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

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Module No.16
Lecture No.64
Interfacial energy in CH

Welcome we are looking at the phase field equation, we said that the phase field modelling actually incorporate the interfacial energy. So it is very important to understand where the interfacial energy is coming from in this model. So that is what we want to understand in this part of this lecture.

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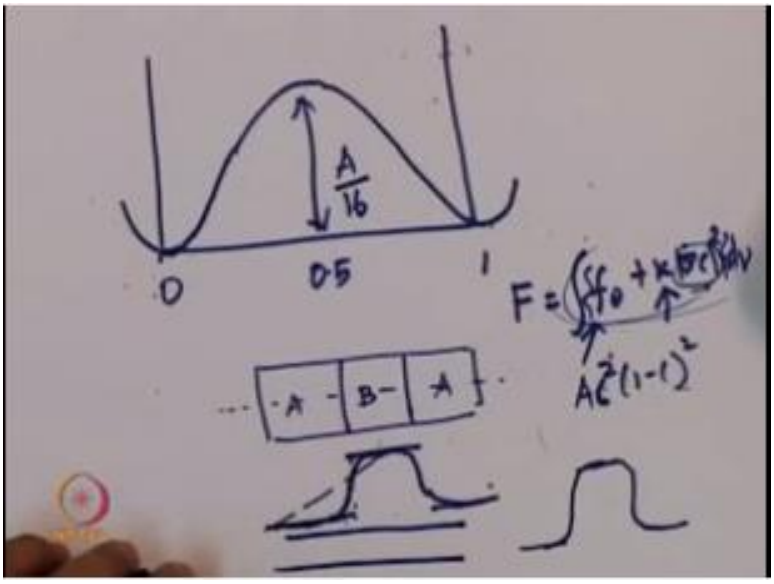

So let us consider the free energy, the bulk free energy density that we were looking at. So it had a 0, it is a minima at 0, it had a maxima at 0.5 and it had another minima at 1 right, this is 0, this is 1, this is 0.5 okay. Now consider a system which is what we are going to solve okay, so it has this to be the A rich region, this to be the A rich region, this to be the B rich region. So I am going to start with the profile.

So if you look at the initial profile it will look like that, remember this is consistent with periodic non condition okay. So this is the profile that I start, in the case Cahn-Hilliard equation you saw that the profile is going to setup like this, so it is going to become like this. Now if you look at what happens in this profile, let us look at a bulk region, what happens in the bulk region, this is our free energy, we said it is f0+k (∇c^2)dv right. So this is what we are looking at, now in this region, because I have taken my minima to be here at 0, so when the composition is 0 that is 0, and this f0 which is nothing, but $AC^2(1-c)^2$ this becomes 0 at C=0.

And because there are no gradients, because composition is uniform here $\nabla C=0$ so the f=0. So in pure bulk A rick region, the free energy is 0. In a similar fashion, if you look at where composition is 1, you can see the F is again 0, because 1 if you substitute in $(1-c)^2$ that term is

going to become 0. Again there are no concentration gradient so that is also going to be 0. In the region where it changes from either 0 to 1 or 1 to 0 there are contributions that are coming.

One contribution is that the bulk free energy which is this contribution is going to increase, because you are going to sample points with all this composition right, any region with this bulk composition will have higher free energy as compared to this. So this is going to have a higher energy, because remember I mean this is the barrier and this barrier height was decided by A, it is A/16 because if you put 0.5 here it is $0.5^2(0.5)^2$ so it is $(0.5)^4$ that is $(½)^4$ so A/(2/4), A/16 that is the barrier height.

So it is going to get to sample these regions. So suppose if this composition changes abruptly suppose I can keep up to this as 1, up to this as 0 and then the composition changes adruptly then the contribution from this will be very low, because it will be 0, but the ∇C term which is the gradient term is going to become infinity. So when this is 0, this becomes the infinity. On the other hand one can say that from this point to this point okay, the composition right, what have I done, I have made the ∇C as small as possible.

So the contribution from this part is going to become very low, but because now it is looking at compositions of all these points, most of the points are away from the minima, so there is going to be huge contribution, that is going to come from the bulk region okay. So now that contribution is going to become very large, so the system is going to adjust the ∇C the gradient and composition in such a way that most of it, it will keep it clear, because this is also 0, this is also 0.

But it has to support an interface from a B rich region and an A rich region. So in that region it is going to choose that ∇C which as compared to this will minimize the energy. So if it takes very small ∇C then it will have lot of contribution from here, if it takes very large ∇C this contribution will be lower, but there are ∇C contribution will be high. So the system chooses an interface which will be an optimum of these two.

In other words, the A in the F0 and k here in the ∇C term together determine what is the interfacial energy. Now thermodynamically the interfacial energy is the excess free energy. So how do we define, we define it as the free energy of a system which has just this A and just this B you add them up to subtract from a system which has these interface. And now we have two interfaces, so it will be the interfacial energy will be two times the interfacial energy okay.

So, but we know that for the bulk we have setup the free energy to be 0. So if you measure this quantity integral of $F0+k\nabla C^2$ for a system which develops these interfaces that is the excess free energy associated with the interface itself, because if I take an all A or all B then I would have gotten 0 from this. So now because I have some part A and some part B, the interface forms and the excess free energy associated with the interface is just obtained by the evaluation of this free energy.

So that is what we want to do now, and in this case I do not want to take a initial profile which is a sinusoidal, but I want to take an initial profile which looks like this. That is the code that I have.

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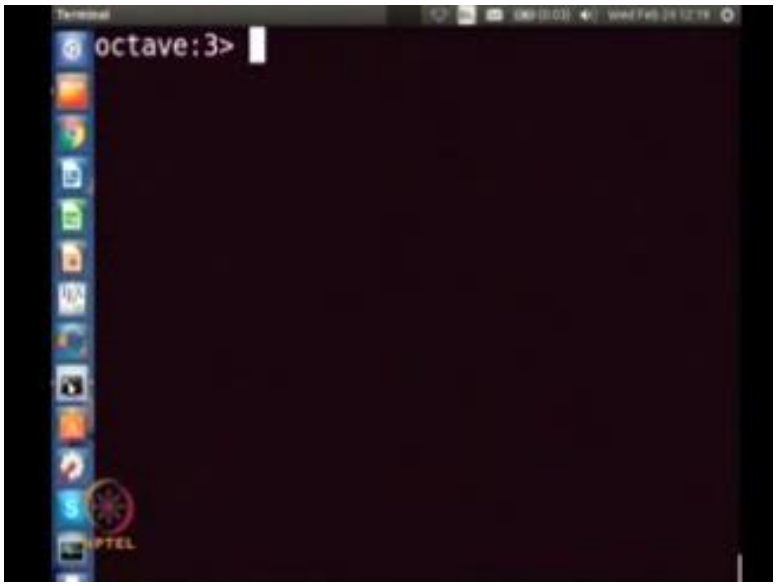

So let us take the.

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FFT Cahn-Hilliard code that we had.

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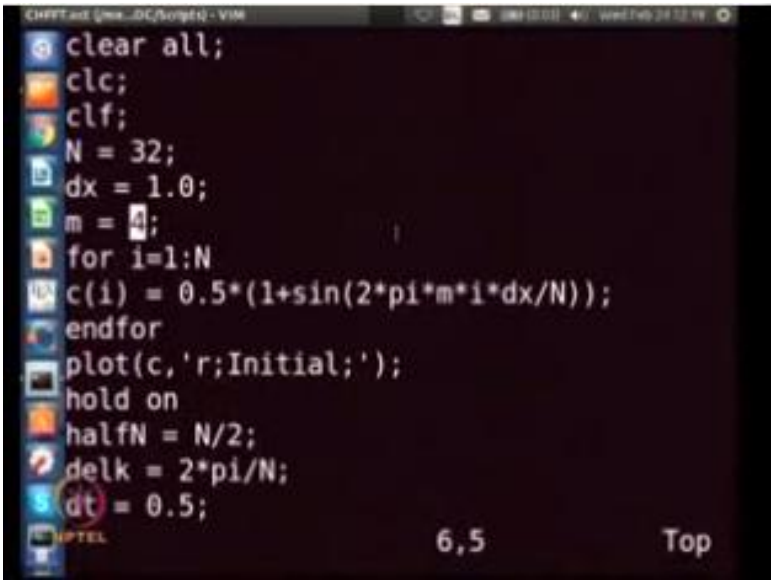

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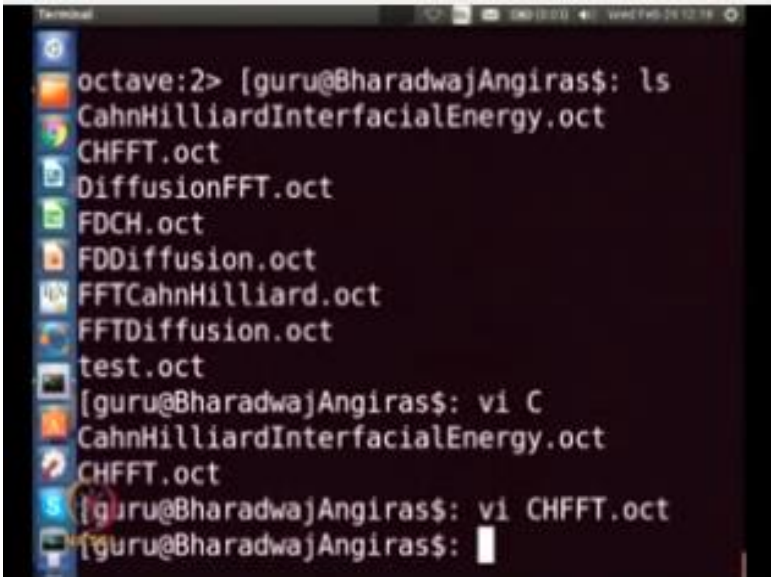

Called this Cahn-Hilliard FFT.oct so I am going to say interfacial energy Cahn-Hilliard.oct vi interfacial energy.

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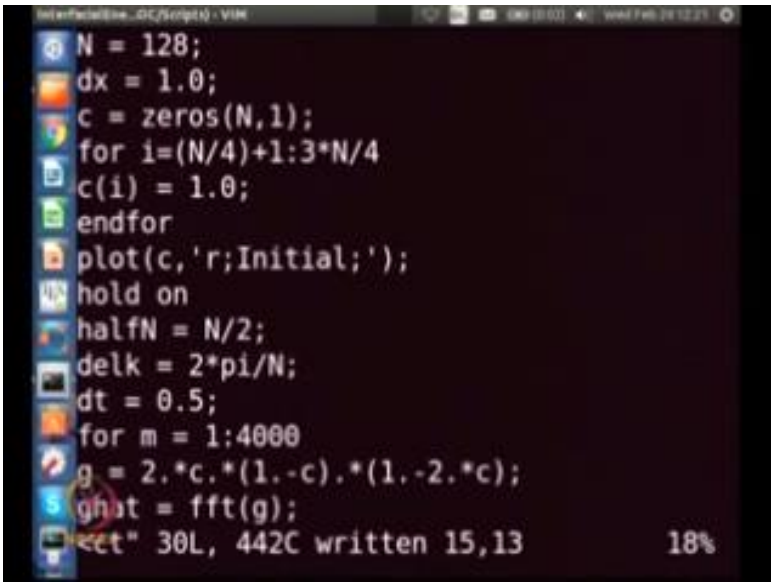

Cahn-Hilliard, so I am going to take it on a bigger system okay, and I am going to change the initial profile, so do not want any m. So I am going to make the initial profile like this for -=N/4+1 that means what quarter to 3N/4, s quarters. I am going to say c(i) is 1 and so for the first quarter and the last quarter I am going to make the composition to be 0, so I want to first define c=zeros (N, 1).

So I have 128 so I have defined a composition which will be vector with 128 zeros of which the first quarter and the last quarter I am going to leave it as 0, but the middle half I am going to put as 1, so this is the initial profile okay. So we plot the initial profile, we evolve the system and now we need to run for long time because we want to achieve equilibration.

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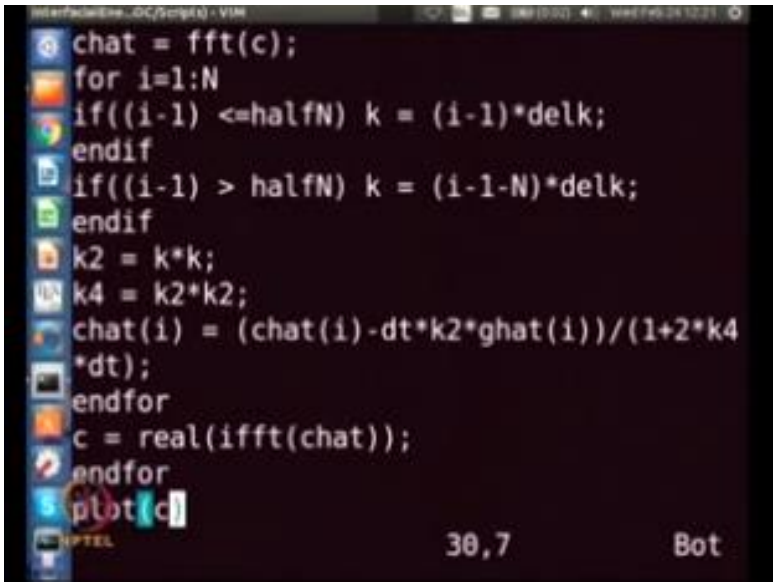

And once we get that, so we get to the solution, we will plot the final solution. After this is where I want to calculate the energy, now energy calculation means that we need to calculate $AC^2(1-c)^2+k\ \nabla C^2$ at every point and you add that up. So that is basically the excess free energy itself, because for the bulk phases the free energy is 0, if I integrate this quantity that will be the bulk free energy itself, so that is what I want to do now.

To do that now I know the final composition profile. So I am going to do the Fourier transform of composition, I will tell you why I do this. FFT(c) okay and I implement the periodic boundary condition stuff, so I am going to take these four, five lines and I am going to put there. So I am going to put the 5 lines here, so I am going to implement periodic boundary condition for doing.

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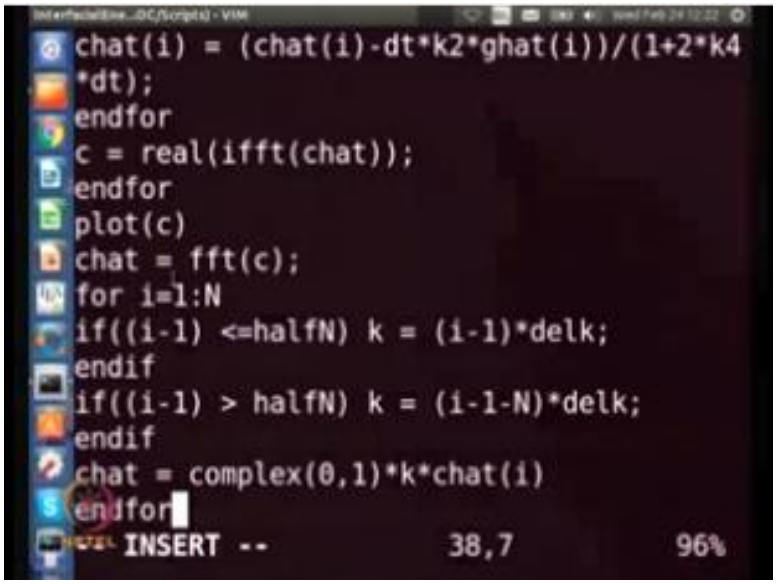

What I am going to take the chat = complex (0, 1) multiplying k, multiplying chat of i okay end for okay. So what is being done here, see I want to calculate the concentration gradient, because I can do Fourier transform if you take concentration to be C and if you are in Fourier space so you can see that.

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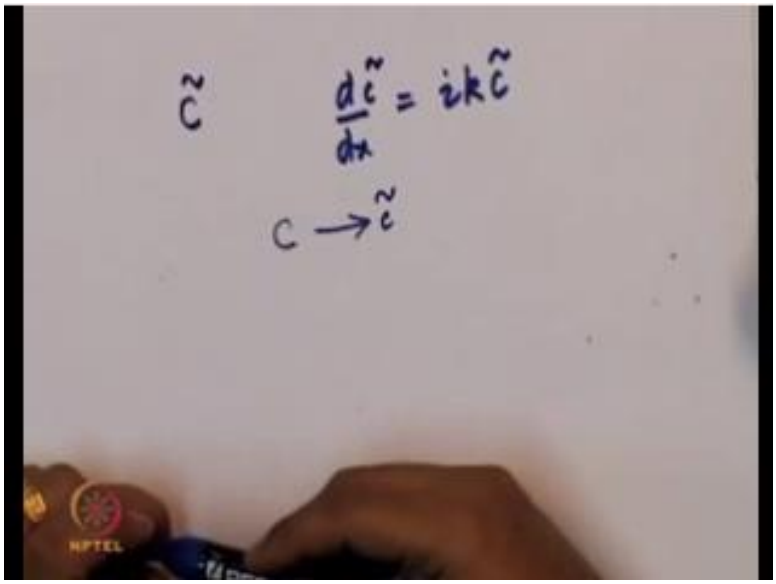

Suppose if I have C tilde right, if I have C tilde then d/dx of C tilde is nothing, but ikC tilda. So if I take the composition to C tilda then the derivative of the composition is just obtained by multiplying with ik and taking the inverse Fourier transform, so that is what we are trying to do.

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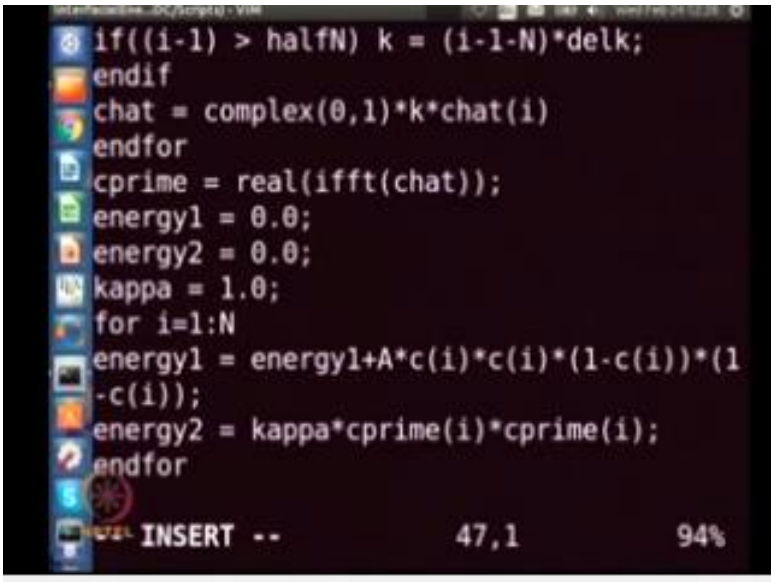

So I will take the inverse, so this complex 0,I means the complex number which I am multiplying with k okay. So now with this, so we have the Fourier transform quantity, so if I take this now back C' is nothing, but real of iFFt(chat) okay. So if I do that then I calculate the C' quantity right. So now I have C at every point, I have now the ∇C at every point $\partial C/\partial x$ at every point.

Now I can calculate energy, so I am going to say energy is equal to 0.0 okay. So I am also going to do another small test so let us split energy into two parts, energy 1 is 0.0, energy 2 is equal to 0.0. So for i=1 to n what are we doing we are saying that energy 1=energy 1+ A is 1, A*A.*c(i).*c(i) okay, okay c(i0 we are doing, so .* is not required c(i)x c(i)x1-c(i)x1-c(i) right. So what is this energy, this is the energy that is associated with $AC^2(1-c)^2$ okay.

Now what is energy 2, that is nothing but the k, so I think I have defined k somewhere let us make sure that we define the k okay I have not defined k, so k is 1 so I am going to define it anywhere here, so k=1 because later it will be useful. So kxC'(i)xC'(i) so this is the second prime end for. So now I want to write down the total energy.

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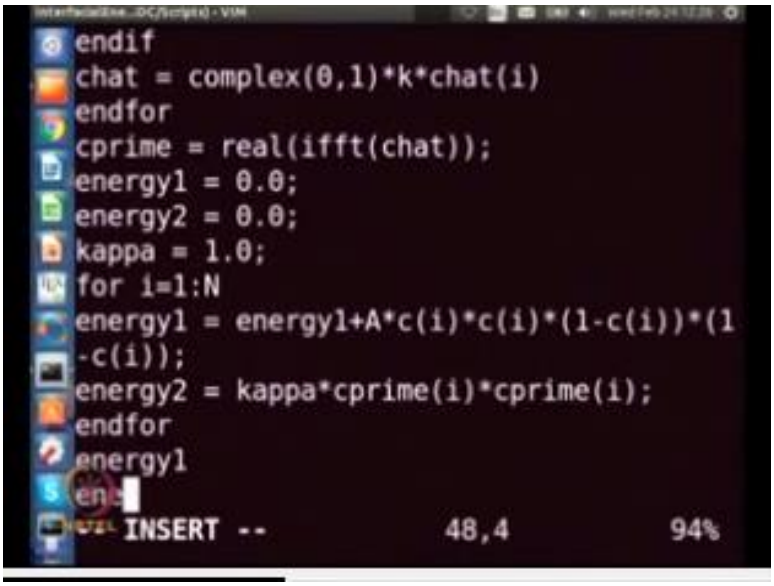

So energy 1 I want to print energy 2 I want to print and 0.5 times energy 1+ energy 2 I want to print. Why 0.5 because here also it should be 0.5, because there are two interfaces, remember there is an interface at quarter distance, there is an interface at three fourth distance. So interfacial energy is per unit area or per unit length, whatever, so we want to get for two interfaces this is the total energy.

So for one interface this is half the energy, because everything is symmetric okay. So we want to get this as the energy, so want to print out these three quantity, so that is what we want to do with this.

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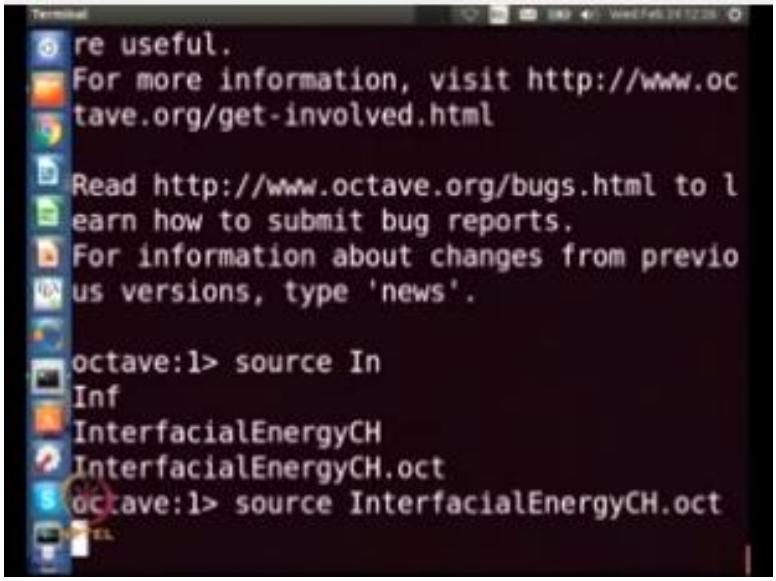

So let us go and source interfacial energy CH.oct okay.

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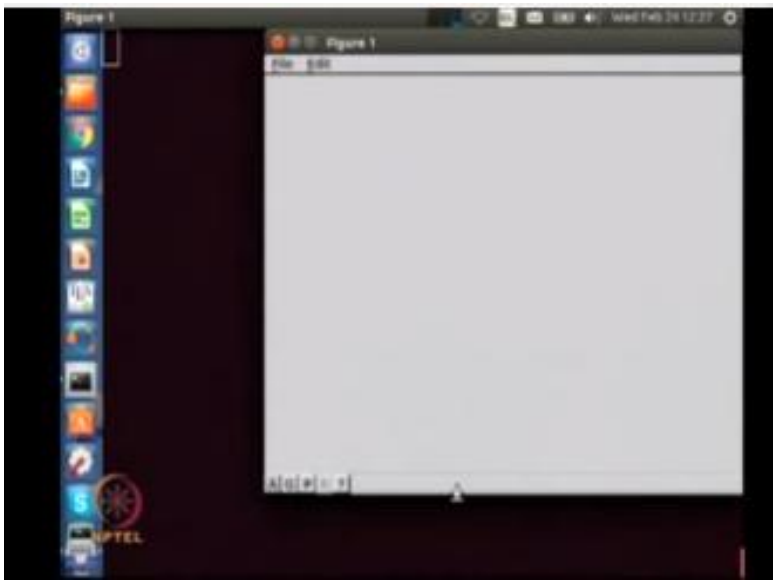

So we are going to see.

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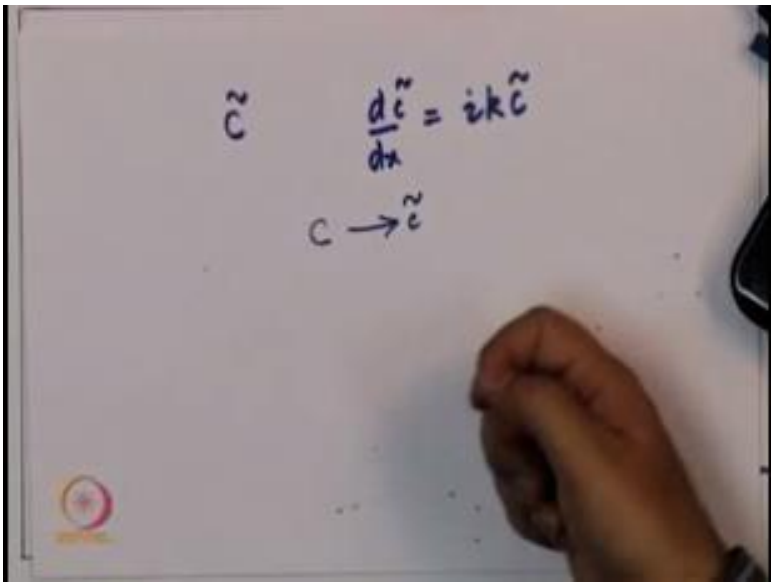

So the free energy if you know the free energy expression you can integrate it, if you subtract the bulk free energies from there you will get the excess energy associated with the interface which is bind of solution of the interfacial free energy. So using our Cahn-Hilliard code we are just trying to calculate that quantity.

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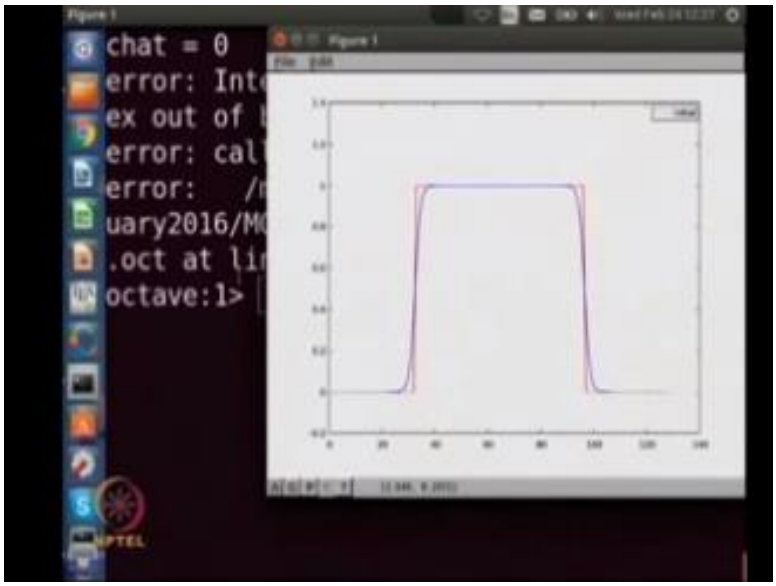

So I got this solution, so you can see that it forms one interface here and another interface here.

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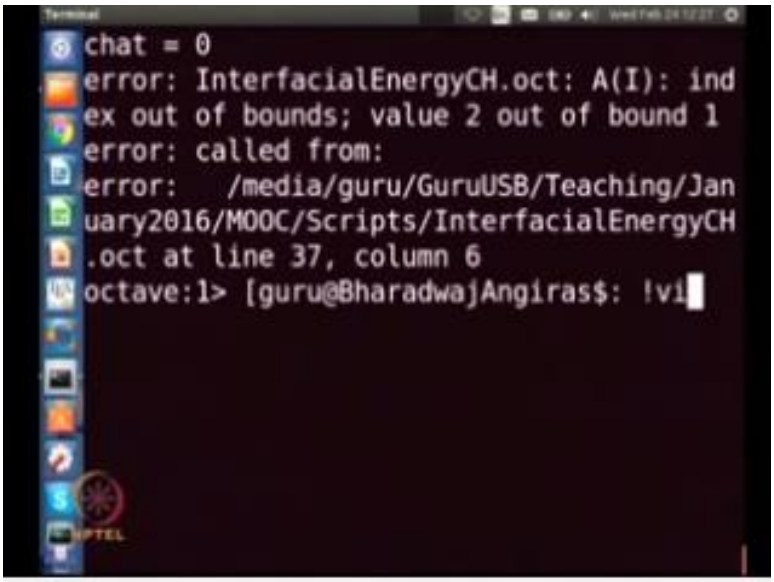

But there is some problem in the code, so let us go find out what is wrong line 37.

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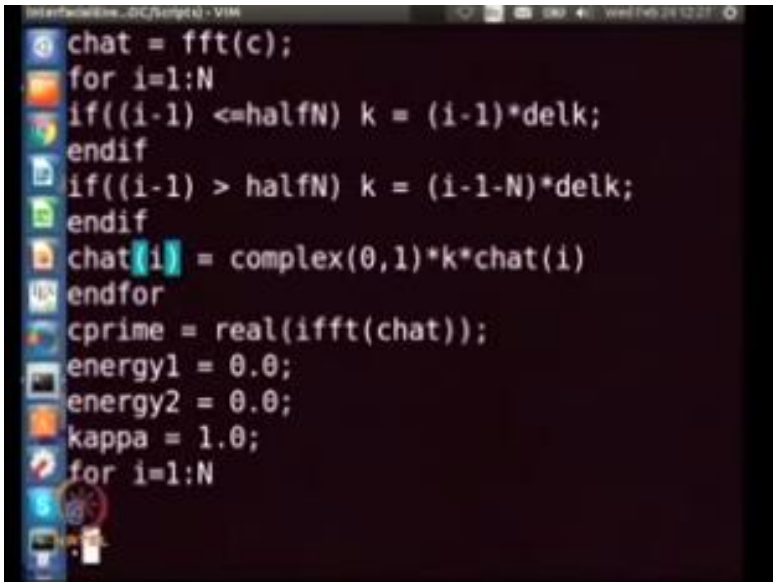

Okay, so I keep forgetting this chat of i is complex 0, 1 into chat of i okay.

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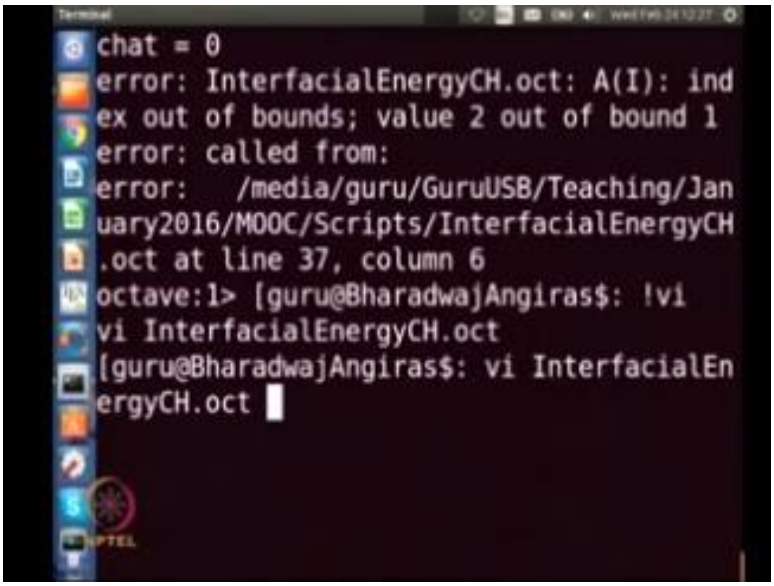

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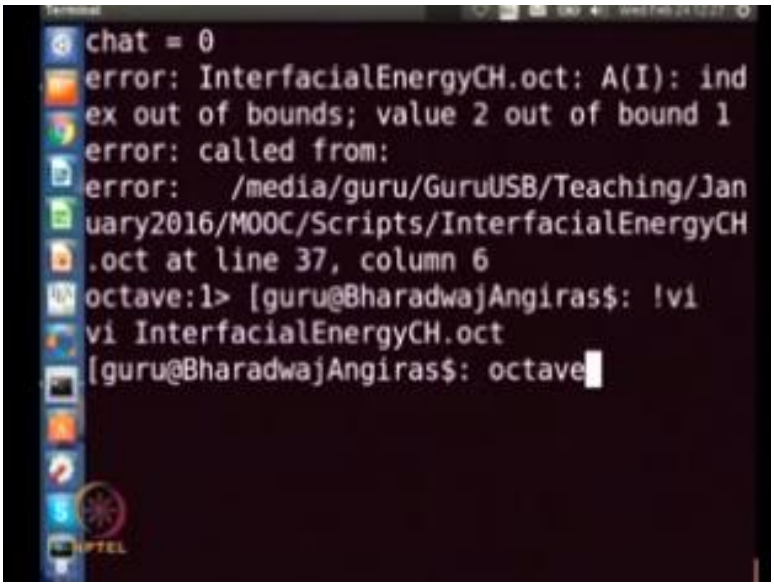

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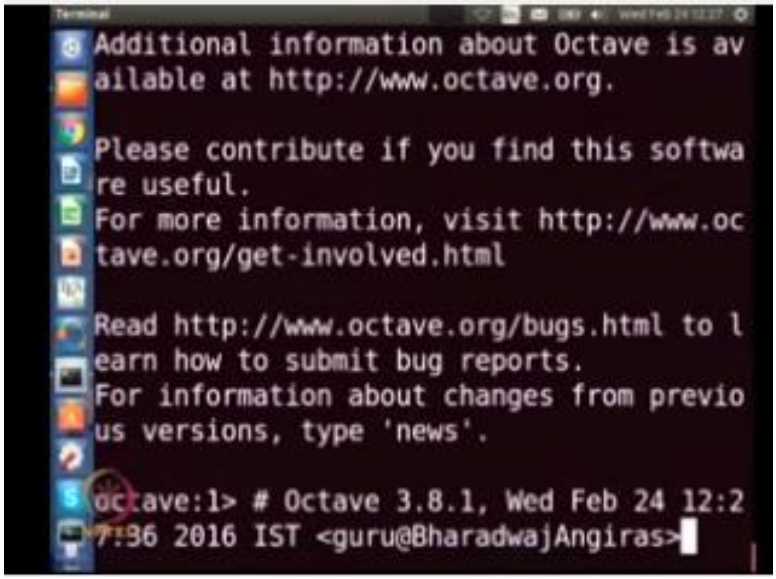

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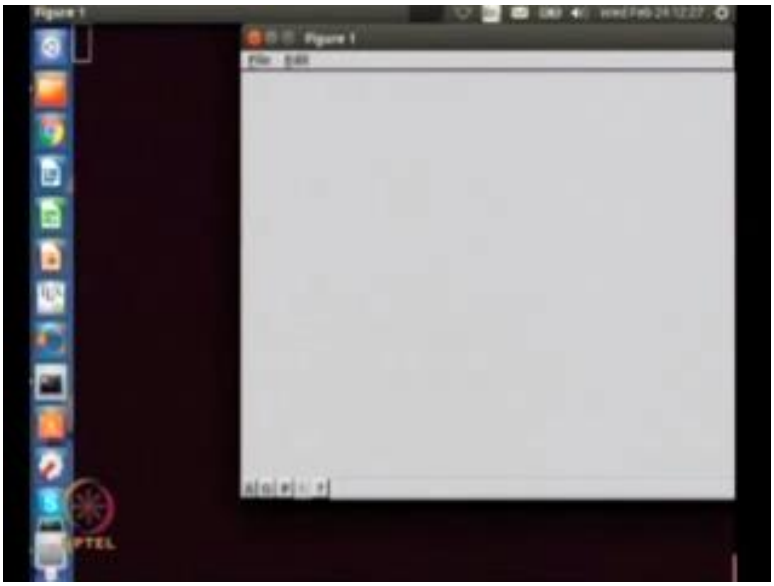

So that is the mistake, so now probably it will give me the solution. So we calculate that, so the trick that we have used is that the derivative, the $\partial C/\partial x$ can also be obtained easily if you have the Fourier transform okay. It is also going to be very accurate, so that is another thing as part of an assignment you will try to do the same thing, but you will calculate the interfacial energy using finite difference formula for the gradient and composition.

And you can see how much is the error, the spectral techniques are very, very accurate in 1D they are accurate as 1/N, in 2D that goes at $1/N^2$ whereas in the case of finite difference the error goes as H^2 okay.

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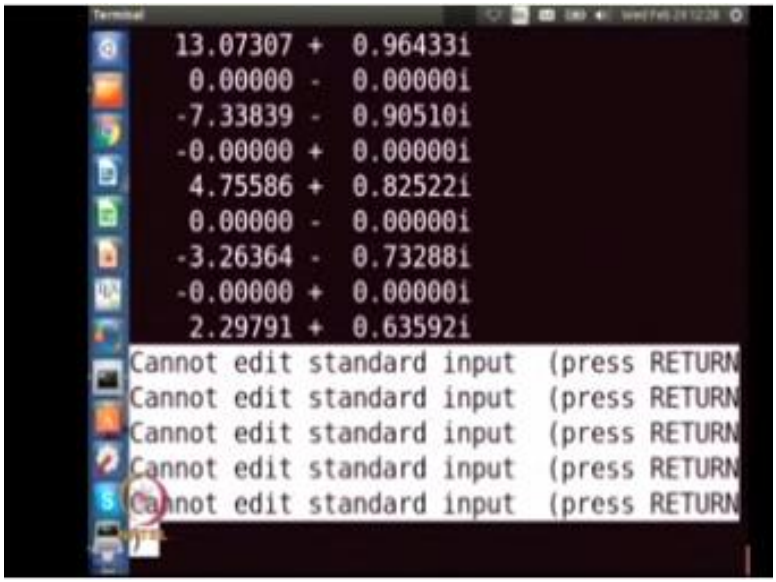

So now okay.

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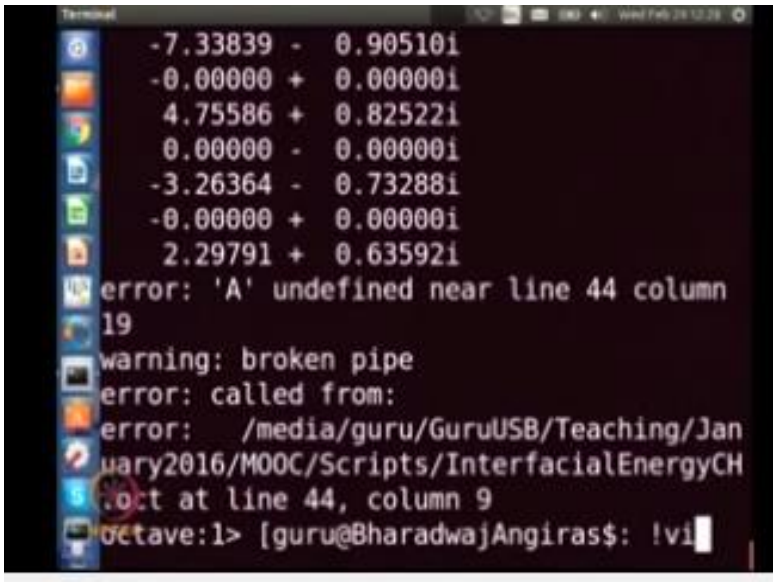

There is something wrong, so a line 44.

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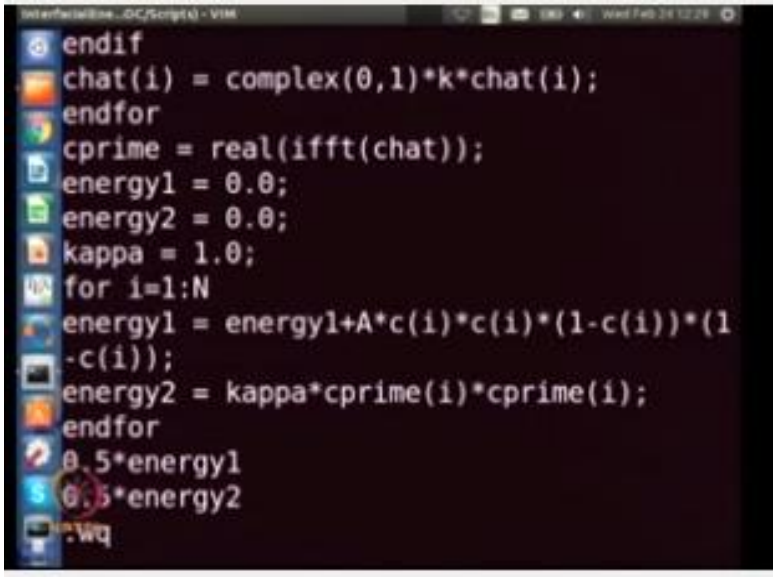

Okay, I need to find out first thing it was okay, so this I do not want, that i okay. So okay I did not get what the problem was, so let is run again.

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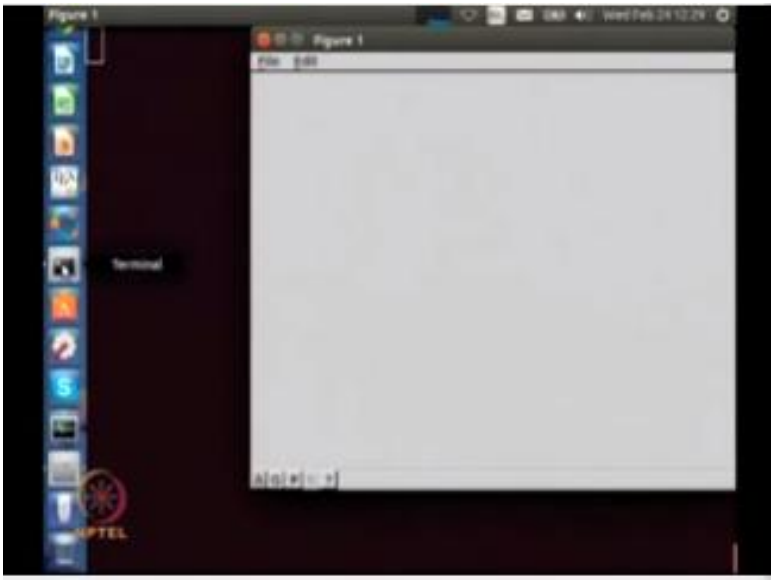

Okay, so there are also ways of solving in 1D atleast some of these things analytically and getting to the solution, which is what we will do in the next lecture okay.

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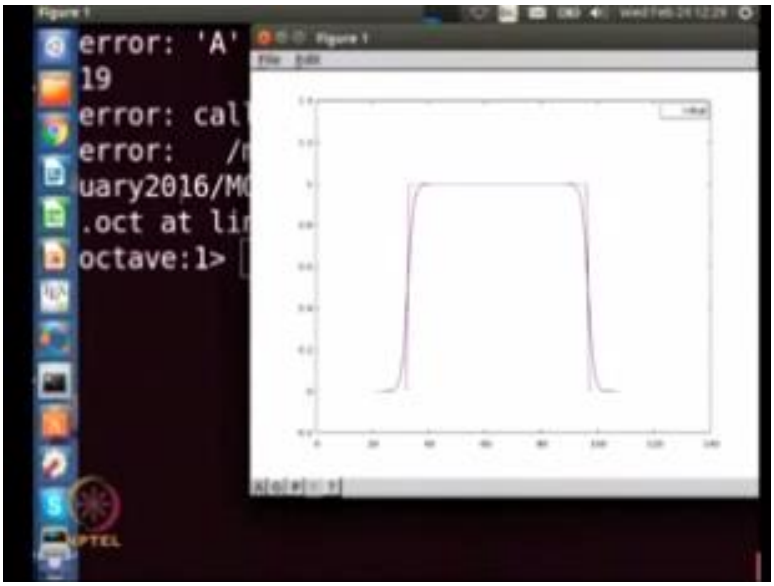

So in this part of the lecture we have done everything numerically.

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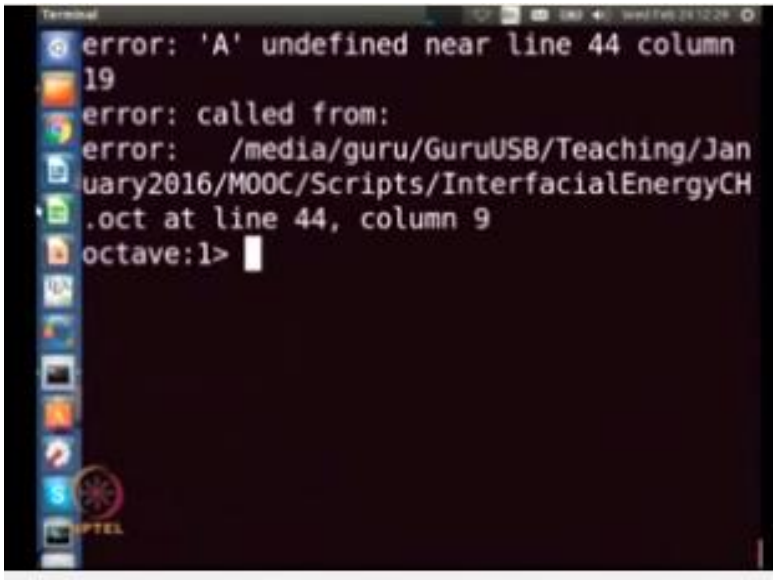

And we are going to do it analytically in the next okay, line 44 there is a problem.

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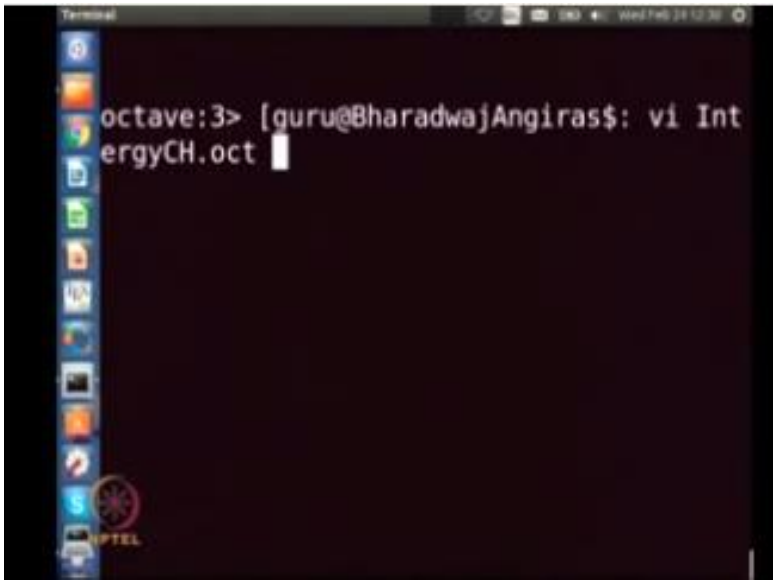

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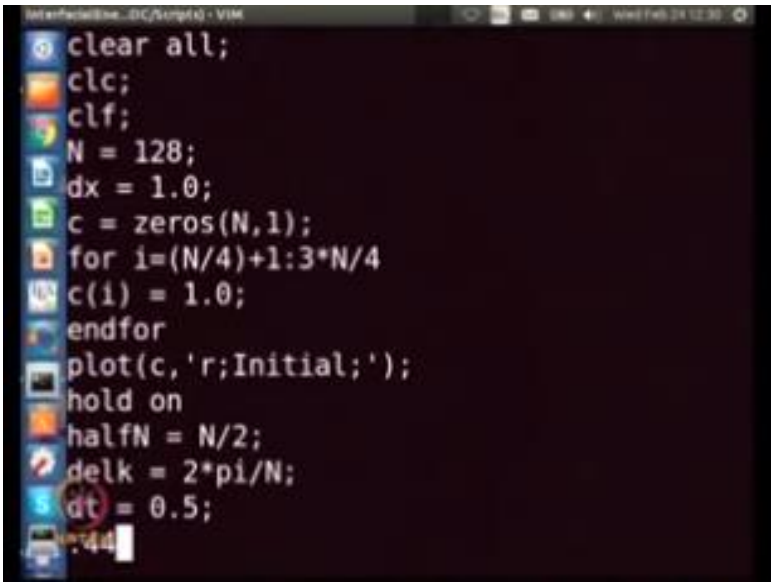

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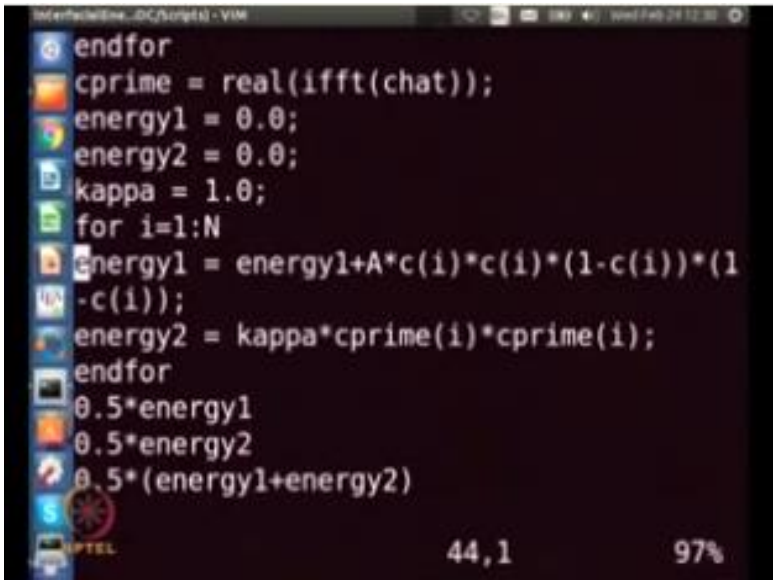

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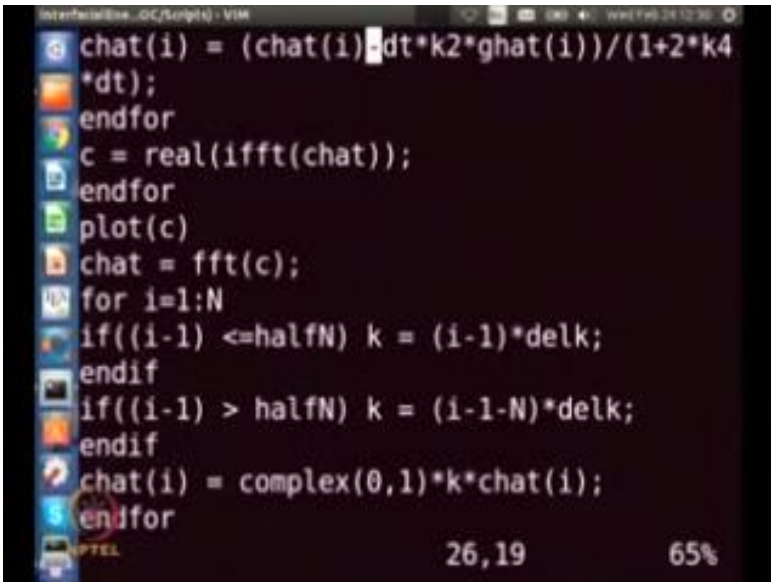

Okay, A was not defined that is the problem.

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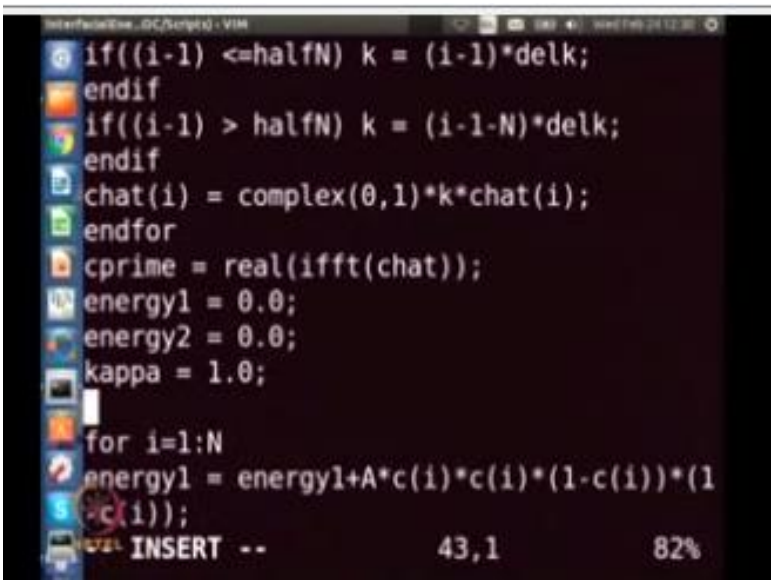

Okay A was also not defined, so let me define A also here A to be equal to 1, because that is what we have used in the.

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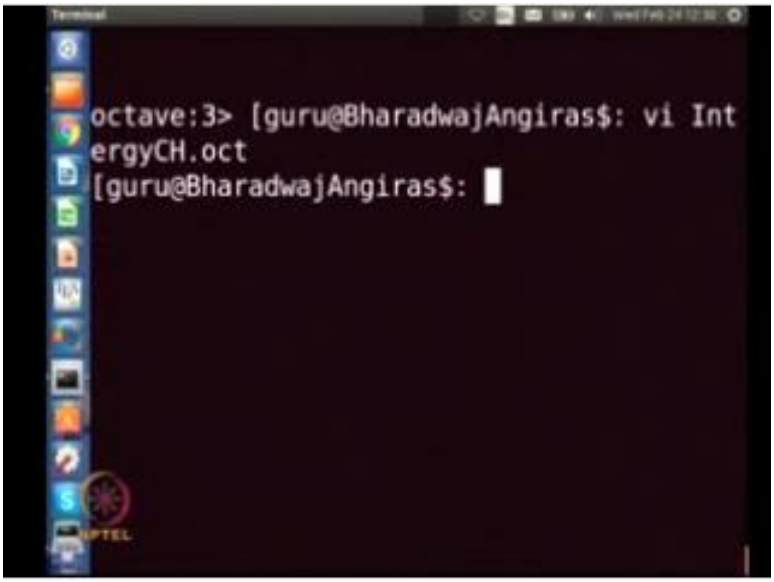

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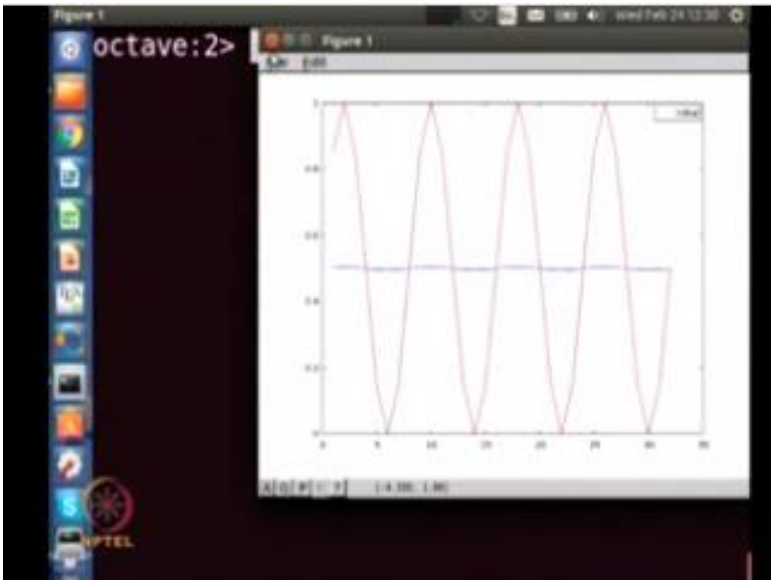

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Sorry, so I run the --

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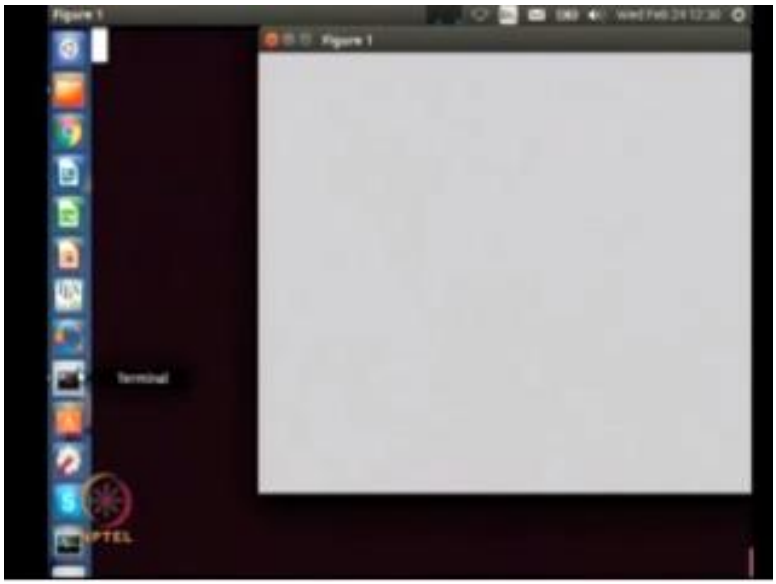

Okay, but one more thing that you can notice is that the Fourier transform technique is also really fast, that is because it allows us to take larger Δt Fourier transform itself is not easy, so it is a costly thing to do, but after you do the Fourier transform.

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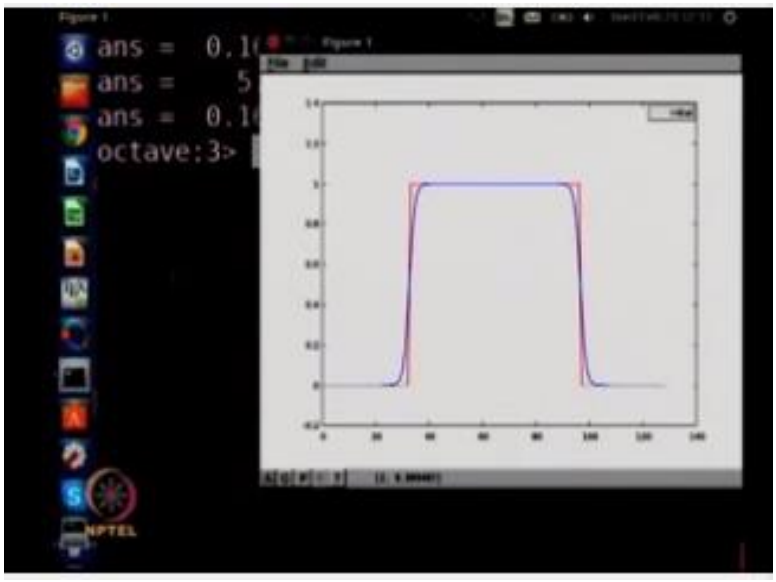

You see that the solution is very fast, because we are able to take larger Δt. So the interface, the red line is the initial one and you can see that most of it is kept at bulk A rich and B rich region. But where the interface was, where I put a very large gradient, you know in one grid size, it went from 0 to 1, now it has made it to be a smooth function. So there is a gradient here, but it is not making the gradient from here to here that is because, you know the gradient term will be very small the bulk free energy density contribution will be very high.

It is not preferring what I gave either, because even though the bulk free energy density was 0 everywhere in this part the gradient energy gave a very large contribution. So it made adjustment between the two and it gave me the solution.

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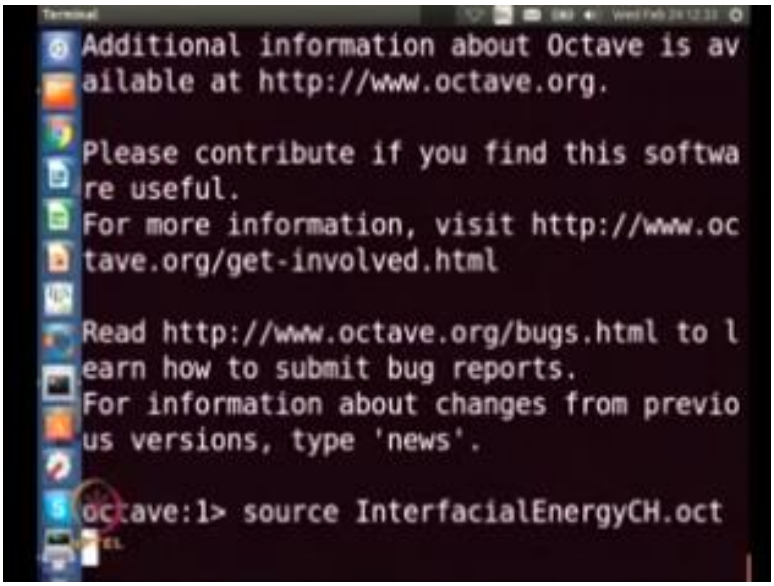

Now if you look at this solution you can see that no, there is something wrong with this, so the second term also should be 0.1666 so the total energy should be 0.3333 okay. So I do not know where the mistake is, let me find out. So we took the Fourier transform of C and we calculated the ∇C and we calculated C' as this okay. So probably I should plot C' with C okay, so I know what the mistake is.

So energy 2 is equal to energy 2 plus I am not summing it up and I am just taking some energy 2 plus right, so that is the mistake okay.

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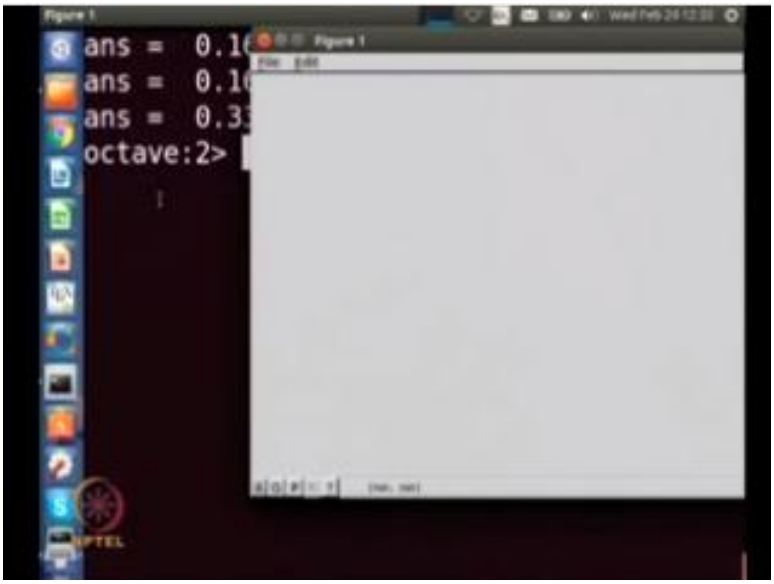

So now I think we will get the right solution finally and the solution when you get so, so you can show when we do the analytical solution, we will be able to show that for the F0 that I have chosen for the kA I have chosen the interfacial energy is one third okay 1/3. And you can see that, that is what the solution we are getting. What is more interesting is that you can see, that the contribution that comes from F0 is exactly equal to the contribution that is coming from $k\nabla C^2$.

That is how the system is actually finding out the interface that it wants and how does it determine what is the interface with either you have F0 or C giving large contribution or the first profile I made were all the contribution the interface as it came from ∇C. So it will keep reducing the contribution from ∇C by making ∇C to be smaller and smaller in the process the F0 contribution will keep going.

The calculation will stop when both the contributions become equal okay. So this we can show analytically which we will do later, but at this point all you need to see is that the contribution between the two is exactly the same. Now you can see what happens, so let us do one small experiment before we stop this lecture. Let us take a k to be equal to 2 and k to be equal to 4 and then see what happens to the solution.

So let us go back to the code, so I want to put this A in k at the beginning itself, so we do not want to put that here, because it is very useful to have it here itself let us define k and A and in the solution also let us put the k and A. So this is dt, so Ghat when it is calculated it should be two times A times ∇C right. So this is where A goes in and this is where k goes in, it is two times k times k^4 okay.

So now we have k=1, so let us run and make sure that our code is working fine and then we will change k let us make k to be 4 for example and see what happens to the interfacial energy and interface with, so both we will look at okay.

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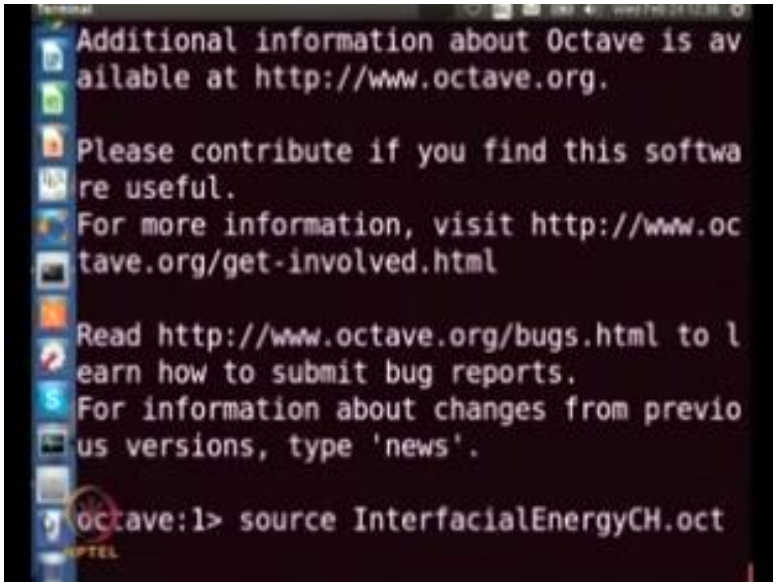

So we get this 0.3333 is the energy and you can look at the profile and so you can look at the profile, the profile is like this right. So it is somewhere between 23, 24 to some 40 or something right. So that is the interface, now let us take this thing and make k to be equal to 4. Now because we have increased k then the gradient contribution is going to become more, so what should the system do. That is what we are going to check.

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Okay, so we have increased k, so the k contribution is going to increase and we know that interfacial energy should be in such a way that both the k contribution and F contribution should become equal, so what happens you can see that it increased okay. Now this is 0.33, 0.33 so it has become 0.6. So when you increased k four times interfacial energy became two times. So it goes as root k.

In the same and you can look at the profile and so I do not see the plot okay, so you can do this exercise and look at the plot of the okay, so there is a clear figure here, so which I just try to know for plot.

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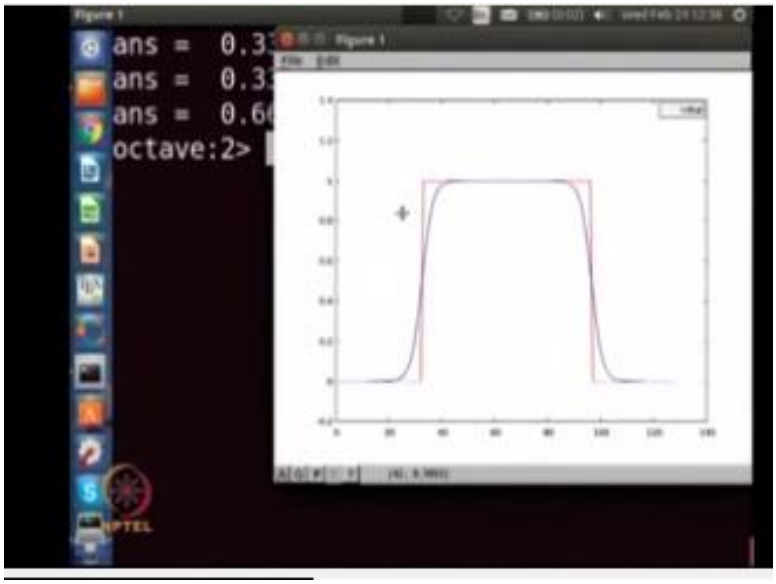

And similarly you can also change the interfacial energy by just changing A instead of taking A to be 1 for example you can take A to be 4, then the contributions from the bulk free energy density is going to increase, so k also should correspond adjust in all cases, I mean whatever be the A k that you take the contribution that comes from F0 terms should be equal to the term, the contribution that comes from k density squared term to the free energy.

So that is the thing that we will show, we will show later, so now you can see that the interfacial width also has increased, so it has gone beyond the 40, whereas previously we have to 40 okay.

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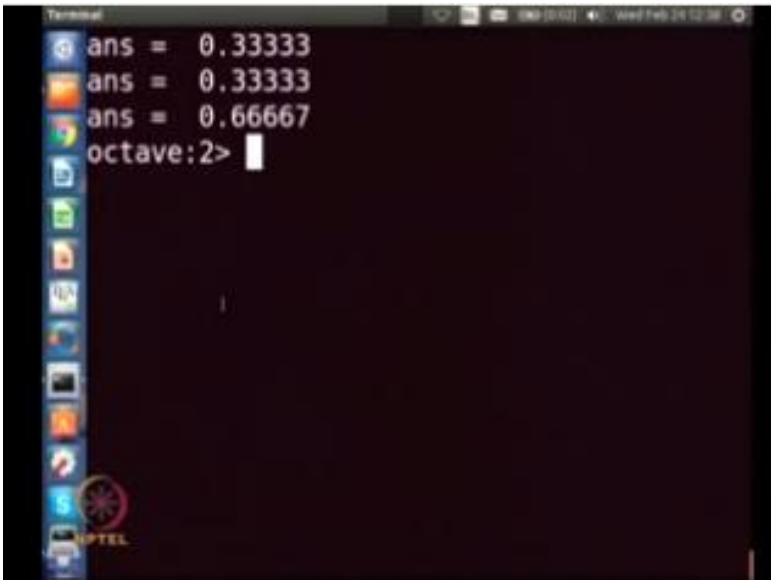

So you can pay around with A and k so I will stop at this point, we will come back and we will look at some of the analytical solutions and analysis of the solution which we will do in the next lecture, which will give us a much clearer picture of what is happening in the phase field model, then we will move on to 2D and most of this course will be done on 2D systems only okay. Thank you.

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