have guttered of those surfaces here, there is no surface right this is continue this discontinuous, I have orbit ally chosen some reason and I am working on it, now sometimes people tend to say that when you implement periodic boundary condition the system is infinite, that is not quite correct okay.

The system is not having any boundaries or surfaces, but that does not make it an infinite system, because this you can understand very easily suppose by mistake instead of taking one full wavelength, I took half a wavelength and did my calculation and assume periodic boundary condition, right then I will have a problem because in that case I am not having something that is like this, but instead I am going to have something that is like this.

Right now periodic boundary condition you have implemented, so when this system where you have taken one full wavelength, and repeating it will correspond to something which is like the infinite system, because we have gotten the full information and everything else is repetition, this is not I mean this is a completely different system if the composition is like this yes! Of course you can take this and the periodic boundary condition works and makes it infinite but.

So this is the concept related to representative volume element unless the unit cell that you are assuming over which you are implementing periodic boundary condition is actually completely representative of the system. It really does not the results are not equivalent to what you would get from an infinite system, in other words there is a system size effect,

unless you have gotten rid of it completely periodic boundary condition does not imply infinite system.

But in all cases where periodic boundary condition is implied, it implies that there are no surfaces or boundary synthesis, so it is a way of getting rid of surfaces and boundaries and if it is chosen appropriately the system will mimic an infinite system. But it is not necessary that every time you implement theory boundary condition the system will actually mimic, an infinite system so this is something that you need to keep in mind, so let us go implement a periodic boundary condition for an initial profile, which is sinusoidal like this okay, of course as usual we are going to open,

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Every time you open a terminal, go to the relevant directory I do it several times so that you will remember many a time because you will not do this you will get lots of error messages, so we don't want that okay. So then we open a text editor and,

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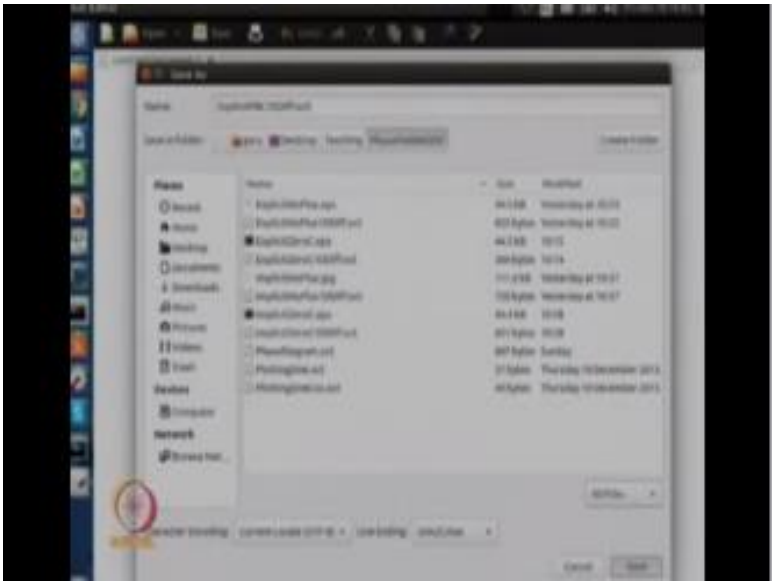

We save a file, let me save as it has to be saved in the same directory from which you have invoked octave, that is another reason why I am doing it every time to show you, let us do so this is also 1ddiffusion equation, but with periodic boundary conditions. So explicit PBC to say that it is periodic boundary condition, and one be diffusion Oct on the deft auto city right explicit periodic boundary condition 1d diffusion in off there right so this is the file.

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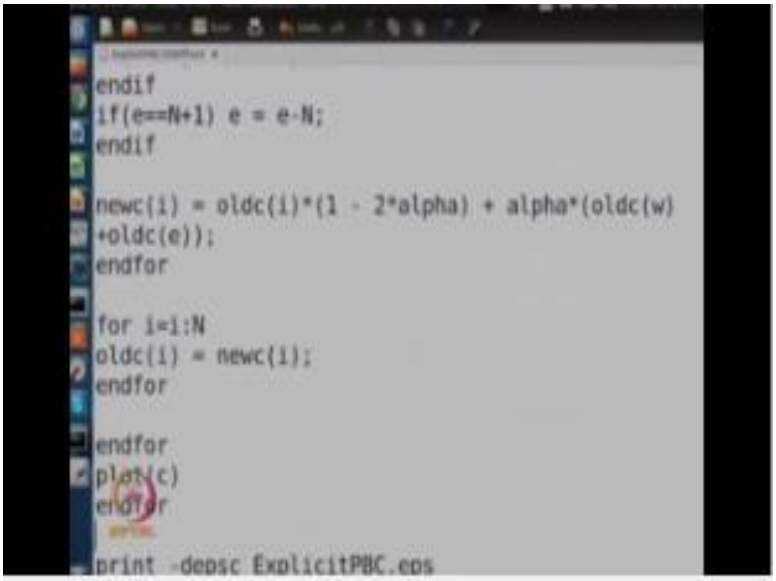

Of course, what do we do we start with clf and clear, okay the next step is to put the δ t = 0.01 δ X = 0.5 okay, so let us move that and d=1.0, α = d, into δ T divided by δ l X × δ x, okay, so we have defined α I am going to define the system size I am going to define n = 128, you will typically see that when we use spectral techniques, the numbers that we take for the system size is 2^n okay, it is like 32, 64, 128 256 / 12 24 2048 and things like a 40 96, so we go in this because Fourier transforms work better if you take the system size to be 2^n, it is not necessary in the case of finite difference, but just to indicate that sometimes you can take the system size it does not have to be from 0 to 100, it could be one to 128 so that is why I am taking it to be 128 okay.

And typically if you are using Fourier transform asters, spectral techniques for solving it is always better to take the number something like this okay, so I have defined the total number of points, so I am going to define the initial condition for defining the initial condition I am going to define what is known as m, is basically the number of wavelengths that you are going to include in the domain, okay now our case we said it is one single wavelength okay it could be more than one wavelength, you can put 2 then it will put 2 sides are ways you can put three it will put 3 sinusoid ally and so on okay.

So let me make m = 1 so far i = 1 to n, what are we going to do? so I am going to define a old c and a new see ok hold c of i =0 .5×1 + sign 2 π × m × I × L X / n okay, so this is very important to note what is it that we are doing? we are saying that the initial profile is sinusoidal but remember sign goes from 0 to - 1 to 1, but our composition profile should go only from 0 to .

So I am going to add one to sign that is going to make it go from 0 to 2 then I am going to × that by0 .5 so that the composition, is now going to run only from 0 to 1 that is the reason why it is here sign of course2 π m into I into del X / n i into del X will tell you what is the current point, and the M will tell you how many wavelengths you are going to include, and this distance divided by total n total numbers that you have.

So I should have this capital right so for I = 1 to n, we are going to have this right so this is the old c, I am also going to define a new c, of I so that can be 0 because that we get updated so n. Okay, so the point behind this is to put a sinusoidal profile which goes from 0 to 1, which means it will be about average about 0.5 okay, so this is one-way of putting a sinusoidal profile and a new c I am just initializing the variable here, I am not giving it any value because new c will be obtained from the old c, using our explicit formula and so that will automatically get the right values when we need it okay.

So this is the initialization that we have done, and let us plot, old c should be plotted and it should be plotted with a red line right, so whatever is red we know is the initial profile and then we have to say hold on, right because we want to plot everything on to the same plot, and then what we are going to do is that for, so this is again important k = 1 to 20 for j = 1 to 500 right this is our usual trick.

So the 20 plots I am going to make and each plot is after 500 time steps, so that is the reason why these two are there, and then we need to do the actual evolution actual evolution, will be done with using I so we say for i i = one to n okay, we are going to define west as i – 1, east as i + 1 right, then I + 1 point is the West for a yeast point i - 1 is the west point but we do know that when we have West Point as 0.

So we put that condition if West = 0 then what am I going to do, West = s + n so this is the basically the implementation of here are periodic boundary condition, end ever yes east = n +

1, that can happen east is = East – n, need to consistently use right, and if okay, so what is this? So this is basically implementation of boundary condition right. So now because of this you know only point which is expected to go below one is the west point, and that is only for the first point that we have taken care of only point that will go greater than n is basically, the east point we have taken care of that.

So this will take care of it, is not necessary of course to do it this way you can go from I = 2 to n – 1, and for i = 1 you can always make West is this and n is that, but this is another way of doing it said there are more than one-way of implementing it this might not be the most efficient way because for every w/e you are going to execute at if loop was so it is costlier in terms of optimization of the code.

But it makes things easier in terms of understanding so let us keep it this way, okay so we have now defined so what do we do we say new c (I) remember, we are still in this I loop is = old c (i) + α times, old c of i should multiplied 1 +1-2 α right, 1 - 2 α is what the old c should multiply + what do we have + α times old c West + old c east, point this is the new see remember that is the expression, so c at time T + delta T is = cat time T into 1 - 2α + α times C ati – 1,and C i i + 1, that is what West and East is what we are calling in this for right.

So you do this end the for loop for evolving, so after some time loop so we also end the other one but before ending the time loop of course we have to say for i = 1 to N, what do we do old c of I is = new c (i) okay, remember we are doing explicit keeping this whole scene new c is not really required but again, I mean you can do it in whichever way you want it is not necessary that it has to be done only in this manner, okay.

So this is not far so we need another n for which will be for the j loop de loop is for 500 time steps, so it will do this 500 times and it will end that loop after ending that of course it has to plot, plot C and then end for so it will plot20 times and then it will plot and so, then we can print the figure print- de psc is explicit periodic boundary condition dot okay.

So let us run through once more what is it that we have done we have done the clearing and then defining variables and all that, and we have made the initial profile here and we have plotted the initial profile, and we have held on to the figure and then we have this plotting loop time loop and actually evolution loop, in the evolution loop we define the east and west

points and we implement the periodic boundary condition on them, and then we go through the usual explicit scheme okay And then we end the loops we plot and then we come out and plot difficult okay.

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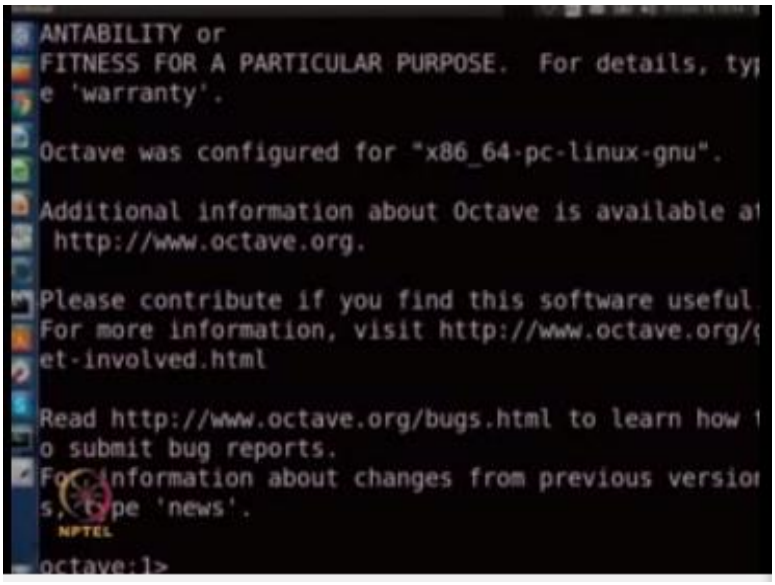

So this, so latest source I think this is explicit.

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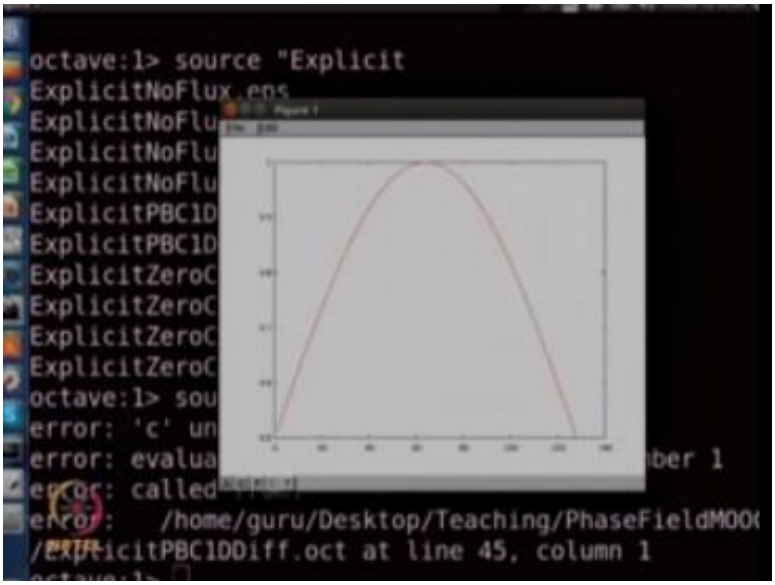

Periodic boundary condition one day diffusion doctors of it okay. so there is a problem somewhere I have made a mistake so it says to see undefined near line 45 column set let us go.

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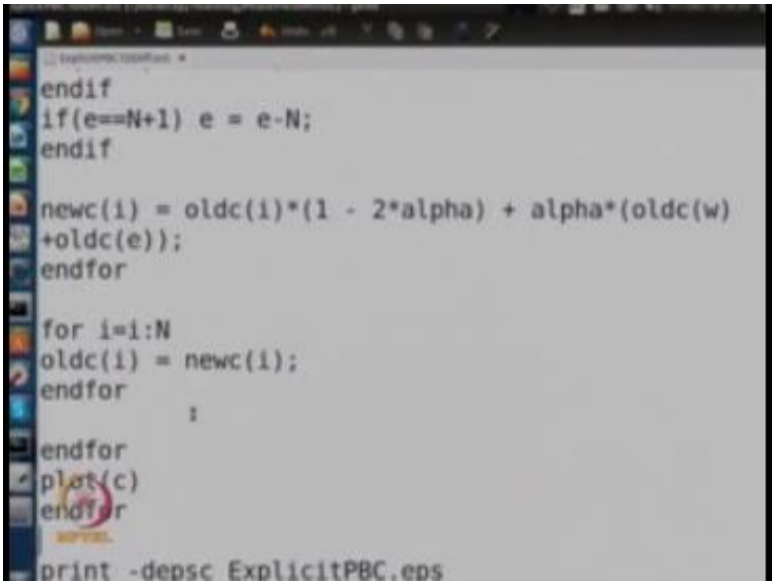

Where is line 45 ha plot I should say oldc, because oldc is what is going to be the latest value at that point okay.

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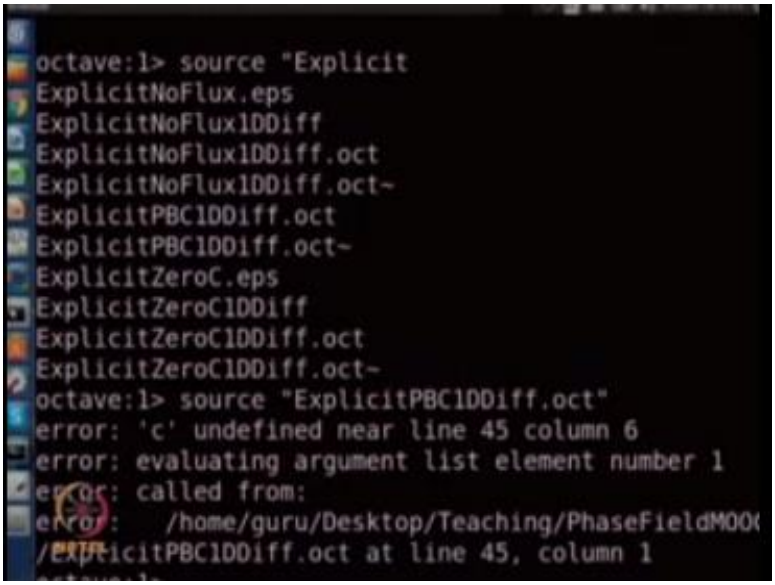

So I did not know what the C was okay, alright.

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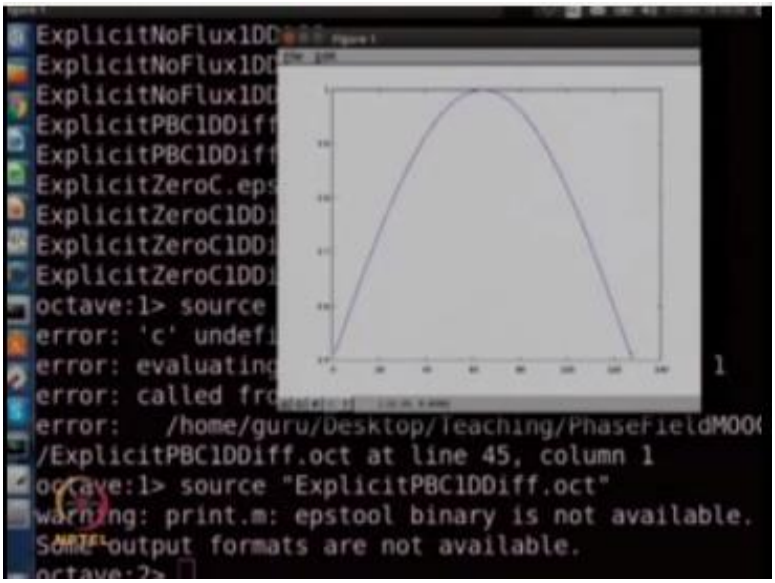

So again I am writing this code as we are doing the lectures because I want you to also understand it is not like I do not get error messages I do get it all the time in fact I get more than what I get when I am lecturing because here at least I am prepared even then I make this many mistakes if I am writing a code by myself I make much more of mistakes, but you should be able to read the error message or look at the result and what is happening and try to figure out what went wrong or why or how okay.

Now something has gone wrong because I do see that there is just one figure I mean blue but this is not what we expected right.

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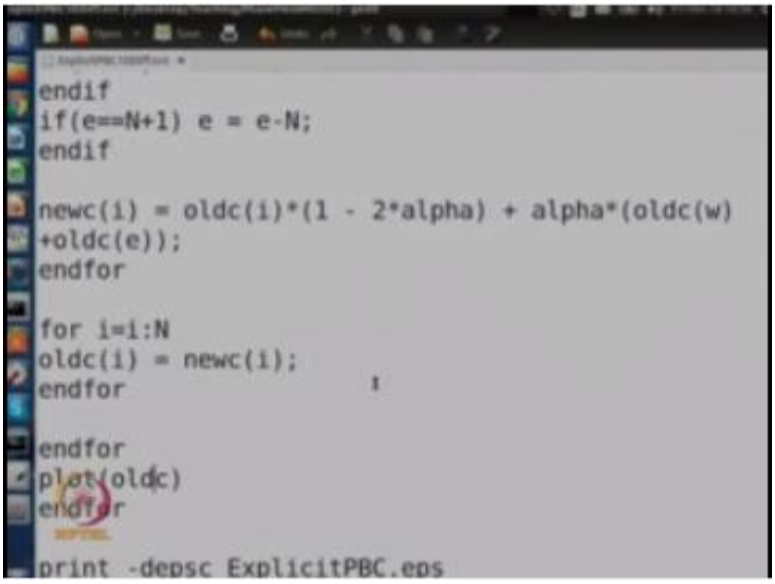

So we wanted it to run for some time.

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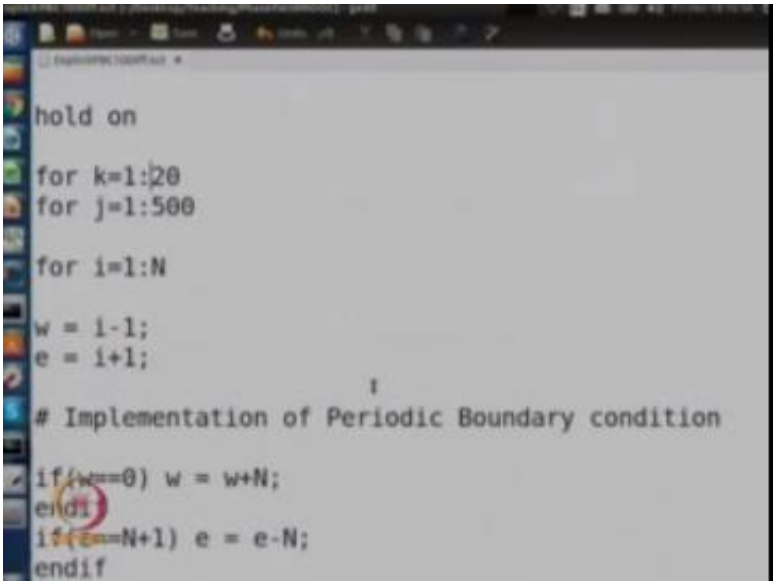

So I think the number of steps it ran is not sufficient.

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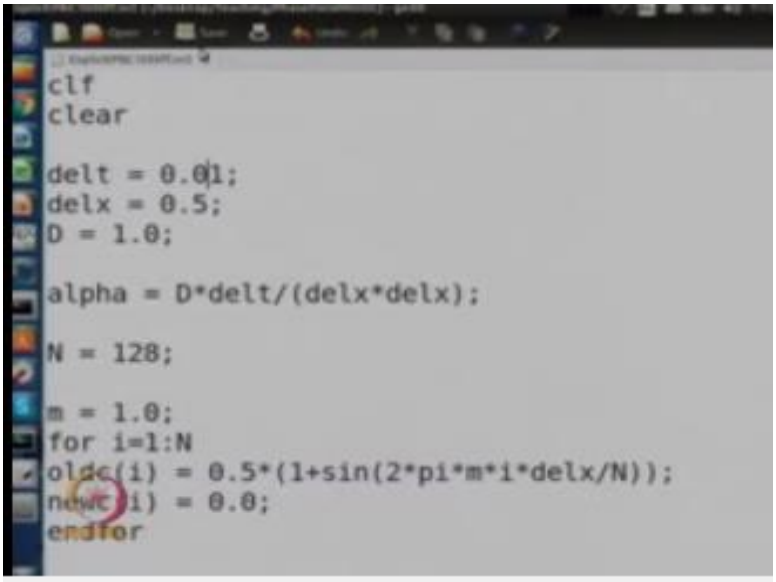

So let us make the ΔT to be smaller maybe 0.01.

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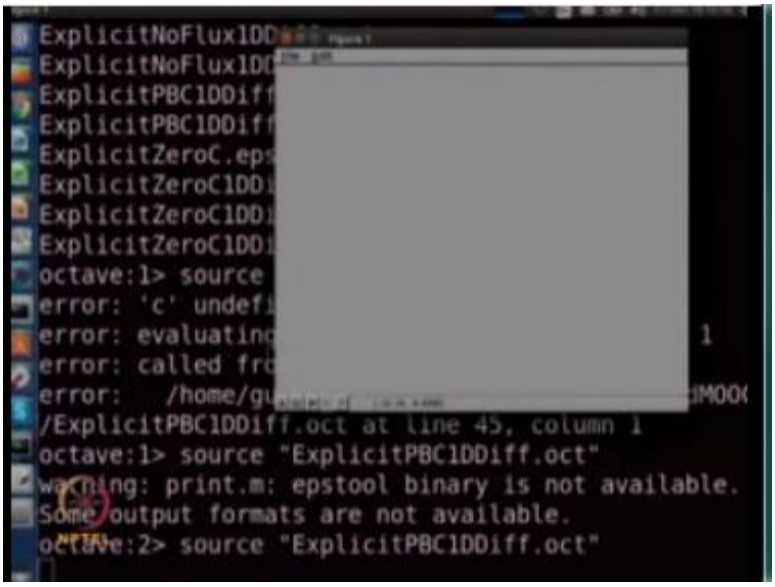

And let us try to source book it is not clear so why the evolution did not take place in all probability the time steps was too small because it was 0.001 20 x 500 is like another 1000, so that is like just one time unit ram. So that is probably the reason why it gave no difference between the initial profile and the final profile, so let us see what we get here okay, we are getting similar result again.

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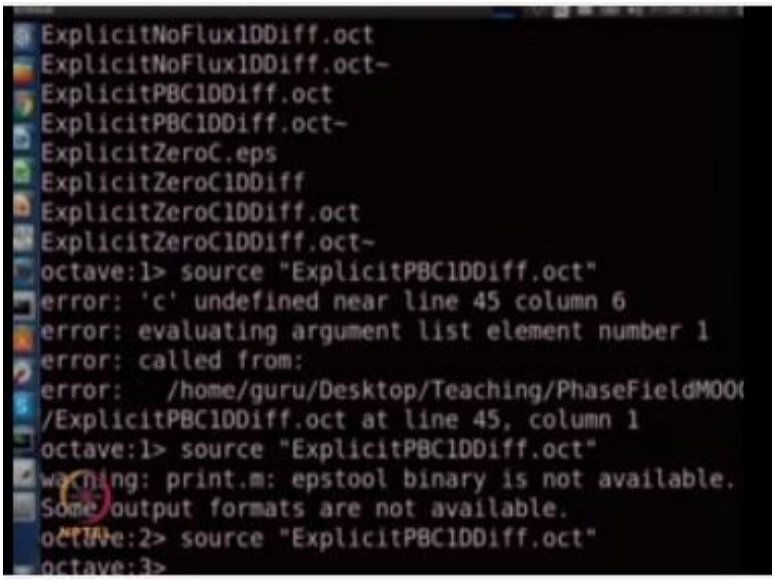

So I think I will go and change things a little bit.

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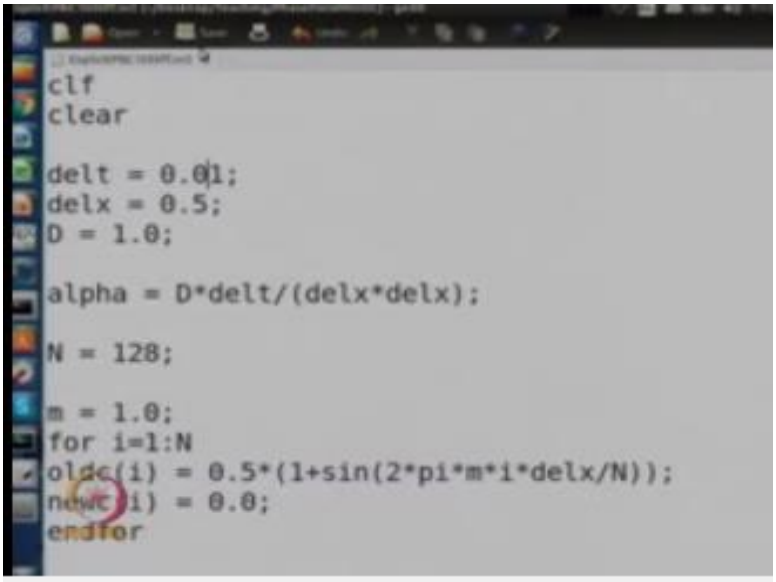

Let me put for example, may be okay.

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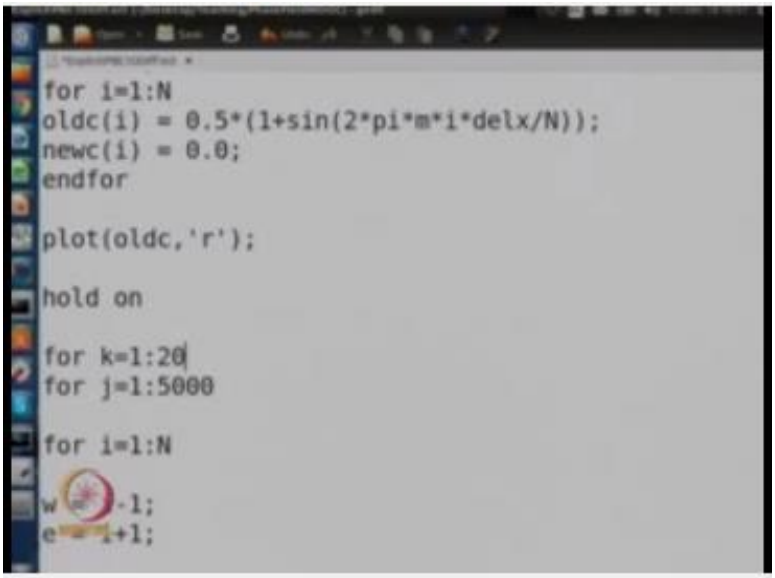

So let us make this 5000 and this 200 let us see what happens.

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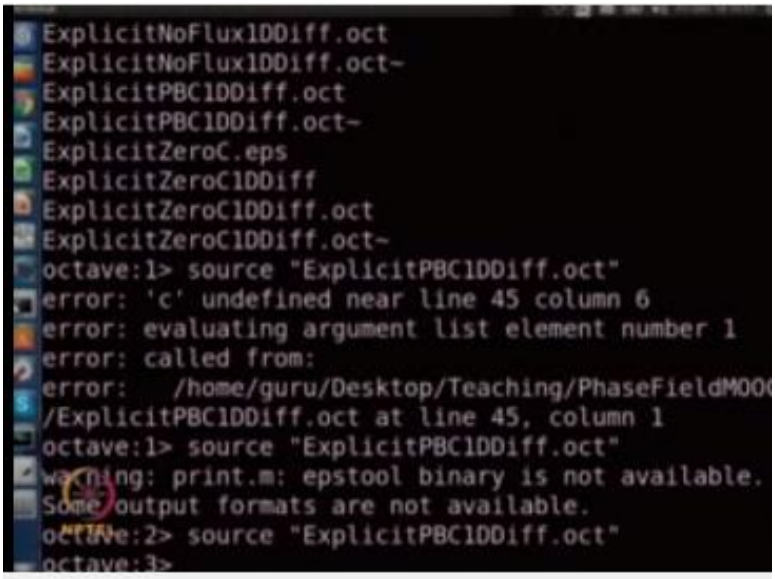

It is going to take much longer to run of course, but probably that will give us better composition profiles see the other thing that I am surprised is that we have only one half of the figure. So it is not sinusoidal okay, so maybe we have to put m = it is not one wavelength that we are finding okay. So I think M has to be made two we will come back to that let us see what this okay.

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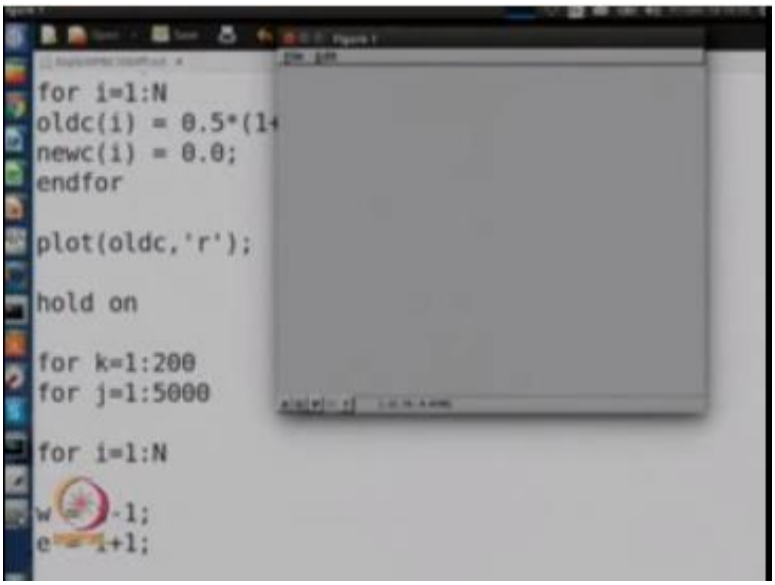

So is the code is going to take some time and once the results come we will, I will store the figure and in the next lecture we will show how it looks and are probably I will play with the parameters, so that when we come back in the next lecture we can use the proper parameter so we get the results within the timeframe. So for now I am going to stop here and these scripts will also be available for you to work on them on your own. So you will be able to also work with it and see what happens. Thank you

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