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

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Module No.18
Lecture No.70
Spinodal decomposition in 2D

Welcome we are looking at a phase field modeling we looked at one dimensional implementation for Chan Hilliard equation and Allen Cahn equation so this lecture onwards we are actually going to discuss phase field modeling that is with respect to micro structural evolution how to write the equation how to implement it and how to analyze the solution so this is what we want to do for the rest of this course as a starting point we want to do to classical problems one is spinodal decomposition the other one is order disorder transformation where we want to look at the domain structure evolution.

So this is what we want to do in this lecture to begin with so let us look at what is involved in building the phase field model so you can consider these two cases where we are writing for spinodal decomposition and order disorder transformation the domain structure evolution as prototype problems and whatever is done in this problem is what needs to be done in every problem so the first thing that we want to do is to say that we are going to look at a system we are we are looking at the micro structural evolution in a system let us consider the spinodal

decomposition scenario. So let me consider a system which is undergoing spinodal decomposition so what do I mean by that.

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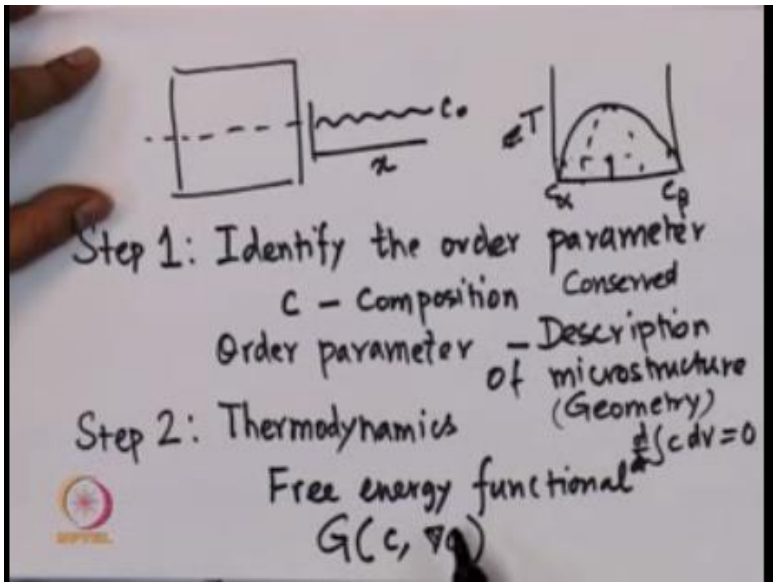

So we take a system initially let us say that the composition is uniform everywhere and so in terms of the phase diagram so inside the miscibility gap so there is a spinodal regime so I choose some other compositions over here okay so because and the temperature is something like this so we start from here so the end compositions are also marked for us so the entire system is taken with this composition with some minor fluctuation so if you go across any line and if you look at composition so the composition is something like this okay.

So this is some c_0 the overall other composition this is the position and this is the fluctuation how is this system is going to evolve is what we want to look at so first decision that we want to make whenever we are writing a phase field model is to decide what is going to be the order parameter okay so that is the order parameter is the one that is describing the microstructure in this system okay.

So step one in phase field modeling is identify the order parameter so in the first case we are identifying the order parameter to be composition this is the case that we are considering now once we identify the order parameter which is basically used to describe so what is the purpose of this order parameter order parameter is nothing but a description of microstructure so wherever order parameter namely the composition becomes this value that is going to be the α phase and wherever it is going to be this value that is going to be β phase and so on.

So we are going to describe the micro structure using an order parameter that is the first step the second step is the thermodynamics so what do we mean by that we want to write the free energy functional in this case functional because it is a it is a functional because the free energy is a function of composition and gradients and compositions okay so this is the approximation we are making it could be higher order gradients as we saw in the derivation of the Chan Hilliard equation it is possible to take higher order derivatives we will probably look at one of those cases late.

In this course but for beginning we want to take a free energy functional and the free energy is a functional that is in terms of the order parameter and its gradients it is written this basically describes the thermodynamics this basically describes that my free energy versus composition the free energy versus composition has a double well and there is energy associated with the interface region where the composition changes and things like that and that it leads to this kind of phase diagram is all built-in into the free energy function.

So first is the geometric description of microstructure is basically the geometry or the topology and the second is a description of the thermodynamics of the system okay now the order parameter that we have identified is a conserved order parameter because composition the integral of composition over the volume if you take with time how it changes that is 0 because integral cdv is sub C_0 it is a constant so d / dt C_0= 0 so we have the description of microstructure we have the thermodynamic description for the given microstructure. The step three is to actually write down the phase field equation so in step two so let us write it in little bit more of detail.

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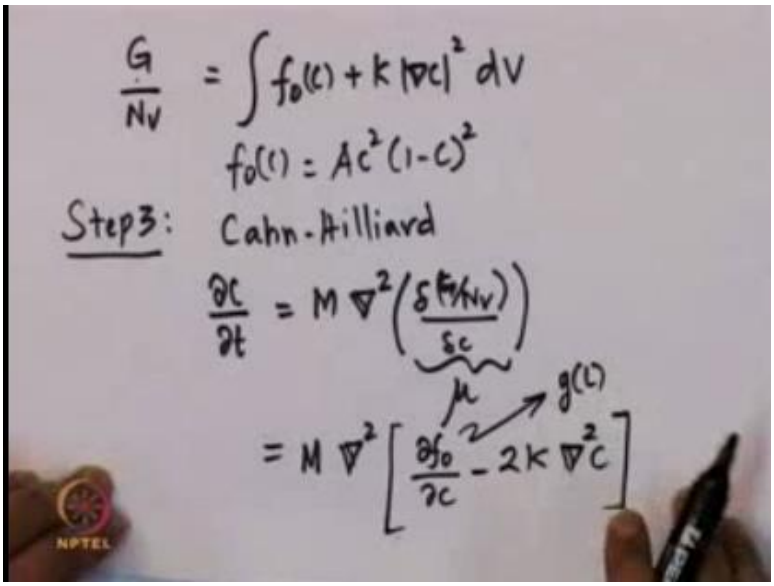

So G(G/ NV) let me say is we have chosen to be f_0 (c) $+\varkappa\nabla c^2$ so dv so this is the simplest that we can think of where f_0 (c) is a function like Ac^2 $(1 – c)^2$ so I now have a description of the thermodynamics now the step three is to write the evolution equation because C is a conserved order parameter we want to write the Chan Hilliard equation what is the Chan Hilliard equation it says $\partial c/ \partial T$ is equal to so I am going to assume the mobility is a constant $M\nabla^2$acting on μ which is nothing but $\nabla G / Nv / \nabla C$ because this is nothing but the μ the chemical potential.

So that gives me $M\nabla^2 + \nabla G / \nabla c$ the μ is nothing but the Euler-Lagrange equation so that is nothing but $\partial f_0/\partial C - 2\varkappa\nabla^2$okay now let us call $\partial f_0/\partial C$ as some function g(c) okay so now we have the evolution equation which is given by.

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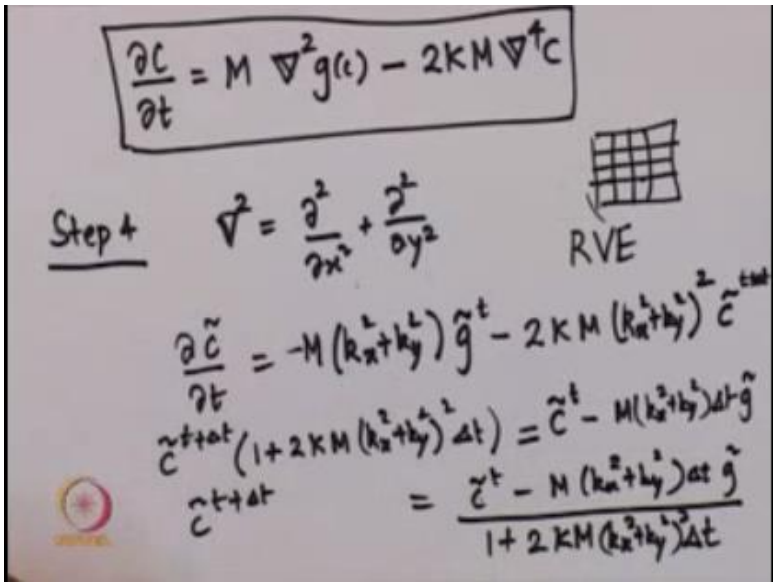

$\partial c / \partial t = M\nabla$ acting on g(c) -2 $\varkappa$ $M\nabla^4$ c okay so this is the third step now the fourth step is of course solving this equation so step four this is what we want to do now we have already done it in one dimensional case we want now want to do it in a 2d case okay so let us take what is involved in solving this equation in 2 dimensions okay so ∇^2in 2 dimension is nothing but $\nabla^2 \partial x^{2+}$ $\nabla^2/\partial y^2$ so already this is a second derivative which means it involves points to the left and to the right of a given point so you can evaluate g at every point in my domain right I have this domain so I am going to split it into lots of points and at every point I know so I can get on the left right and top and bottom for the y so that is possible.

In addition when you have $M\nabla^4$ c terms it is $(\nabla^2)^2$so it has$\nabla^4 / \nabla x^4 / \nabla y^4 + \nabla^2 / \nabla x^2 \nabla y^2$ in other word sit is going to have these cross terms also and it is a fourth derivative which already involves the points to the left and left of left right into the right of right top and above top and bottom and below bottom and so on and so forth and ∇^4 in addition is also going to have these cross terms so in other words doing the finite-difference implementation of this is going to be very involved but we are going to do a Fourier spectral implementation so semi implicit Fourier spectral implementation in that implementation as we have discussed earlier the periodic boundary condition is implicitly assumed.

So periodic boundary condition means that there are no surfaces that we consider so all points have points to the left right top bottom for that matter right so even this point has points to the right which are nothing but the points here even this point has points to the left which are nothing but these points and so also the top and bottom point so this points have points to the top which are these points and these points have points to the bottom which at this point so that is how the periodic boundary condition works.

So there are basically no surface points okay now that is implying when we when we do the periodic boundary condition implementation what it means is that we are assuming that the microstructure that we are considering is a representative volume element RVE that is this region that we are looking is a representative area of the entire microstructure so whatever is happening here if you look at that is sufficient to get the complete information about the microstructure so that is an implicit assumption that is made if you are using periodic boundary condition and because we are looking at microstructures and this is true even when you look at experimentally the micrographs what we are looking at is some portion of the microstructure.

We are assuming that the portion we have chosen is representative of the entire surface and that is how we make our analysis based on these small regions that we look at under a microscope so we are going to assume that this is given to us assuming that then you can do a Fourier transform based implementation so that means $\partial C\sim / \partial t$ is nothing but M so it will become now we are doing it in 2d so the ∇^2 will have the kx part and ky part so we are going to have-so $kx^2+ ky^2$ acting on $\tilde{g}$-2$\varkappa$ M so-$k^2$and another - k^2

So this is going to give a k^4 so that is basically $(kx^2+ ky^2)^2$ acting on c~ okay we are also going to assume that $\varkappa$Ma everything to be one as usual but for now let us say that this is at time t + Δt this is at time t so then that gives c~ at time T +ΔT is nothing but this quantity is going to come 1 + 2 $\varkappa$ $M(kx^2+ky^2)^2$ x Δt so that is going to come is equal to c~ at time t -$Mkx^2+ ky^2$ Δt $\tilde{g}$ so c~ t + Δt is going to be c~ t - $Mkx^2+ ky^2$ Δt $\tilde{g}$ / 1+ 2 $\varkappa$ $M(kx^2+ky^2)^2$ Δt so this implementation wise you can see so this is the final step now we are going to go to the computer and solve this

problem implementation wise you can see that this is no different from the one D implementation except for in addition to kx now we have ky that is added.

So this is what we want to implement now and we want to write a script in octave which will solve this problem so let us do that and look at how the solution looks in 2D in 3D also it is a straightforward generalization so in addition to kx and ky you will have kz in three dimensions so that that is all that is there in 3D but because of the computational resources that will be available to us I would like to do everything on a laptop and that is not possible if you want to do 3D simulation.

So I am going to restrict myself to 2D simulations except for this additional complexity there is nothing new that we have to deal with when we do 3D simulations so if you understand this you should be able to do 3D simulations also fairly comfortably okay so let us try to implement this problem now so let us go to the computer.

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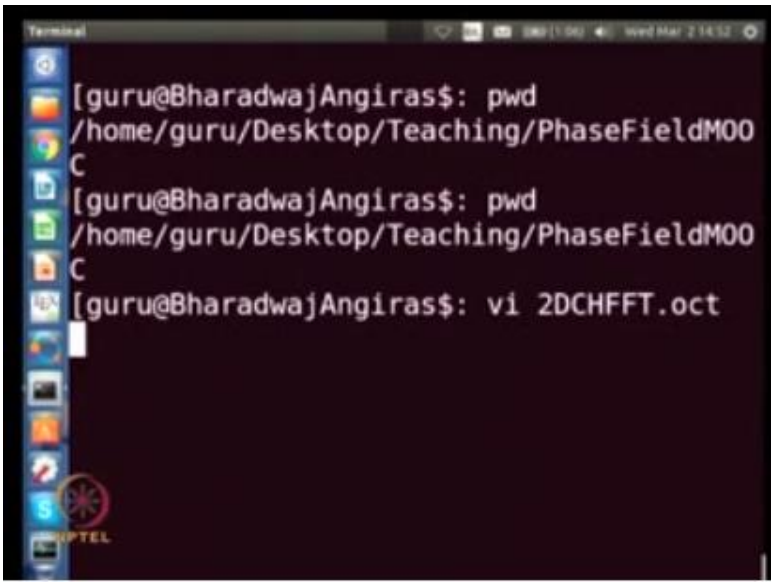

As usual so I need to check the time in the right directory so I am in the right directory so I let us call this as 2D Chan Hilliard FFT.OCT so that is what I call the program.

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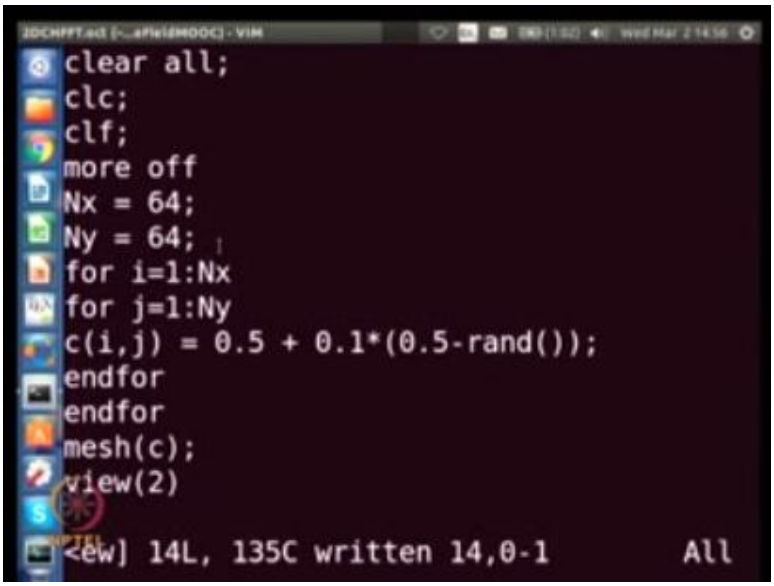

So first thing is clear all clc clf so I clear everything that is already there I am also going to introduce this command called more off the purpose of this command is that when we want to plot things and unlike 1D you know those were just profiles so you can keep on the same plot but now we are going to look at micro structures so the microstructures are going to evolve so we want to get a movie kind of feel if I do not put more off the all the entire script is executed and then all the figures are shown one after an other that which is not what I want to see.

The microstructure as it is developing to do that if you put more off then what it will do is that it will show the figure it will do the next computation it will show the figure corresponding to that and so on and so forth okay so this is just to get you a proper microstructure as the system is evolving see that I have put more off okay so now what we are going to do of course we want to start with an initial profile.

So let us say that we have total say some 64 points now here it is possible because now we have to say Nx and Ny right because there are two points because the x and y if you have z N_Z also you have to say so let us say that I take a square domain the region where I am going to evolve my micro structures o it has Nx 64 Ny is 64 so now we have to start an initial profile and the

initial profile is going to be a noisy profile so I am going to take some average composition I am going to pickup pick it up as 0.5 because that is where the unstable region is and I am going to put some small noise about 0.5 + or - some small noise.

So that is what we want to do so let us do that so you say for i –1:Nx for j= 1:Ny what do we want to do we want to define c(i, j) so I am going to define composition as what 0.5+or - I want to do so I am going to take this 0.5 - rand okay so now the rand function is going to return a random number between 0 and 1 so if you subtract it from 0.5 you will get either a positive number or a negative number which is of the order of 0.5 so I want to multiply it by the small number which is nothing but the noise so now this will be 0.5 + or - some number which is of the order of 0.05 okay.

So that is going to be the initial composition profile so that is the reason why we have put it like this end for and end for so this is the initial profile so we want to plot and see now this is a 2D information so it is going to be a 3D plot so I am going to plot it as mesh(C) okay view 2 is to look at this mesh from the top I will show you how it looks and then so let us just run this part of the code and see how it evolves.

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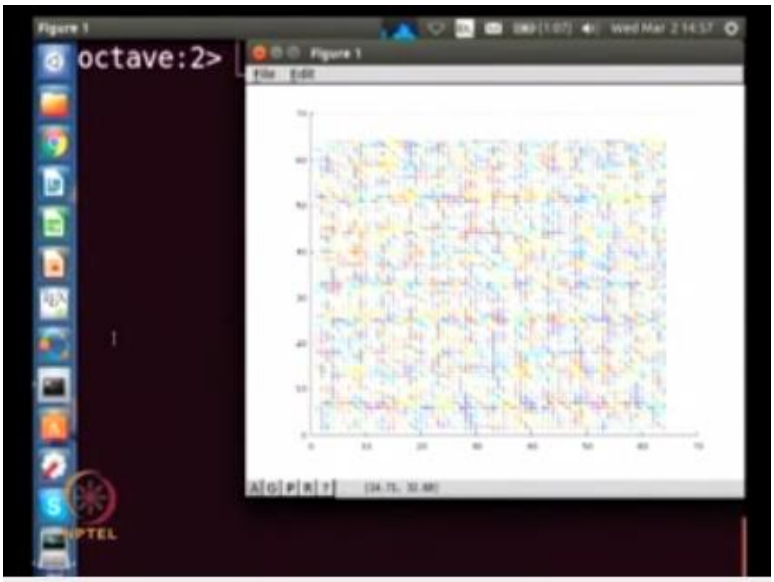

So let me see let me see if I am the right directory so I say octave and then I say source to 2D okay so you can see that this is the microstructure I get and these colors basically tell you what is the value so it is more or less all the colors that you see which means I and you can see it is a 64 x 64 system and so what we have done is to look at the projection so if I actually want to show you how the micro structure itself looks you can see so I have taken about 0.5 the noisy profile right so it is all compositions which are about 0.5 but with some noise.

So that is what it is and when we take this view to basically we are looking at a top-down right so that is basically how it looks like now this is the microstructure that is going to evolve okay so let us go back.

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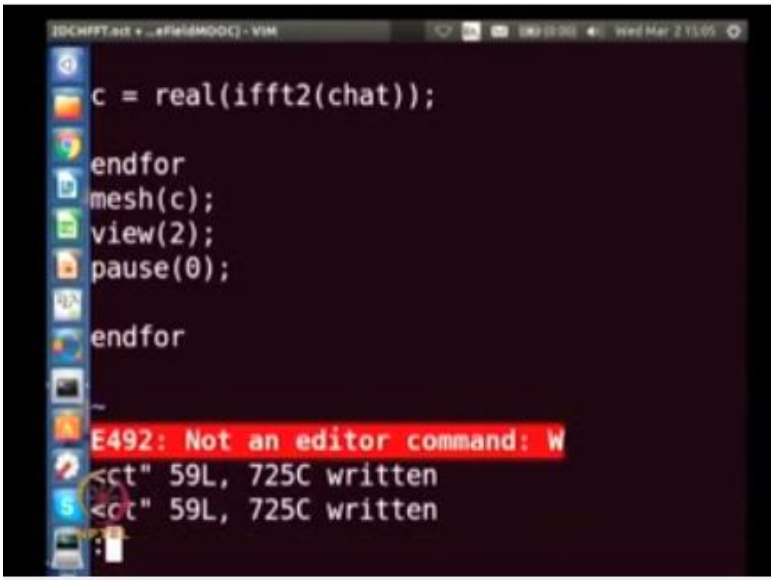

And let us introduce another command called a pause 0 pause 0 means after showing this figure it will stop for 0 seconds and then it will move on to the next figure which it has to apply okay so pause 0 pauses 1 for example will wait for one second and if you just give pause without any comment without any number it will wait till you give some keyboard input before it move on to the next figure so let us put pause zero and try to evolve the system.

So what does evolving the system involve evolving the system would involve calculating the G and taking its Fourier transform say taking Fourier transform of C and so on and so forth so let us do that far i = 1 to 2 m okay that is the time step but I also want to plot it once in some number of steps so let us say 1 to10 4 let us not call it I let us call m1 to 10 n = 1 to 8 okay so end for end for now the n 1 to 8 is the inner time loop after this is over I am going to plot this composition every time right and pause 0 so every 8 times steps once this is going to be plotted.

So that is what this inner loop for and like that it is going to go 10 steps so total number of time step is going to go is 80 so the final end for is meant for that part and we want to also define dt so let me define dt to be equal to some 0.5 okay we also want to define half Nx is = Nx / 2 these are needed because we want to implement periodic boundary condition half Ny is equal to Ny /2

okay and ∇kx is equal to 2 π / Nx and ∇ky is nothing but 2π/ Ny right so we want to have all these defined previously we just refined half N and ∇k but now because there is x and y you need to define them both once we have done that so let us calculate in the inner loop first we want to calculate g what is g 2 times A.

So let us also define these quantities let me call A is equal to 1 m = 1 kappa = 1 okay so two times a .* c .* 1.- c.* 1.-2. * c so it is 2Ac 1- c (1 -2)c so that is what g is so we calculate g and then we take the Fourier transform so g^ is nothing but f (t2(g)) so f(t2) is to indicate that it is a two dimensional Fourier transform okay so C^ is nothing but f (t2) of c okay so now we have the Fourier transponder now what we are going to do so we are going to say for i = 1: Nx for j = 1: Ny right.

So we want to implement the periodic boundary condition so this is end for so these end for our for the for loops for the Nx and Ny so first we want to do this so we want to say if i is less than or equal to write less than or equal to so i-1 i -1 is less than or equal to half Nx then kx is equal to i -1 into ∇kx right so that is what we defined and if i -1 is greater than half Nx so then kx is going to be i- 1 –Nx into ∇kx right and end if okay so we are going to repeat the same thing for the while loop also so let me take me for okay so j -1 is less than y then ky = j -1 times delky in this case ∇ky ∇kx they are all the same but I am writing it generice nough so that it can be used in the other cases also right.

So it is not necessary that Nx and Ny are the same it is not necessary that the ∆kx ∆ky are the same and so on and so forth so I am writing for that generic case so now we have implemented periodic boundary condition and for both x and y so we want to define k^2 as kx * kx +ky * ky now we want to define k4 as k^2 *k^2 okay so now we are ready to evolve the system so we say that C^ (i, j) is nothing but C^ (i, j) so c^(i. j) – dt times k2 times h^ M times dt times k2 times g hat (i, j) right i, j.

So that is the entire thing now divided by 1 + 2 * M* kappa * k4 * dt right so this is what the new C hat is so you evolve it now we have to take C to the real space because C is equal to real of inverse fast Fourier transform of 2D now C^ okay so we take it to real and that ends the loop

so then we plot and we pause ass and then we keep doing it so this is the complete loop now let us so we have the entire code now ready so let us try to run it and see what happens okay so let us source.

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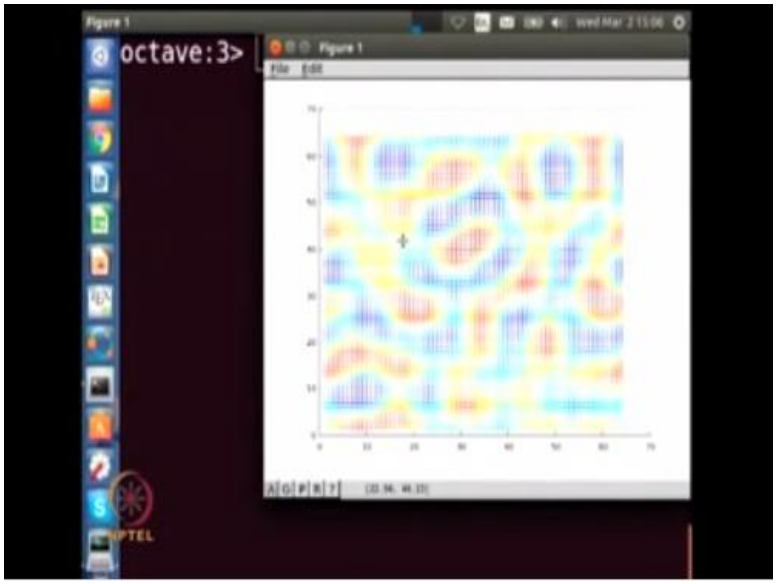

So I get yes so as you can see the microstructure is evolving okay so you get all these red regions you get all these blue regions and they correspond to a and b rich regions okay has you can see the microstructure is cautioning so the system has come out. So let us do it once more so that we can look at the evolution from the beginning.

So let me have this okay so this is from very early stage we can see whatever was all colors is slowly becoming face separated into regions which are rich in a and rich in b and the random number that is different every time so that is why every time you run a simulation you get a different kind of microstructure if you want to get the same microstructure then you have to use a seed and using the seed same random number sequence can be generated on the computer okay. So the evolution is quite fast here so let me do one more thing.

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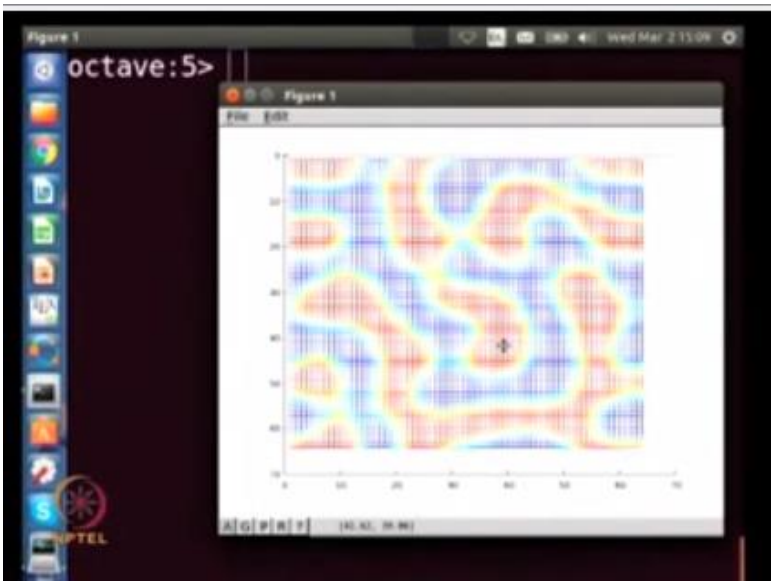

So let us say that we start and we go to the same ten steps but let us plot the microstructure once in 20 steps okay so let me evolve and this is what it is and so this is what it is and this is the initial microstructure within some 20 steps you can see it became that and another 20 steps so it is becoming so you can see all a rich regions and b rich regions of forming and it is it is evolving because we are now going to longer time so you can see that these are coalescing so here at this point they are all coalescing and you know this is this is becoming one and this is probably going to become one together.

So you have this interpenetrating microstructure that is coming up that is very typical of spinodal decomposition now let us take a look at so this is just a projection I am looking from the top let us take a look at how the micro structure itself looks like so this is how the microstructure looks okay so the microstructure goes from 0 to 1 so there are regions where it is all one that is basically the b rich region which is seen as a red patch and there are regions where it is you know blue regions that you see all these values that you see are basically where the composition is 0.

So the entire micro structure consists of composition regions where it is 0 and composition regions where it is one and there is this effect of the interface or the composition part so which

we will see clearly when we look at the simpler precipitate growth case so this is the microstructure you are looking top down and that is why it looks like this okay so in this figure whatever is all blue is basically a rich all red is basically b rich and you can see that the interface is a region where it goes from red to blue.

So this is basically spinodal decomposition modeled using the phase field equation namely the Chan Hilliard equation and implemented using a semi implicit 40 specter technique so we start with an microstructure which is about 0.5 with some noise and it evolves to give you a rich and b rich and a rich b rich regions have this typical microstructure which is what you would see if you did look at a spinodal composed microstructure okay so this is the first part now we want to do the same thing two-dimensional implementation for the Allen Cahn equation we will do it next in this lecture thank you.

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