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

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Module No.10
Lecture No.42
Spectral techniques II

Welcome we are looking at the numerical solution for the diffusion, equation and we just looked at the Fourier transform based a spectral technique for solving the diffusion equation, in which finally we showed that if you have.

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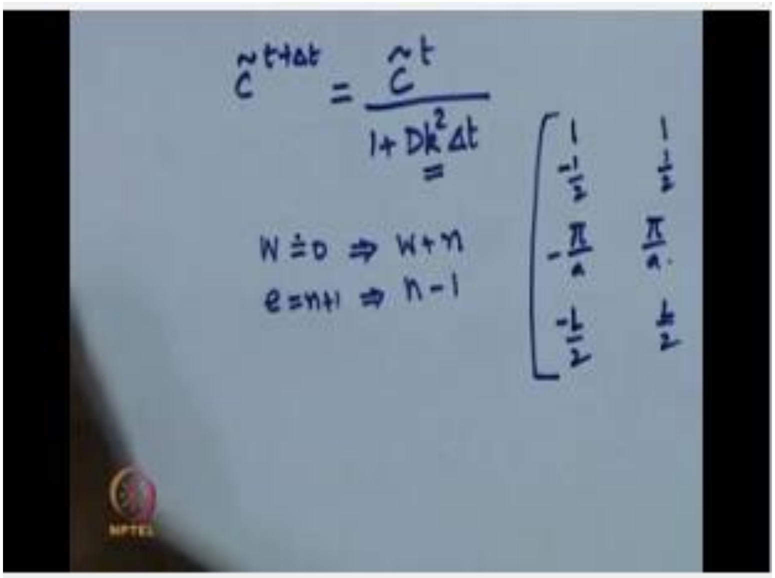

Fourier transform of the composition field this, is spatial Fourier transform then the time evolution is just given by, ~t c / 1 +D K^2 Δ T, now in this equation there is no boundary condition that we have implemented, that is because Fourier transform automatically implies periodic boundary conditions, this is the reason why we discussed periodic boundary condition earlier, so Fourier transform based techniques automatically assume that it is periodic boundary condition.

So the way the periodic boundary condition is going to enter, multiply our calculation is in terms of this k, and as you will see in the implementation that I am going to show you the implementation for the Fourier transform is exactly the same way in the earlier case, where we implemented periodic boundary condition, may be said that if W which is the West Point becomes equal to 0, then you replace it by w + n.

And the east point if it becomes n + 1, we said replace it by n – 1, in a similar fashion we are going to take the reciprocal vector and, we are going to restrict it and this is a common trick that you would have seen between – ½ and + 1/2okay, So sometimes it is π / a - π / a 2 + π by a, this is how periodic boundary condition is implemented in solid state. For example or – L/ 2, L /2, this is how it is sometimes represented.

So we are going to use this whatever be the length some – ½ to +1/2 , that is range of k values that we are going to keep, anything goes outside we are going to bring it back by either subtracting or adding depending on, whether it goes out at this end or it goes out at that end, so this implementation of the periodic boundary condition is the only tricky thing that we need to care about when we do the spectral technique. So let us write a small script, which will solve the diffusion equation using the spectral technique ok, so let us as usual go to the directory.

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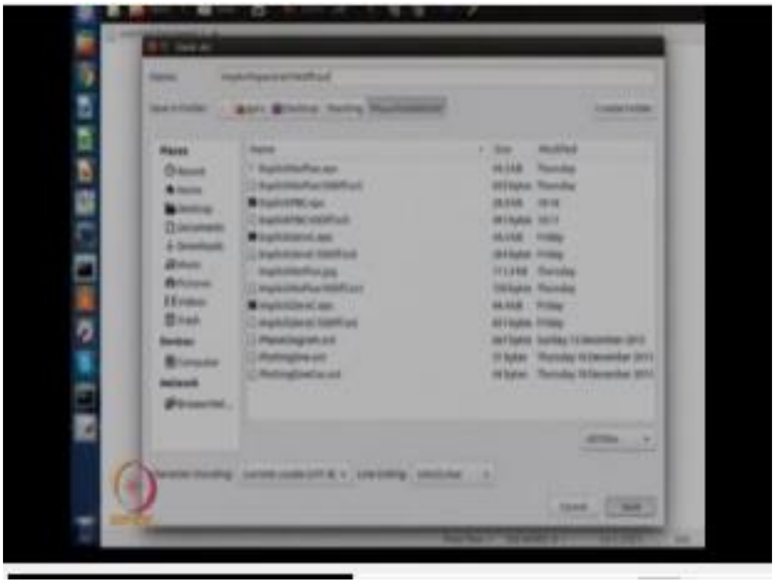

In which I am going to invoke octave and, I am going to open an editor, which is a simple text editors that is the G edit, so and I am going to save a file an Oct file, going to save it as remember in the same directory in which you have invoked octave is where you have to save the file, and I am going to save this file as, implicit because that is what we are going to do spectral1d diffusion. So it is implicit spectral 1d diff dot Oct.

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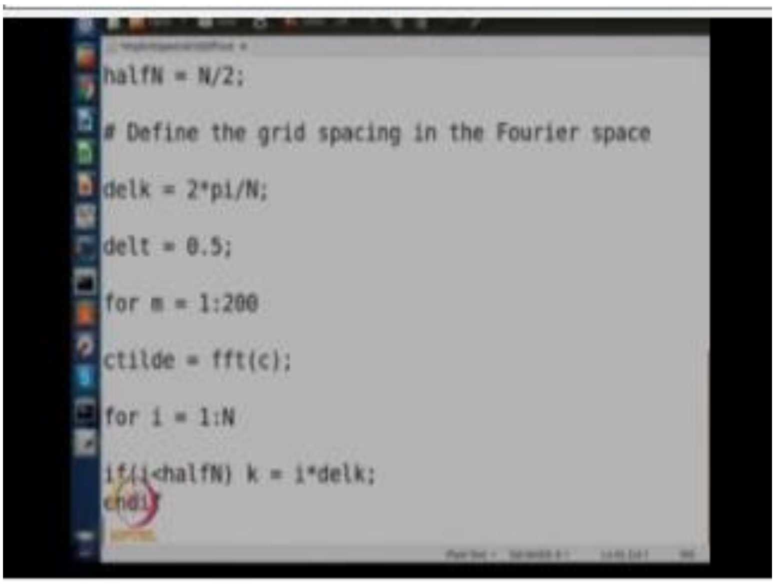

So this is what I am calling my file, so as usual we first clear all the data, we clear the figure, ok and then we say what is the number of points, and like I said input EA transforms it is preferable to have it as a power of two so n = 1 28, so I am going to make a sinusoidal profile so that is as usual see zeroes, [n,1] or so it has put zeros everywhere, so I am going to say m = 1, and then I am going to say for j = 1, to n what are we going to do? We are going to say C F J, 1 = 0.5 × 1 + sign of what 2×π× m × j / n okay.

So let us put some comments here so which will be helpful, clear the memory, and so we find system size, so that is defined system size make an initial sinusoidal profile, so that is what we have done and it has a single wave, so that is y m = 1, and I am going to plot the initial profile, see with some red square boxes okay.

And then I am going to say hold up okay, so this is rod B initial profile. Okay so after we do that we are going to define, so for periodic bc implementation, so we need to do certain things to get the periodic boundary condition implementation. So I am going to define a half length of the box okay, so I am going to call it as 1/2n = n / 2, okay.

And then I am going to define the grid space, so define this is defined half length of the box, so and then I am going to define the grid spacing in the Fourier space okay or reciprocal space, it's called so how do we define? We say that Del k remember, which it is not Del X anymore it is Del K = 2×π/ M, okay.

So that is how we define it and dt which is Δ t is 0.5, so to be consistent with our earlier notation let us call it as Δ is 0.5, this is the time loop okay, so now what we are going to do wear going to say for the M =12 some 200, let us run for some 200 time steps what are we going to do? First were going to take a Fourier transform.

So I am going to call this Fourier transform as C tilde right, that is what we call in the expression so let us call it as, so what is C tilde? It is Fostoria transform of c okay, then what do we do for I = 1 to n, so we are going to go $^{\times}$ the loop, in the loop first we define a B implement the periodic boundary condition, What is how is it done if, I < 1/2 n then k = l, to the k = i times Del K okay, That is ended.

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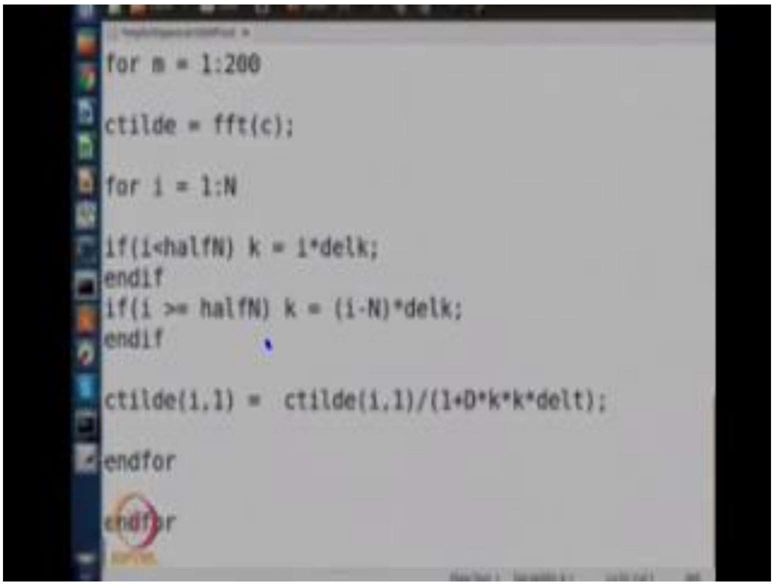

On the other hand if, I ≥1/2 n, then what are we going to do we are going to say k = i - n times del n okay, so now we have defined k I want to define k^2 or I can leave it as k^2 because, we just need k^2, so C had of I , 1is equal to what is it we know that it is C hat of I , 1 divided we haven't defined d, so let me go back and define the parameter D where I define the N so I am going to say B = 1right.

That is the diffusivity we assume so it is going to be d $^{\times}$ k $^{\times}$ k $^{\times}$ Del t right, 1 + D $^{\times}$ K ^{2}d $^{\times}$ Del T so if you take the c Tilde so sorry! I should call it as re right the Fourier transform is called see tilde/ s, so I should call it as C tilde C hat is another notation for the Fourier transform, c tilde = C tilde x 1 + D K ^{2} t.

So now the c tilde that you have on the left hand side, is in the new type ok so now if you end this for loop or so, this end for is for this I loop, so you have evolved it there in time and you haven't it, ok and now you can keep doing it for the number of steps that is n for this is for them loop which is the time loop, and finally when you come out you need to take the inverse Fourier transform.

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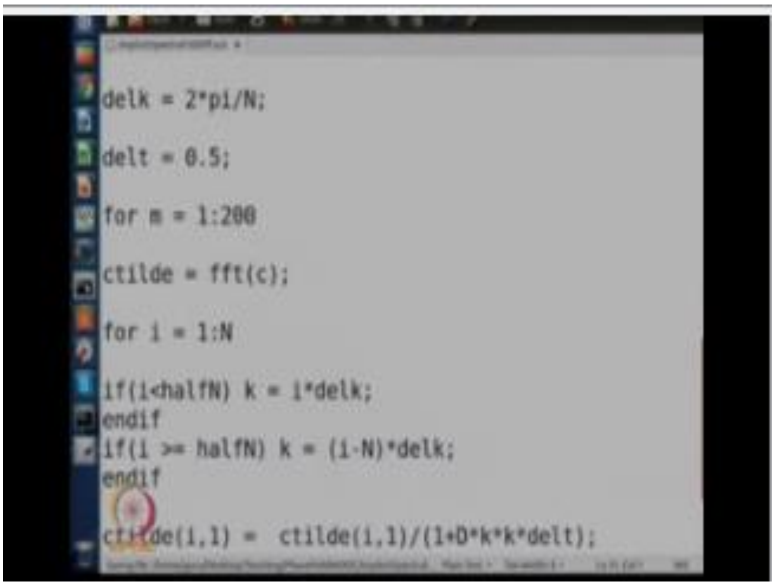

So I FF T so now let us get back to c, c = to i FF T which is inverse Fourier transform of C tilde, right you if you take C tilde and do the inverse fast Fourier transform you will get c, a but we only need the real part because C is real, so let us keep it only to the real because the new to Fourier transform it has real part and imaginary part and the c we took as real.

So it went and then when it comes back because of numerical errors it might have collected some imaginary part, but that is not part of our solution so let us remove it. After you do that plot C, right so there is a hold on that I introduced I suppose so this will plot on the same plot what the solution is after you valve it for 200 rights, steps okay. So that is what this code does.

Now let us try to go back and run this, so for running I have to say source this is an implicit one, I think spectral is what I called 1d tiff tortures city okay, so as you can see I get the solution but I do not see the solution, so maybe I had it to run for longer time to get the evolution, so let us run it for, let me run it for longer time.

So let me learn it for some 20,000 time units and that is going to take slightly longer to run, I will just start the calculation we will look at it later, so what where doing trying to do using Fourier transform is very simple you know, it has again become an algebraic expression you did a Fourier transform on the variable and then you went to the partial differential equation, you found that it can be reduced to an ordinary differential equation.

And now we are trying to solve that ordinary differential equation, and when we solve the ordinary differential equation so it is an implicit method, so it's quite simple unlike the case of finite difference technique, where implicit method actually involves solving the setoff algebraic equation by doing some matrix inverse and multiplication and all that.

In this case that has simply become an algebraic expression as if it is like an explicit method, so then you can directly solve the equation and you can plot the solution, and now I as an exercise for this problem I would like you to try several initial conditions, so let us list them out and for example you can take

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An initial condition in which you take one third of the distance to be zero,, another one-third here to be zero, and the remaining one-third to have a value of one, for composition so this is one initial condition, for which you can try see remember because the Fourier transform assumes periodic boundary condition your initial profile should be periodic, if not it will not work.

The second thing that you can do is that you can take some constant $C_0 = 0.5$ and you can put some noise about 0. 5, ok some random noise about 0.5, and you try to evolve this system of course you know that all the noise should die down and it should become a constant after a long time, so these are and a couple of problems that one can solve using the spectral technique given the code.

So you can take the script you can modify it and you can try to solve these cases, so that brings us to the end of this section, so let us remind ourselves what is it that we have done we have looked at the diffusion equation, we looked at its solutions using analytical means, we have also looked at its solution using finite difference technique, and pure spectral technique.

The next step is of course to go do the same thing with the continuity equation, or the phase field equation, which is a nonlinear diffusion equation, for doing that we are going to stick to the spectral technique, I am going to spend most of my time and trying to do special technique maybe for some 1d problem we will try to do the finite-difference technique, but you will see,, why finite difference becomes too messy? For solving an equation like carnelian equation which is nonlinear, so we will solve primarily using the spectral technique and it's fairly easy to solve in 1d.

And what we have done and we will do as part of tutorial for the force is to solve the diffusion equation in two dimensions, because the using Fourier transforms we are going to solve things in 2d as far as the continuity equation is concerned, so it might be a good idea to try to solve the diffusion equation, at least in 2d and see how the solution looks like and things like that, and then we are going to solve the Alanson equation, and then combinations of carnelian Alanson.

So that takes us to the phase field part but before doing that I need to show where the phase field equation comes from? so we are going to do a little bit of mathematics to derive the continuity equation, I didn't derive the equation earlier I just wrote down the revation but deriving the Colin Hilliard equation involves a little bit of mathematics, it involves a Taylor series expansion, which is in multiple variables something that some of you might have seen but it is not very common.

After you expand the free energy, it is a free energy functional because it consists of both the composition and its gradients, so the Taylor series expansion is in terms of composition its first gradient and second gradient third grade, ii it's so those are known as gradient curvature aberration etcetera, so in terms of those we are going to expand the free energy functional, when you expand you will see that the free energy functional consists of lots of property tensors.

So we need to understand tensors and how to deal with the tensors? And what kind of properties they have to obey? For representing the underlying symmetry of the crystal that you are considering, for example what happens to these tensor quantities if you assume that the system that you are dealing with is isotropic or cubic, we might not go in this course beyond cubic.

So but we will indicate ways in which you can go beyond the cubic systems, so you can say that how to deal with cubic anisotropy, for example the underlying crystal is cubic so what happens to be the fencers? And in terms of then those properties then you can reduce the free energy functional to a simpler form, and that involves some gauze green theorem kite of the theorems and once you have reduced it then we need to look at the chemical potential.

So chemical potential can no longer be derived as a partial derivative, but it becomes a variation a derivative because we have a functional instead of a function, so how to write variation derivative becomes an issue? So once you have written the variation derivative and you get the chemical potential then we need to substitute it in the modified the flicks' law, that we said that the flux is directly proportional to chemical potential.

And once you have done that to get to the time dependent part then we will use the usual arguments, and write the evolution equation which becomes the continuity equation, and in the case of a Alanson I am just going to write the free energy functional and directly I am going to show you what the evolution equation is, because in that case we assume another type of constitutive law to get to the evolution equation, by Ricky okay.

So that is the part so that involves a little bit of mathematics, so the next several lectures are going to be on these mathematical topics they look disjointed because I am going to talk about certain mathematical entities, and their properties and, how they behave etcetera then I will move to the next mathematical entity, so we will keep doing this but once we come back and try to derive the continuity equation they will all fall in place okay.

So the next few topics are going to be mathematical topics, but there is no continuity that you can see at this point for these topics because they are not really continuous things, I mean there they are different mathematical aspects but we need all of them if you want to understand the continuity equation, so we are going to do these bits and pieces of mathematics, and then we are going to come back put them all together to derive the continuity equation, which we will do from the next lecture onwards thank you.

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