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Phase field modeling; The materials science, Mathematics and Computational aspects

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Module No.10
Lecture No.43
Implicit spectral method

We are looking at the solution for the implicit spectral method in one dimension for the diffusion equation and the solution that I wanted to show so there are some parameters that are not chosen properly so I have now corrected that and I am going to go through the code once more and then we will run this code and see how the solution looks like.

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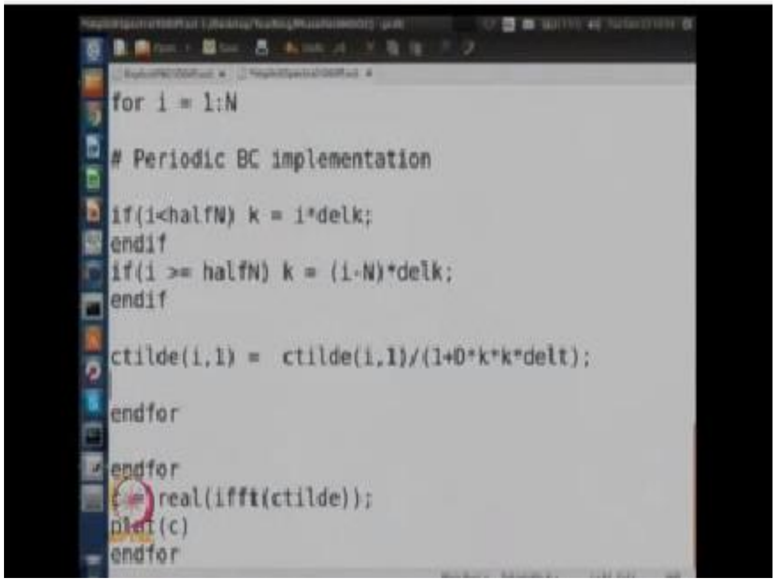

Okay the first step is to clear the memory and figure so clear all and then clear figure and we define the system size which is 128 we define the diffusivity so let me say system size and parameters so the diffusivity is also defined then probably it is a good idea to define ΔT also here instead of defining it later so Δ T is defined later as 1.0 so I am going to make it1.0 here.

I am able to take a del t of1.0 because remember we are dealing within X implicit method so there is no constraint on what Δ T you have to take for the calculation to be stable of course smaller Δ T will the calculation will make the calculation more accurate but stability is not a problem so I am allowed to take a larger Δ T so I have taken a ΔT of 1 and then we make a sinusoidal profile.

So we first define the C vector it is a column vector and we say that there will be two waves in this domain which is 128domain and the two waves that is why Miss equal to 2 and we make a sinusoidal profile and this composition profile so I have made a mistake here it should be .5 right it should be .5 times 1+ sign so because sign goes from -1 to +1 if you add 1to it sign will go from 0 to 2 if you x. 5 it will go from 0 to 1.

So that is the reason why this .5 multiplication is there so we have made a sinusoidal profile okay now what we are going to do so we are going to plot the initial profile and we are going to say hold on so that the other profiles will be plot tin on the same thing now we need to implement periodic boundary condition this is a spectral technique so we need first define half the length of the domain that is called half n and then we define the Δ K because remember we are in the Fourier space we are going to solve this equation in full space.

So we do not need the Δ X we need the domain discretization in the reciprocal space so that isΔ K so that we have defined and then I have as usual there is a loop for plotting there is a loop of our evolving the composition and then there is a loop for actually evolving using the implicit top technique so that I need to take the Fourier transform so C tilde is phosphonate transform of C then I go 1 to N and this is where the actual boundary condition is implemented okay.

So I should probably also modify this so this definition of half length is for periodic boundary condition implementation actual periodic boundary condition implementation is being done here so I will say periodic BC implementation so that happens here and then we say the new composition is nothing but old composition / 1+ D K^2 and the K is what is defined and K is defined consistent with periodic boundary conditions.

So that is only trick in this code if you do then the new composition we know but this new composition is in the reciprocal space okay so we evolve it for all the reciprocal space points and we evolve it for 500 time steps because that second end far is for the time loop1 to 500 right so we have this 1 to 500 and that second loop ends there so this is the end for the second loop and then when we want to plot the composition we want to plot it in the real space so inverse fast Fourier transform of C tilde that will give me the composition we want only the real part because this Fourier transform and inverse Fourier transform will have both real part and imaginary part.

So we want only the real part because I am in the real space and the composition is a real value it is not imaginary and it does not have any machinery component but numerically when you are doing you might pick some imaginary compound component that is because of errors and we want to get rid of it.

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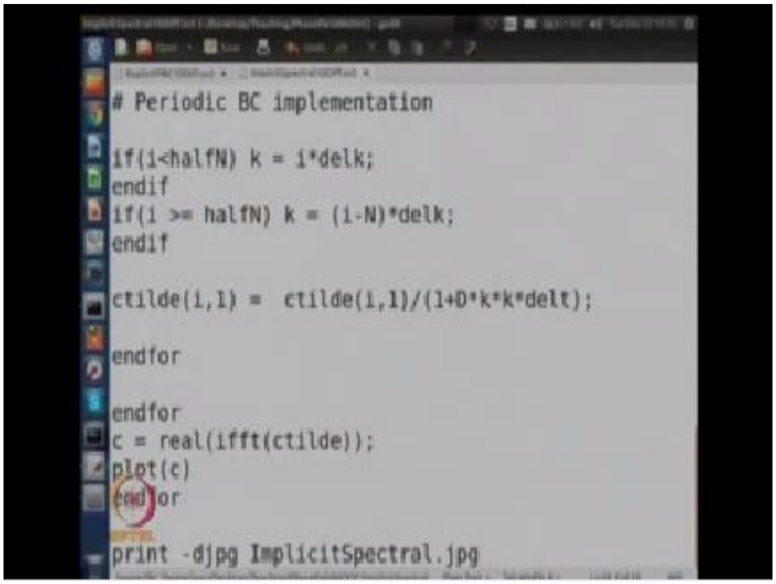

So C is real part of inverse fast Fourier transform of c tilde so this CI plot and then I end so this end for will make sure that I have plotted for several times now the lost thing of course you can print - B jpg that to the device jpg I can say that implicit spectral . jpg okay.

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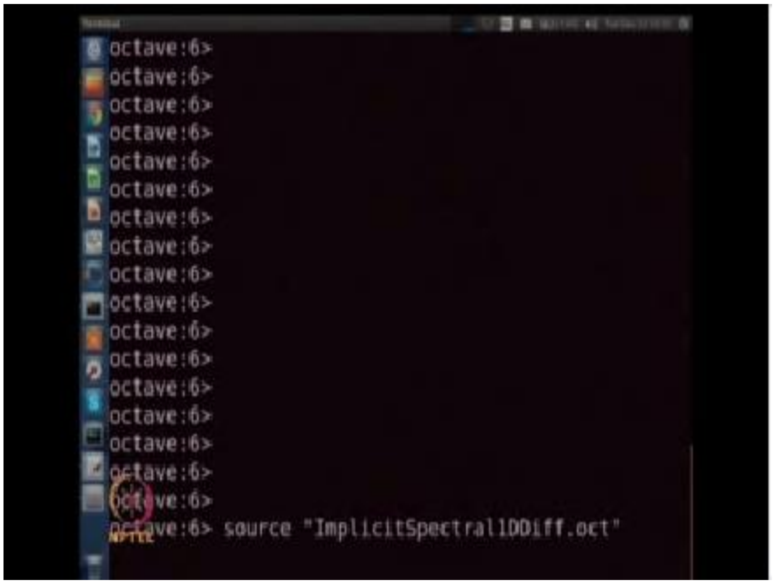

So let me say this and let us serve on this so I have the source implicit spectral only diffusion .okay so again because this is sinusoidal profile the composition evolution is expected in the same way as it was in the finite-difference case namely that wherever.

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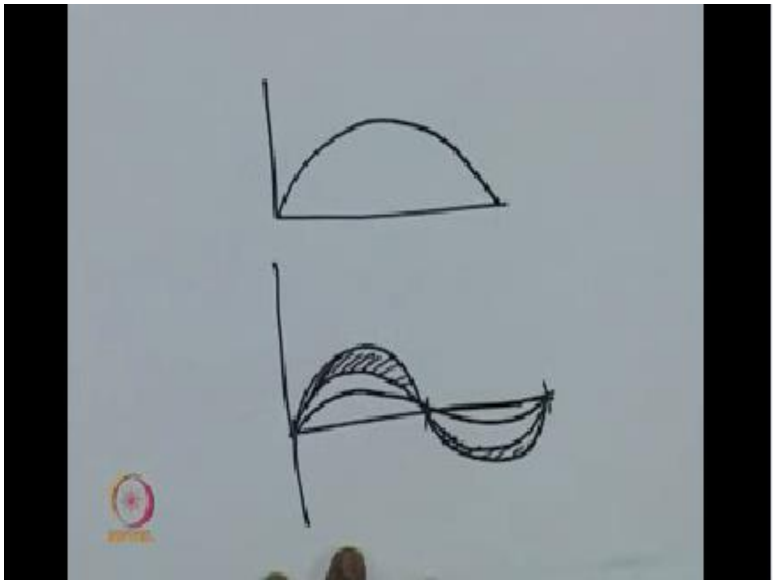

The curvature is a positive that region is going to increase wherever curvature is negative that region is going to decrease and that this system is going to go towards homogenization.

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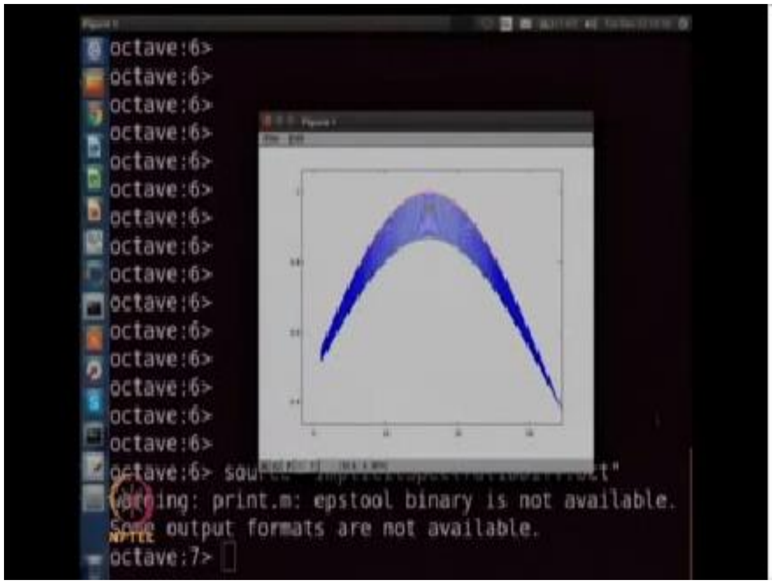

And that is precisely what we see here so you can see a redline and you can see several lines which are basically the evolution of the composition so let me just take one of these parts one wave length and you can see that for the display so this is the same as you know we can go closer and take a look at it so this is basically the composition evolution as a function of time.

So it starts at red and then the composition is coming down and in the other part the composition is going up so whatever extra amount of composition that is coming down here is going to go into that region and is going to bring up the composition so here also we see that finally the composition will become a straight line ok so this is the spectral technique1d diffusion equation solved using spectral technique and like I said as part of exercise we will do several initial profiles thank you.

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