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

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Module No.10
Lecture No.41
Spectral techniques I

Welcome we are looking at numerical solutions to the diffusion equation as well as analytical solutions and the trick is always to reduce if you are looking for analytical solution the PD to ODEs and solve them. And there are several ways in which you can turn them into ODEs we saw variable separable, we saw the dimensional analysis based variable substitution which reduces the equation to a ODE. So now I want to talk about another way of reducing the PDE 2 ODE which is based on what is known as Fourier transforms okay.

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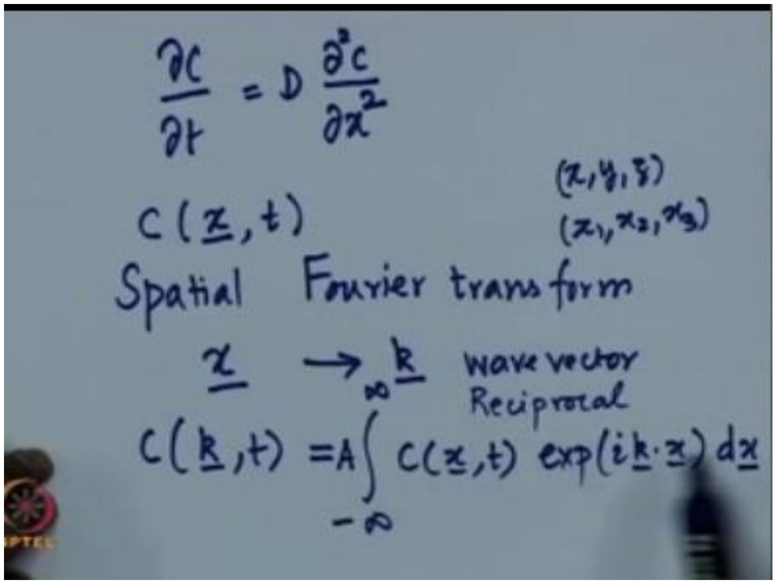

So the equation that we are trying to solve is the diffusion equation and we are going to perform a Fourier transform on the variable C. Now C is a function of both position and time okay, the line below x indicates that x is a vector because of the position is basically given by XYZ are x1 x2 x3 okay. So x is a vector and t is when we say Fourier transform there are two Fourier transforms one can think of one is what takes the time domain into frequency domain which is a Fourier transform which is extensively used by electrical engineers for example.

When you are doing analysis of signals you are generally trying to take what is there in the time domain and put it in the frequency domain right you can analyze voices for example using that kind of Fourier transform. But that is not the kind of Fourier transform in which we are interested it is very natural in material science to look at this Fourier transform because this Fourier transform takes from the space to the Fourier space sometimes it is also known as the reciprocal space all the diffraction experiments.

For example, take the information about the arrangement of atoms in a crystal from the real space to the reciprocal space that so that is equivalent to a Fourier transform 2. So what we are talking about is the spatial Fourier transform okay. And in spatial Fourier transform we go from

X to K so this is the wave vector space okay are the reciprocal space. So if we assume so the Fourier transform is typically given C(k, t)= integral minus infinity to plus infinity you take C(x,t) multiply by exponential Ik.x and then you volume integrate over the X okay. So that is the Fourier transform there are factors sometimes people use 1 by 2Л or sometimes people use 1 by root 2Л.

So there is some constant factor here so let me just call it some a we will not specify it is not very important for our purposes today, but if you do a Fourier transform actually you need to look up the documentation of your Fourier transform to see what is the number that is used there are many different ways in which this constant can be introduced some introduce it only in this way which is known as the forward for a transform you take the spatial domain information and you integrate out the spatial part.

So it becomes just a function of wave vector some introduce it only in the reciprocal or in the reverse or inverse Fourier transform where you take this and multiply by exponential minus ik.x and then integrate it over DK that is you do this in the reciprocal space, so some do it in that fashion. So some do it symmetrically in both the forward and inverse four transform by putting1 by root 2Л so you need to look up.

And generally sometimes people prefer 1/ root 2Л in both because that is symmetric and you do not have to remember which way the constant is coming. The other thing to remember is that four transform is defined with exponential minus ik.x and the inverse Fourier transform is defined with exponential ik.x so again so this is a convention you can design define it whichever way you want but you need to look up the documentation if you are going to use Fourier transform for your purposes to know what is the right definition okay.

So let us say that this is the Fourier transform definition that we are going to use then using this we are going to reduce this equation to a ODE so that is what we want to do so how do we do that let us take the equation.

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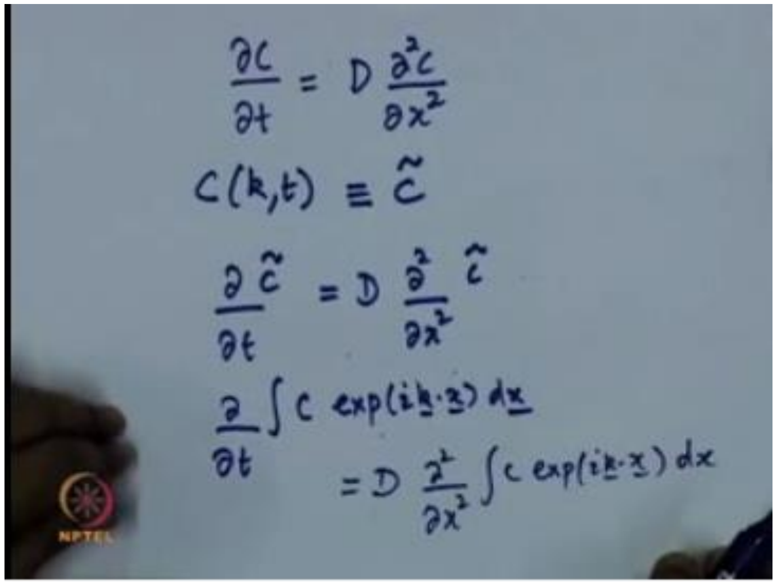

$\partial C/ \partial t$ is D $\partial^2 C/ \partial x^2$ now I am going to replace C by its Fourier transform C(k, t) I am not going to write this kt, xt etc but I am going to put a tilda so C(k, t) I am going to call as C tilda okay. So $\partial/ \partial t$ of C tilda is equal to D $\partial^2/ \partial x^2$ acting on C tilde. Now what is the C tilda we know that C tilda is nothing but integral C exponential (ik.x)dx is equal to D $\partial^2/ \partial x^2$ acting on C exponential (ik.x)dx right.

Now you can inter change these two operators there is $\partial/\partial t$ there is integral so I am going to take $\partial/\partial t$ inside if you take this operator it will just pass through this entire thing because nothing here is except for C which is a function of T. So this integral the entire integral will give C(k, t) and that is the only time dependence. So the partial derivative in that case becomes an ordinary derivative.

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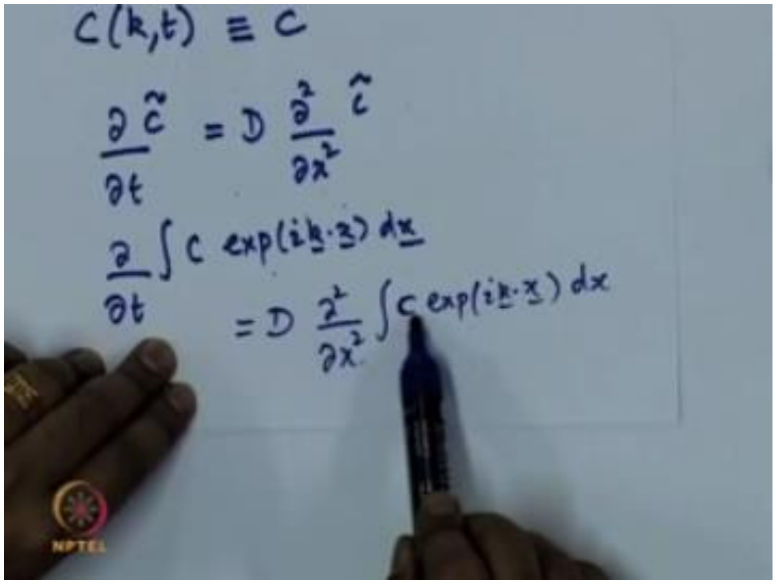

So you have D by DT of C tilda right because it is nothing that is happening there is equal to on the other hand if you look at on this side on the on the right-hand side we see that ∂/∂x will act on this quantity right because these are like coefficients in the front. And so this is going to 1 ∂/∂x is going to get the ik out the other ∂/∂x is going to get another ik out, so you will have i^2, k^2 that is $–k^2$ when this apps.

But after that it is going to leave the C exponential (ik.x) dx are the same so that is going to be C tilde still.

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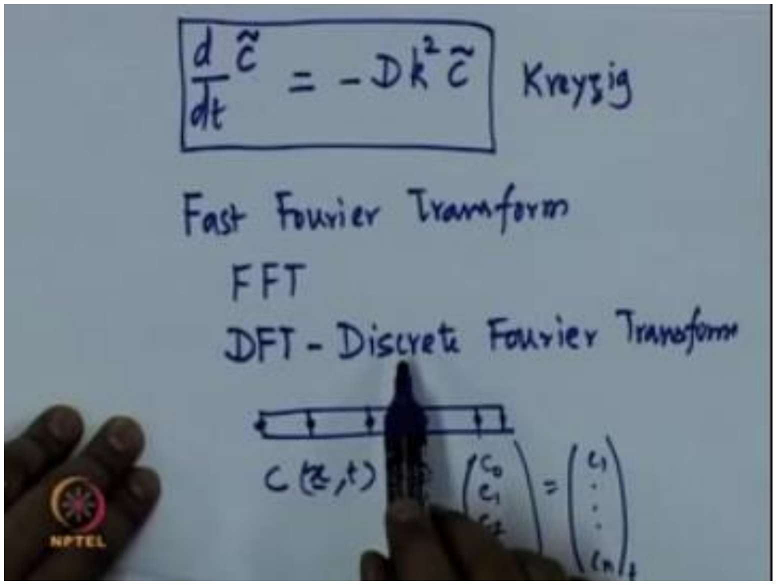

So you end up with this equation $-dk^2$ C tilde. As you can see this is an ODE which can be solved because it is a ODE in d/dt you just need the one initial value to solve this equation and so transforms I mean using for transforms like this to solve ODEs is a very common trick. Now in our case we are going to do this numerically now I am not going to show you how to solve beyond this point analytically but you can look up textbooks.

For example derivation of this itself is available in crazy book okay. So it is given as one of the solved problems using Fourier transforms to solve the diffusion equation in his case like I said he talks about heat conduction equation okay but it is the same so you can solve this. Now let me say that if I have a numerical way of getting C tilde from C right then I will be able to solve this equation for doing that we need to know about what is known as fast Fourier transform, the fast Fourier transform algorithm FFT as it is commonly known as is one of the one of the best node algorithms.

It is one of the top algorithms of the last century and it has transformed the way several experiments are done based spectroscopy techniques for example they are not possible unless you have a way of calculating Fourier transforms very fast and the FFT algorithm gives a way of doing the Fourier transform very fast. But the Fourier transform that FFT does is basically a discrete Fourier transform so it is sometimes called as DFT it is discrete Fourier transform.

What do we mean by that see I when I want to solve the equation numerically like I told you I am going to take this system and I am going to split it into node points and these node points is where I will have the value of the composition. So C x, t is nothing but a vector C right at any given time T so it will give me C at 0th position C at one position C at two-position etcetera up to CN minus 1 position are we sometimes right it has C 1 etcetera up to CN at time T right.

So this is a set of discrete values and you can go for a transform on that and you can get a set of discrete numbers in the Fourier space okay, so that is what the Fourier transform does. Now let us say that we do a Fourier transform so the equation that we want to solve is.

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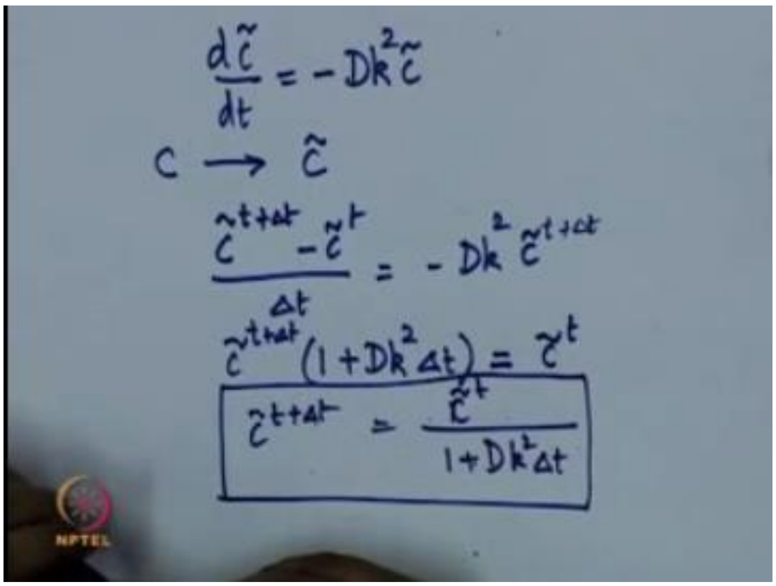

DC tilde by DT is equal to minus Dk^2C tilde, suppose I have given C and I can generate C tilde discreetly at every node point I have C the spatial nodes and I define see tilda in the reciprocal space again at the certain reciprocal points, If I know that you know this I can discretize so it is C tilde t+Δt – C tilde t/Δt=-Dk^2C tilde and I am going to take it at t+Δt you can also take it at t, but as you will see say t+Δt is possible because this is just see this has just become a linear equation just it is Dk^2C right.

So it is just algebraic so I can now take C tilde and then on this side t+Δt it is already there 1 and Δt multiplied and this minus when it come share it becomes plus $dk^2\Delta t$=C tilde t right I multiplied here I brought this term here I took C there. So if you know the initial configuration for composition at some time t=0 if you know what C tilde is C tilde at time t+Δt is obtained just dividing by $1+dk^2\Delta t$. So it is a very, very simple implementation which will solve the diffusion equation.

This technique is known as spectral technique spectral because it uses the Fourier spectrum or a Fourier transform. And in terms of accuracy this is the best that you can hope for it depends on your discretization how many k points you are going to take and integrate in and things like that. And because it is implicit you know because all the right hand side is at time t+Δt so everything is at time t+Δt so because of that there is no restriction on the Δt that you can take okay.

So here is a point at which point it is also better to say something about the issues there is this problem which is known as the stability this is because on computers we do not represent numbers, but they are only represented in an approximate manner. So if you have this approximate manner representation that there will be errors in your representation these errors if they interact with your algorithm on your method of doing calculation and if they start growing such a method is said to be unstable.

The explicit method which works very well because you can take very small we can just write a direct algebraic expression and evolve the composition profile I has severe restrictions on the Δt that you can take for a given Δx, if you take Δt larger than that then it runs into stability problems the errors start growing and the system starts giving you nonsensical results. So this is the problem of stability accuracy is different given in a problem which is table if you take a smaller and smaller Δt you will get more and more accurate results okay.

So in the case of implicit method where we take the right hand side in the future time where it has to be solved by solving a matrix equation so it is costly in terms of solution, but it is favorable in terms of the larger Δt it allows you to take in fact you can take whatever Δt you want the system will never become unstable that is the problems associated with accurately representing the number they do not interact with the method and grow the error okay. So these two are separated so you might have some accuracy issues because numbers are not represented exactly on the computer.

So when you do calculations that error will be there but it will never interact with the algorithm itself and give you wrong results. So implicit method is always preferred and you can see that when you do a Fourier transform you finally end up with a very simplified equation which can be implemented in an implicit fashion which means you will get the solution fairly easily and straightforward as I am going to implement and show you in the next part of this lecture thank you.

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