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

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Module No.9
Lecture No.35
Plotting spinodal

Diffusion equation:

finite difference method

Welcome we have solved the diffusion equation analytically for certain boundary conditions and we looked at two such methods of deriving analytical solution of the classical diffusion equation now we want to solve this equation numeric okay so what does it involve when we have to solve this equation numerically is what I want to discuss next in this part of the lecture so let us take the diffusion equation.

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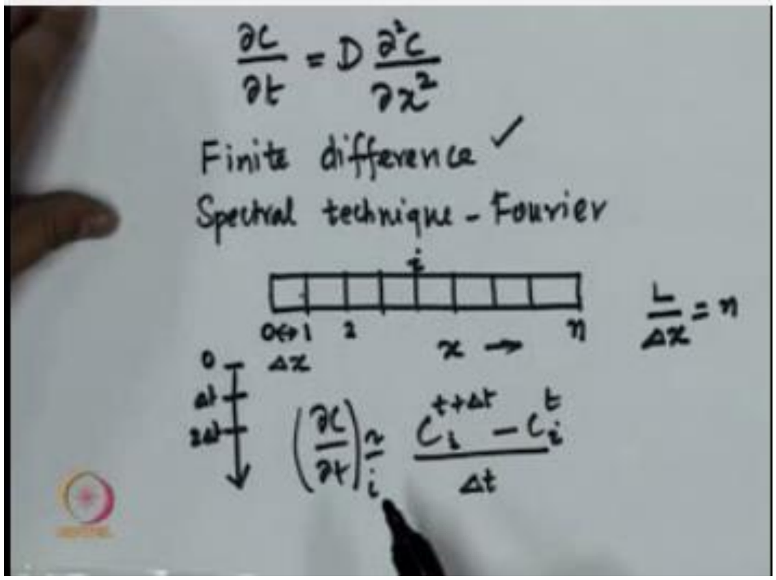

So we have $\partial c / \partial t$ which is $D\delta^2 c / \delta x^2$ this is the equation that we are trying to solve when we solve numerically there are two different ways in which this equation can be solved the one is using an approach known as finite difference approach the other one is to use a spectral technique specifically we will use Fourier spectral technique so first I am going to use the finite difference techniques to solve this equation what does involve in solving this equation finite difference suppose I have the domain this is the x domain in finite difference technique first we discretize the domain okay and the discretisation points for example this is 0 this 1 this is 2 etc up to it goes to n points.

So each discrete part is Δx right n times are n-1 times Δx is basically the entire length so this is Δx this is 2 Δx this is 3 Δx this is 4 Δx etc so up to n so it will have n Δx as the total length so you take the total length and you divide it into Δx pieces so you will have some n number of such pieces so that is what we take for this special part and I am going to refer to each one of these points that I have discretized by some i refers to any discretization point any special discretization point of course we also discretize it in time so we also have the time access and we have 0m time and then we have Δt time and 2Δt time etc…

So the solution at any given time at all these point that I have discretized if I given then I have given the solution so this is the finite difference taken for doing this okay so we are going to use the difference formula to approximate the derivatives this difference formula typically derived from Taylor series expansion that we might have seen we will also do it as a tutorial in this course.

So for example $\partial c / \partial t$ is approximated as follows it is C at time $t + \Delta t$ – C at time $t / \Delta t$ and remember this is a partial derivative so I am differentiating c with respective time so I need to tell at what position so I am going to do this at every i^{th} position okay c_i $t / \Delta t$ – c_i at $t / \Delta t$ is basically $\partial c / \partial t$ at the i^{th} position right so this is the discretization for the left hand side now how do we discretize for the right hand side that is what we will do next and for doing that let us take.

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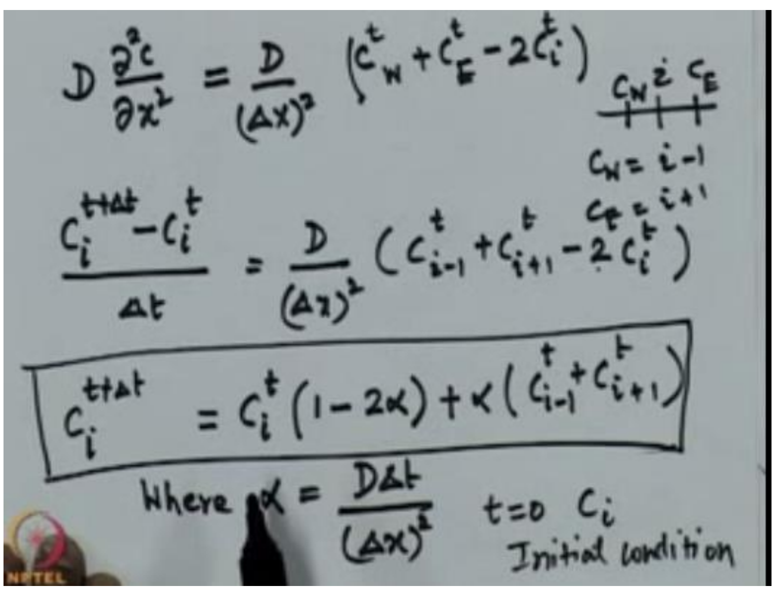

D $\partial 2c / \partial x^2$ = D/ Δx^2 $c_{W} + C_E - 2C_i$ that by Δx^2 is what is here what is W and what is E if you have i^{th} position the point to the west of it c_W the point to the east of it is C_E so this my notation this called the finite difference pencil for example sometimes it is also written as c_W is written as i-1 C_E is written as i+1 okay and in 2 dimensions if you are there are you will also have north south points okay because then the position in this is themselves will run from i and j because there is x and y axis then you will also have j- 1 and j + 1 okay so that is what basically this is now we will come back to the 2 D one later we will first solve it in 1 dimensions so this is the discretization.

Now because this is partial derivative with respective x we also need to tell at what time, there are two ways of doing it the simplest way is to say that all these C's are taken at time T let us start with that and now let us put them together so what do I have $C_i^{t + \Delta t} - C_i^{t} / \Delta t = D/\Delta x^{2} (C_{i-1}^{t} + C_{i+1}^{t} - 2C_i$ okay so let us get all the quantities which are at time T to the right hand side so I get a $C_i^{t} + \Delta t$ so at any i^{th} position if I want to know what is a composition at some future time $t+\Delta t$.

That is related to the quantity at time T as follows so C_i^t have to take the composition at that position in the previous time and this Δt $D\Delta t/\Delta x^2$ so I am going to call that as $\alpha - 2C_i^{t}$ so I am going to get this is $1-2\alpha$ where $\alpha = D\Delta t/\Delta x^2$ okay please remember whenever you do diffusion problems you are always going to get this $\Delta x^2 /Dt$ okay x^2 /Dt okay $D\Delta t/\Delta x^2$ so you are going to keep getting this quantity, okay.

So C_i^t is coming from here so that is 1 and there is $-2C_i^{t}$ and that is multiplied by this quantity so $-2\alpha C_i^{t} + \alpha(C_i - 1)t + C_i + 1$ so in other words what we are saying is that at any position I if you want to know what is a composition in some future time Δt you take the current 1 at that position multiplied by 1-2 α where α is $D\Delta t/\Delta x^2$ add to it α times to the left of that position and to the right of the position.

So this then will give you this solution, now you can see why I need initial condition, to kick start this algorithm at some time T = 0 if I know all C_i that is initial condition, if I have that using that I can get time Δt and then I can put the Δt back here because I know at time Δt I can get into $2\Delta t$ then I can put it back here I know at $2\Delta t$ so I can get it at $3\Delta t$, so in other words you can march in time.

By taking the current value of composition at different positions using that you can predict the future value of composition at different positions, so initial condition is required and one initial condition is substituted; now we also need two boundary conditions, why are they needed? Okay so let go to the position discretization and take a closer look at what the position discretization means, okay.

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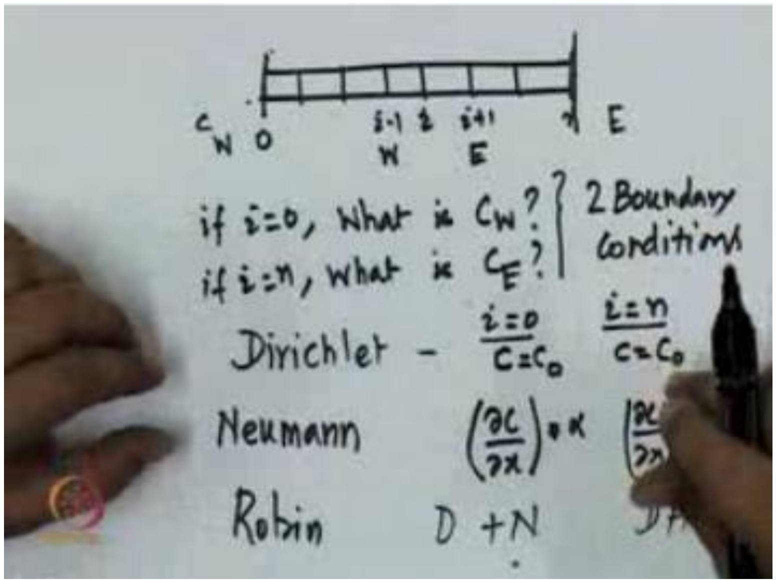

We said that suppose I have a domain then I am going to discretization like this right, I is any position, now if I am in the interior to the left of I and to the right of I so this is I – 1 and this I si + 1 this is what we call as western decibel called as VC, there are always points so for the i^{th} position when you need i-1 and i+1 compositions at this current time you have it but if you look at this end point there is no point top the west and if you look at this right end point there is no point to the east.

So to determine for the end positions when you are at 0 or when you are at end you have to determine what is CW for when i=0 if i=0 what is CW, if i=n what is CE? These two questions we have to determine for that we need two conditions these are the two boundary, condition okay if I give you two conditions.

These two questions we have to determine for that we need two conditions, these are the two boundary conditions, okay if I give you two conditions using those two conditions you will determine what C_W C_E is C_W for i=0 case and C_E for i=n case so you need in addition to the initial condition two boundary conditions to solve this setup equations. Now what are the type of boundary conditions this is not something that we discussed earlier but it is important to have the discussion here.

There are three different types of boundary conditions, actually there is four one more we will look at later, one is called Dirichlet, in the case of Dirichlet at i=0 or i=n you give the composition value itself C is equal to sum C_0 this is Dirichlet. There is a boundary condition that you can give which is known as Neumann in which case at i=0 or i=n you give $\delta C/\delta x$ is equal to sum α $(\delta C/\delta x)=\alpha$. There is also a boundary condition which is known as a Robin which is basically a linear combination of Dirichlet plus Neumann, okay Dirichlet+n=Neumann.

But at any position for example, at i=0 either you can specify this or you can specify this or you can specify this you cannot specify more than one, you cannot specify more than one you cannot say at this position the composition is C_0 and the $\delta C/\delta x$ which is nothing but the flux in the case of temperature $\delta C/\delta x$ is basically the heat flux in the case of a diffusion equation this is a mass flux, you cannot prescribe both the concentration and flux at the same point. Okay.

So either you specify this or you specify that, okay similarly here also either you specify this or this if I tag, okay. So this is something like mechanics problem you would have seen suppose if I have a rod which is fixed or valve for example it cannot have any displacements then it will start developing stresses, if you want to keep it free of stresses for example one end then it might start having displacements but I cannot specify both that displacement is 0 and the stress should also be so much that I cannot say, so okay the loading conditions are going to determine what the stress is going to be if I am going to constrain the position not to change, right.

I am going to fix this rod at this point then depending on loading condition it will develop stresses at this point. Similarly if I say that I am going to leave this end of the rod free then depending on loading conditions it will develop displacements, you cannot say this is free all the same it should also have only so much of displacements that we do not have depending on the loading condition the system will automatically choose similar thing is happening here also, you either give Dirichlet or Neumann you do not specify both at the same point, you can specify Dirichlet at one point and Neumann at the other point which is very common later, okay.

But you cannot specify at the same point both Dirichlet and Neumann, okay the only way you do both at the same point is by using Robin boundary condition which is a linear combination of the two but again if you specify this you do not have any control over this, so the overall boundary condition is what I specified, there is one more boundary condition which is known as the periodic boundary condition which is very important when we look at the special problems so I am not going to discuss periodic boundary condition in this case.

But I want to talk about one more issue namely that when we did the partial derivative of the composition with respect to position we assumed that all of it was done at time t, there is nothing that stops you from doing it at some t+ΔT, okay. The way we have done by taking all the quantities on the right hand side of the equation, right here.

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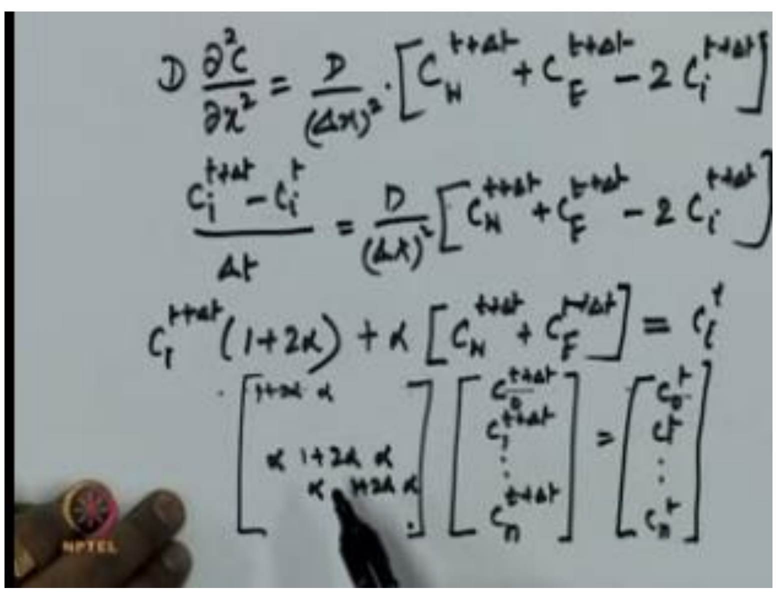

By taking the $\delta^2 C/\delta x^2$ when I took the partial derivative I assume that the time is fixed for the current time t, this is known as explicit method, okay explicit because it is given at this point and then I can calculate, but there is another way of doing it so I do not have to specify the partial derivative at time t, but instead I can do a time $t+\Delta T$, right all the partial derivative says that the time has to be kept a constant, but it does not have does not say that it has to kept at the current time or at the future time so you have the freedom to chose it at future time which is what we do and that is known as implicit method in that case the partial derivative of composition with respect to position is given as follow.

So we say $D\, \partial^2 C/\partial x^2 = D/\Delta x^2\, C_w^{t+\Delta t} + C_E^{t+\Delta t} - 2C_i^{t+\Delta t}$ so everything is a time t+ Δt right so now we have this so let us go back and try to find out what happens in this case so we have $C_i^{t+\Delta t} - C_i^{t}$ / $\Delta t = D/\Delta x^2$ and then everything $C_w^{t+\Delta t} + C_E^{t+\Delta t} - 2C_i^{t+\Delta t}$ and you can pull all the t+ Δt terms ot eh left hand you can push all the t quantities to the right so you get what? $C_i^{t+\Delta t}$ x $1+2\alpha$ right $D\Delta t$ Δx^2 times two and this we defined as α so 2α- sin so it is comes here it becomes $1+2\alpha + \alpha\, [C_w^{t+\Delta t} + C_E^{t+\Delta t}] = C_i^{t}$ right.

Now there is a short hand way of writing this so we write it like a matrix equation so let me say that $C_0^{t+\Delta t}$ C at position $1^{t+\Delta t}$ $C_n^{t+\Delta t} = C_0^{t}\, C_1^{t}$ etc up to C_n^{t} now again the initial condition is known so at every position 0 123 up to n you will know what is the composition at time t what you are trying to calculate it is the C at position 0 1 2 etc at some future time $t + \Delta^t$ and if you look at some i^{th} position so it will become $1+2\alpha$ right for the next position $i+1^{th}$ position it will become α $1+2\alpha$ α etc.

Except for this two points again when you have this position so this is $1+2\alpha$ and α there is nothing to the left up it so you need to use the boundary condition to determine what it is sometimes it will come here if it is periodic boundary condition or sometimes it will get added one of these terms if you have Niemen boundary condition if you have derihslay you will not even consider this variable because of this is fixed for example for C_0 is fixed for all times.

Then that does not have to be part of this solution matrix at all, similarly for this point C_n point it also okay so this is where we need the two boundary conditions this is where the initial conditions is there and you can solve this now this is solving a set of algebraic equations using matrix methods so you might have seen something like gauss Jordan or Gaussian elimination or gauss Seidel some such technique you can use to invert this matrix and left multiply to this solution you will this and if this like α and 1+2 α and terms like that so that is a constant ,matrix.

So once you have inverted you can keep multiplying it and keep getting the solution, there are advantage bs top using this methods even though it is costly in terms of inverting in a matrix and getting the solution on the other hand the exclusive method that we looked at is very, very trivial to implement because it is just a set of algebraic equation right I at sometimes t + Δ t is just some algebraic expression involving C is at some time T so you can write it you can just keep on doing it and you will keep getting the future solution.

So it is for easier at implement but in terms of what is known as stability it has problems so we will discuss what is stability and accuracy issues are and why and how we deal with that okay so we will do that in the next lecture when we start actually solving this problems on the computer. Thank you.

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