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Phase field modeling: the materials science, mathematics and computational aspects

Prof. M P Gururajan
Department of Metallurgical Engineering and Materials Science, IIT Bombay

Module No.15
Lecture No.63
Numerical solution of CH: spectral method

Welcome we are looking at the solution for the diffusion equation.

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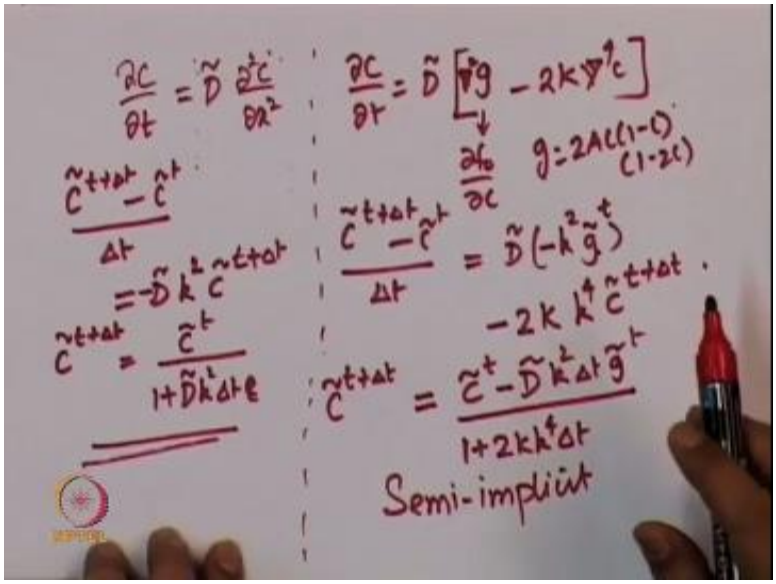

Which is this, and the Cahn-Hilliard equation which is this, okay some $\tilde{D}$ this $\tilde{D}$ is not the same as this times some g function which is nothing but $\delta f_0/\delta c$ function -2κ so there is a ∇^2 acting on this and $\nabla^4 C$ acting on this so that is the equation we are trying to solve. If we do Fourier transform then we can solve these equations Fourier transform technique is much more accurate than finite difference and in that case we take the Fourier transform $t+\Delta t$- $\tilde{C}t/\Delta t=\tilde{D}$ and the Fourier transform basically gets u k^2 in this case $\tilde{C}$.

So and at time t okay, so you can then write $\tilde{C}^{t+\Delta t}$ as nothing but $\tilde{C}/1+\tilde{D}k^2\Delta t$ so this can be at $t+\Delta t$ so this can go and that is how you evolve the solution. So this is a implicit technique so everything on the right hand side is at time $t+\Delta t$ so you can evolve very fast. But in this case such a trick does not work that is because if you do the Fourier transform $\tilde{C}^{t+\Delta t}$-$\tilde{C}^t/\Delta t=\tilde{D}$, now this ∇^2 acting on g so I have to take $-k^2\tilde{g}$ but this can only be at time t it cannot beat time $t+\Delta t$ because t+ time Δt I do not know c and the g function is nothing but 2AC(1-C)(1-2c), okay. So that is the reason why this has to be calculated in real space every time and that quantity should be Fourier transformed so that can only be at time t.

On the other hand the other term $-2\kappa\ k^4\tilde{C}$ this can be at time $t+\Delta t$, so if we now look at it so it becomes $\tilde{C}^{t+\Delta t}=\tilde{C}t$ and then this $-\tilde{D}\ k^2\Delta t\ \tilde{g}$ time t,so this is goes there so it comes $1+2\kappa\ k^4\Delta t$ is the solution so this is known as semi-implicit spectral technique, because some parts is implicit some part is explicit, so this is why we call it semi implicit. But semi implicit is still better than explicit because it will still allow you to take larger time steps.

So now I have two scripts which implement this and remember because this Fourier transform the periodic boundary condition has to be incorporated and that has to be incorporated in terms of this k lying in the range of $-\pi/a$ to $+\pi/a$ so that is how the periodic boundary conditions will be implemented in this code. So what we now want to do is to write the Fourier spectral technique code.

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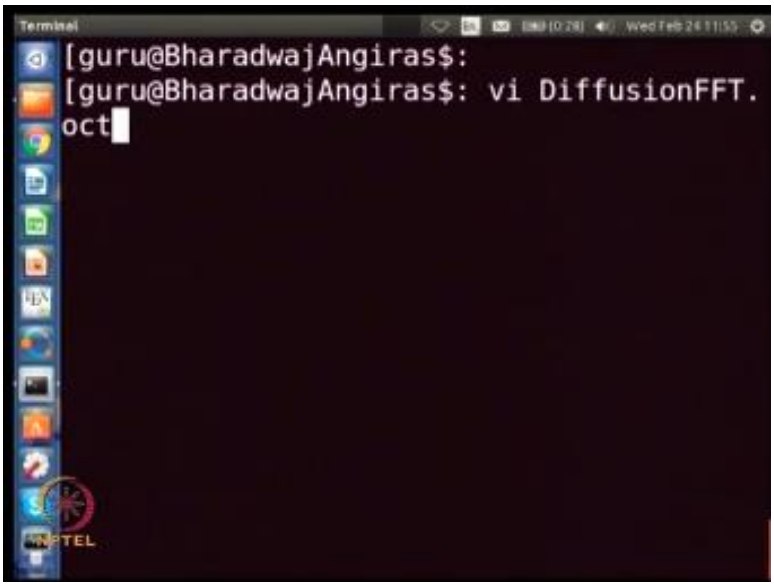

For doing diffusion equation first and then the Cahn-Hilliard equation, okay. so let us write the script for doing the diffusion so diffusion FFT.oct okay.

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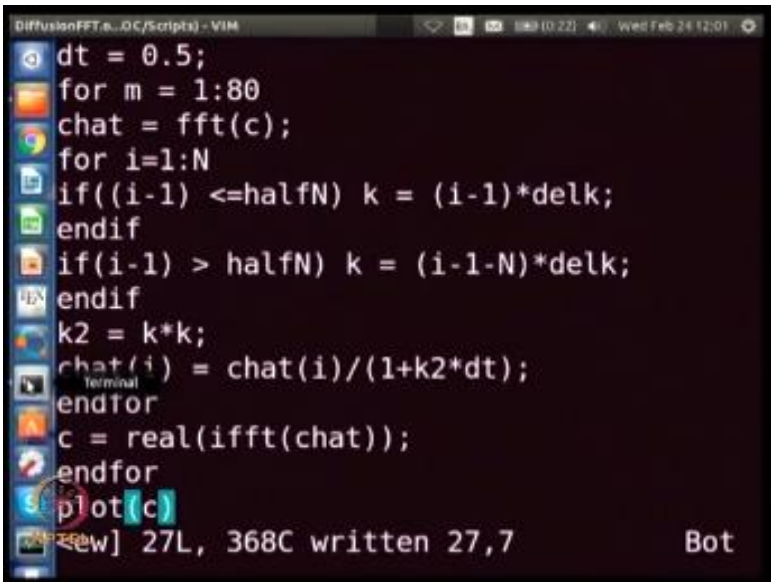

So what is the thing, so first I am going to clear all clc, clf so I am going to clear all variables, functions everything. So start with this thing, so a number of grid points is 32 when we are doing Fourier transforms we are always want this number of grid points to be 2^N okay, so that is very important and I am going to take dx to be equal to 1, okay. So what I am going to do is that, so I am going to put the same profile for i=1:N endfor, so what I am going to do is that I am going to say c(i) is nothing but 0.5*(1+sin())this quantity what is sin (2*pi*m*i*dx/N) okay.

So this is the initial sinusoidal profile that I have made so I am going to plot this and I am going to plot it with the red line and I am going to mark it as initial, okay. So this will be plotted and it will be written as the initial profile, so I am going to hold on so that when I plot the next profile the final profile we will know how it is. So I am going to define and halfN which is nothing but N/2, okay.

So delk so we have to discretized in Fourier space and in Fourier space discretization is that delta k is so 2pi will be split into this N which is the 32 that we have taken okay, so whatever be the number of points that you take so much will be the discretization in the Fourier space okay, so

that is the delk that we have taken and I have to define a time step, I can define a larger time step I am defining 0.5 because this is an implicit technique.

So I am going to say for m=1:80 so that we are going to go the same 40 time steps, c hat which is the Fourier transform of c, okay so and for i=1:N so in the Fourier space what we are going to do if i-1, is less than or equal to halfN k which is the vector is (i-1)*delk and if (i-1) is greater than halfN then k=(i-1-N)delk. So this is the place where we have implemented the periodic boundary condition the reason why we have taken i-1 is we want to include the k=0 point, okay that is in the Fourier space we are having – π/a to π/aall k values.

So basically that –π/a to +π/a is taken by making sure that if it is often we are going to take k to be positive, if it is greater than halfN then we are going to subtract the end so that it becomes negative, so this is the two parts and while doing that we want to incorporate the zero point also so that is done by taking i-1 okay, so that is the periodic boundary condition implementation. So once we have k you can calculate the k^2 as k*k, okay.

So now we have k^2 because we are solving the diffusion equation k^2 is all we need so c hat of i is nothing but chat(i)/(1+2*k^2*dt), right so this is okay, or you do not see why we should have a to know it is dk^2 Δt so it is 2 is not needed at least not in this part so endfor, okay. So we started the time loop we Fourier transform the F and we calculated the vector and we calculator k^2 squared and the evolution is C/1+$dk^2\Delta$t so that is what we have taken endfor, what do we do we take the composition to real space this is a real(ifft(chat)).

Now it is really not necessary in this case at least that you can take this Fourier transform outside the loop you can do everything and then you can come back to real space and come out. But the reason why I have done both the Fourier transform and the inverse Fourier transform inside is that this becomes essential if you are doing the Cahn-Hilliard equation so becomes easier to then compare.

The other reason is there are numerical errors that can creep in so you take the c to Fourier space and you keep doing this so the function is completely real in real space, but it might accumulate

some imaginary parts so by doing this every time Fourier transforming back and taking only the real part then we are making sure that those errors do not grow so that also becomes important sometimes, okay. So now I say plot(c) so this is the code which will do diffusion equations using Fourier transform, right.

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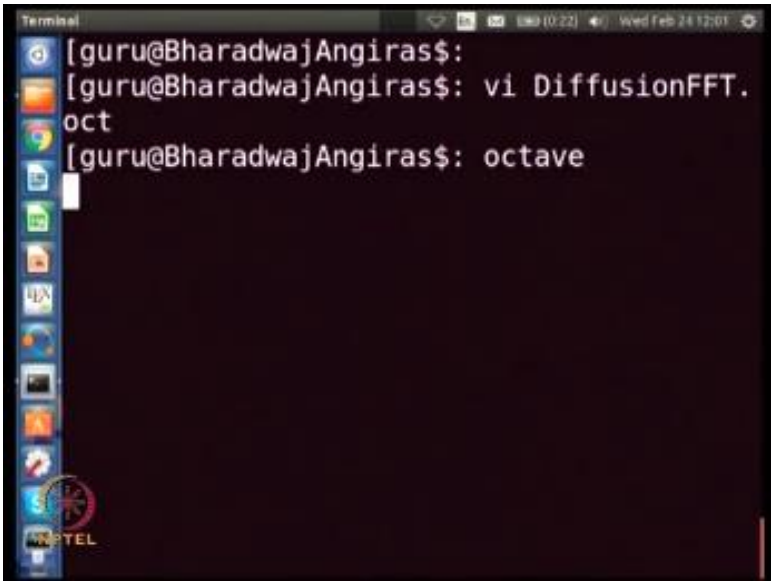

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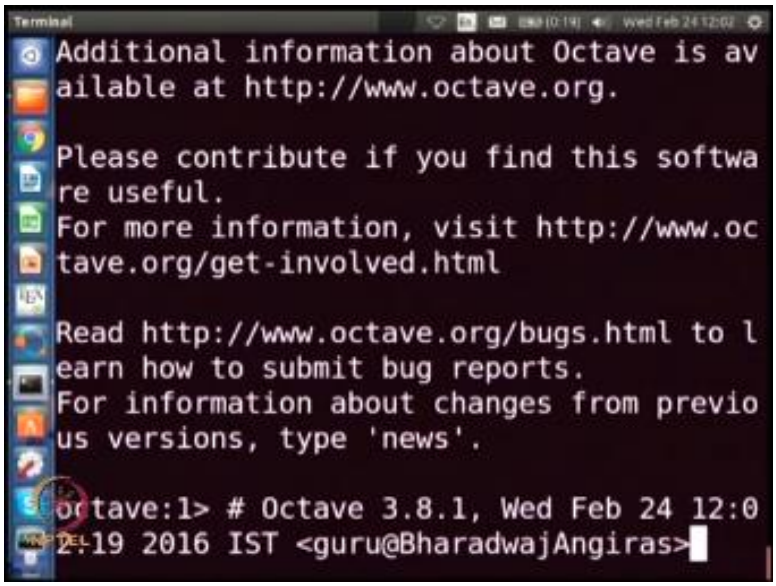

So I say diffusionFFT.oct, okay so there is some error okay the error is here so plot c it should become, okay. So there is an extra so the if loop if i-1 is less than halfN yeah, here there is a this thing that is missing so let me put that if i-1 is greater than halfN so that completes, okay.

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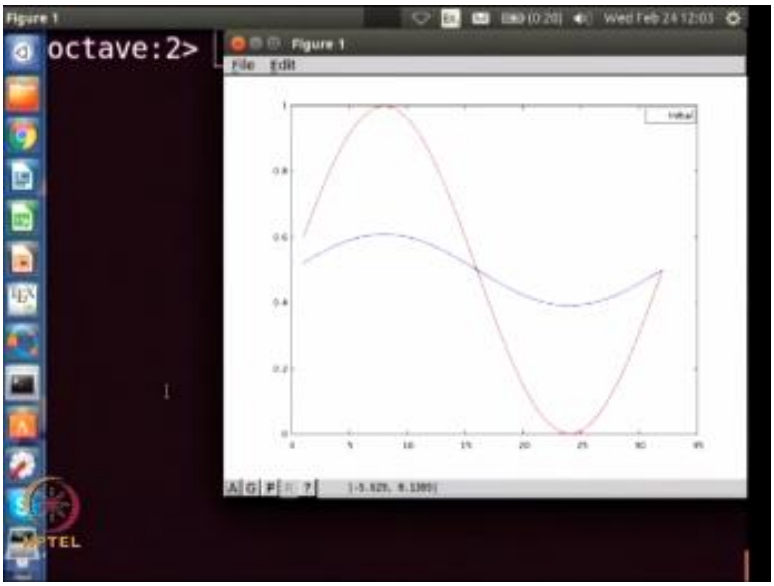

So first thing you notice is that the solution came out very, very fast because instead of running 40,000 I am just running 40, 80 time steps and you can see it is the same solution so this is the initial profile I had and this is the final profile I have, right initial profile was red in this case and final profile which is blue so you can see that it is moving towards homogenization.

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Now let us go to the same thing, same initial profile and okay, let me copy the diffusion.FFT to Cahn-Hilliard FFT.oct okay. Now Cahn-Hilliard FFT.oct what is the difference, so the difference is that now we have to calculate a g and we need to do Fourier transform on that so clear all clc, clf N is 32, dx is 1, m is i so they are all the same so we have taken that, and we have taken the initial profile I have plotted the initial profile and I said the hold on N halfN that delk I have defined dt I have defined and I go to inner loop the first thing that I have to do is that h is equal to I have to define what is, so we called it g so let us call it g, g=2*c*(1-c)*(1-2*c), okay.

Now so this is should be all .*, .*(1.-c).*(1.-2.*c) okay, so it is very important so that each component wise it does and it still says it as g. So now ghat is nothing but fft(g), right chat is fft(c) so now we go in and we do the same thing so we define the k vector and we calculate k^2 but we also need k^4 which is k^2*k^2. Now chat is nothing but a chat, okay so now we have this – k^2dt*k^2*ghat), right so we have that divided by 1+2*k^4 so this is the 2 is coming from the fact that when you write the Cahn-Hilliard equation you have this $\kappa \nabla c^2$ so you get $2\kappa \nabla^2 c$ so this 2 is coming from there, so κ is one but we have taken 2.

So sometimes we will take κ to be half so that also becomes 1, but we have taken it to be κ to be 1 so this 2 is coming from the Cahn-Hilliard equation which is $2\kappa\nabla^4 c$ okay, so that is the 2 that we have it here, okay so $1+2\kappa\ \nabla t$ so we have and again we so this is the reason why in the previous case also I put this Fourier transform of c and the inverse Fourier transform of c inside the loop, because unless the c is in real space you cannot calculate g in real space and after that only it has to go to the Fourier space.

So that is the reason why we did, so we go and we save this okay. So now let us run this source Cahn-Hilliard FFT.oct.

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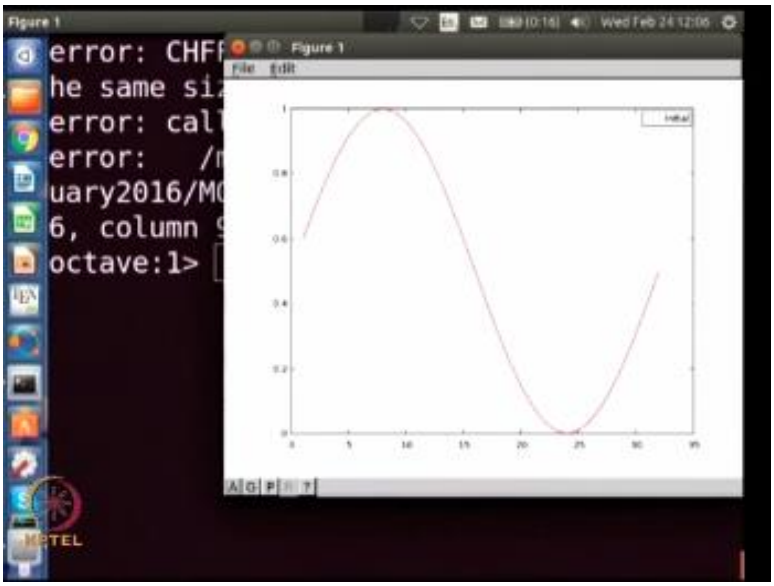

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Okay, so there is a problem what is the problem line 26 column 9 okay, chat, okay so ghat I have to say i right so for every i it has to do it does not know which i it has to do so okay.

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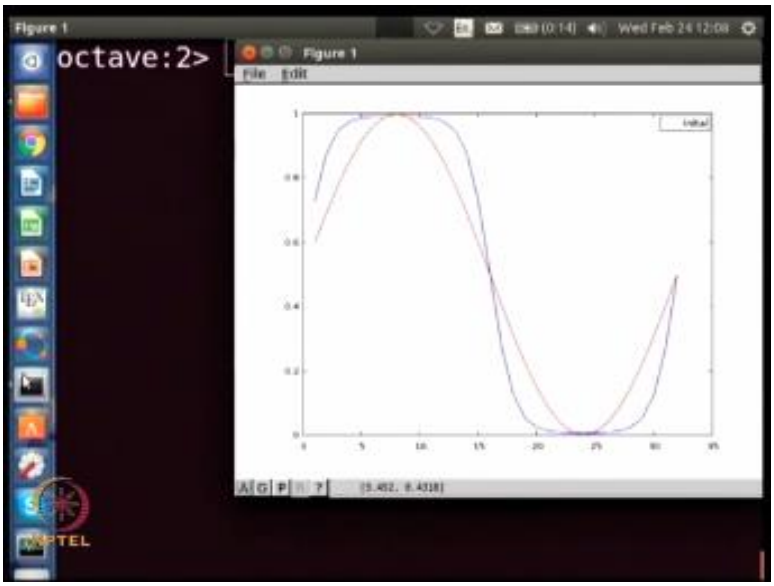

Okay, so now you can see that I started with an initial profile and my profile has become like a box profile, okay. So this is the solution of the Cahn-Hilliard equation, please remember when we solved the diffusion equation the initial profile was like this and the final profile was something that was going towards homogenization. Now we have the A rich regions becoming richer in A and B rich regions becoming richer in B, rather the other way so this is the B rich region, this is the A rich region.

So they are becoming richer in B and richer in A respectively, and you have this interfacet hat is formed between the A rich region and the B rich region so the interface region is the region where the composition changes continuously whereas the in the bulk come in the A rich region and B rich region it goes to the compositions of 0 and 1 which is the bulk composition respectively, okay.

So it is still not evolved completely so when it evolves completely you will see a perfect one which is going to 1 and then it will have an interface and it will go to 0 and it will come, this is what we have looked at but this will not happen for all wavelengths to show you that I would like to change the number of wavelengths.

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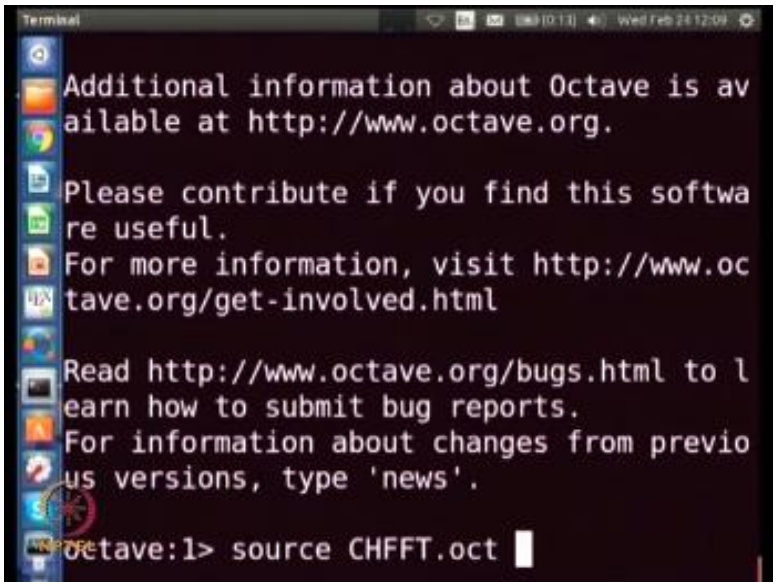

So let us try to do that Cahn- Hilliard FFT dot so let us make m=2 and let us see what happens okay.

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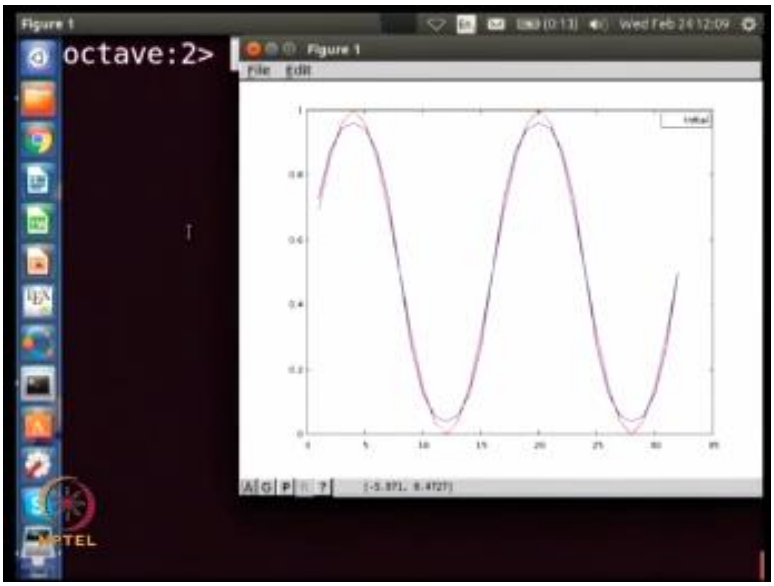

So initial profile has to this thing and you can see that the final profile is actually going towards like in the case of diffusion, right so this is coming down instead of becoming a box profile, okay.

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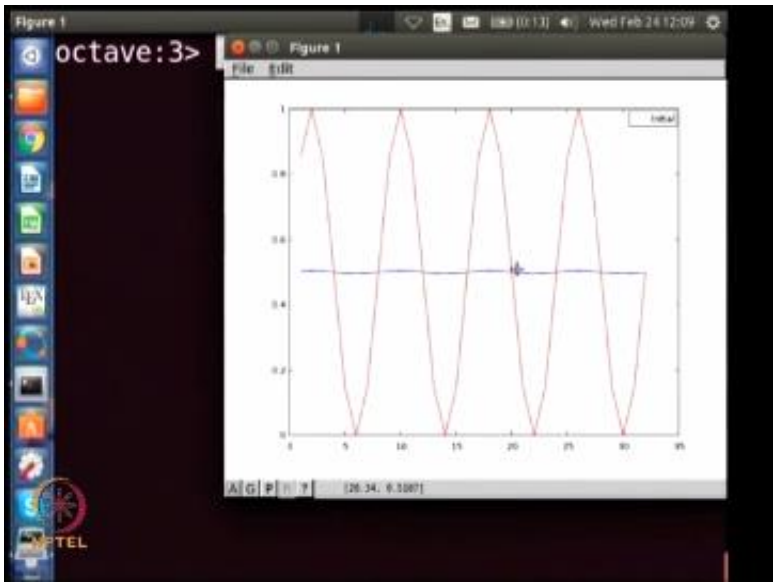

And you can see suppose if I make it m equal to some 4that is still smaller wavelength then you will see that it becomes okay, so this is the initial profile everything has become flat. So which means in the case of Cahn-Hilliard depending on the wavelength the some wavelengths are going to grow you saw one wavelength m=1 that wavelength group, m=1 the wavelength was 32 because we are taking a system size of 32. Now when I make four ways the wavelength is 8, 8 is not growing and we also saw one with 16 when I took m=2 that was not growing, okay.

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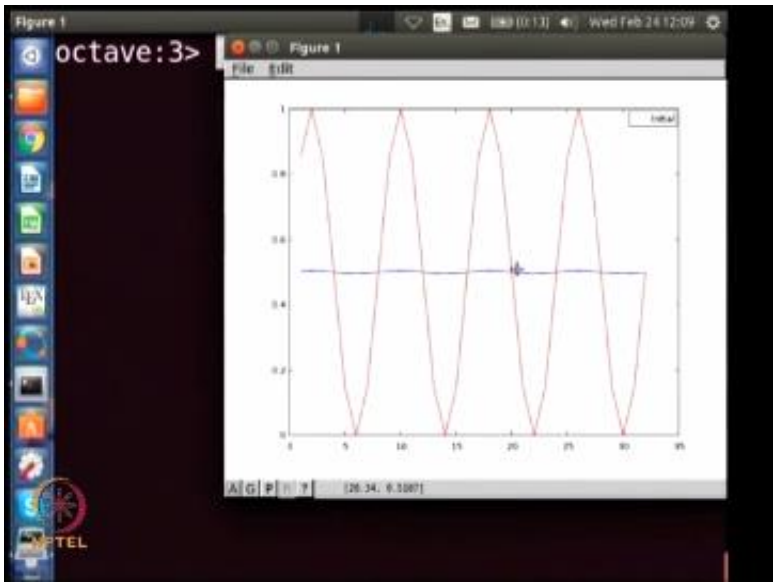

So this clearly indicates that in this case certain wavelengths will grow certain wavelengths will not grow and these smaller wavelengths will be the ones which will not grow. The lowest wavelengths that grows basically sets the wave length limit above that everything will grow 32 grows so if you have something like 40, 64 ,128 they will all grow but whatever is less than 32 16 itself was not growing so the rest of them will not go. So this is the solution for the Cahn-Hilliard equation unlike diffusion equation.

You know diffusion equation the 32 itself was going and anything higher you take also will grow so whatever be the wavelength they will all go to homogenization that is the nature of solution in the case of diffusion equation. In the case of Cahn-Hilliard equation it can go to this homogeneous solution or it will grow depending on what is the wavelength that you are considered, okay so this is important this is what we discussed by looking at the growth rate or beta and this is getting the same thing numerically, okay.

Now there is one lost piece I would like to do with this before we end this lecture, so in the next part of this lecture I would like to take the fast Fourier transform code for Cahn-Hilliard and try to calculate what is the interfacial energy for the system, okay so this system supports interfaces

when m=1 for example it is supported an interface and I would like to set up a system in which I will produce two interfaces and I would like to find out what happens to the interfacial energy, so that is what we will do in the next part of this lecture, thank you.

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