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

Prof. M P Gururajan
Department of Metallurgical Engineering
And materials Science, IIT Bombay

Module No.17
Lecture No.69
AC: numerical solution

Welcome we are looking at the alençon equation so let me write down the equation alencon equation says no fee by ∂ T.

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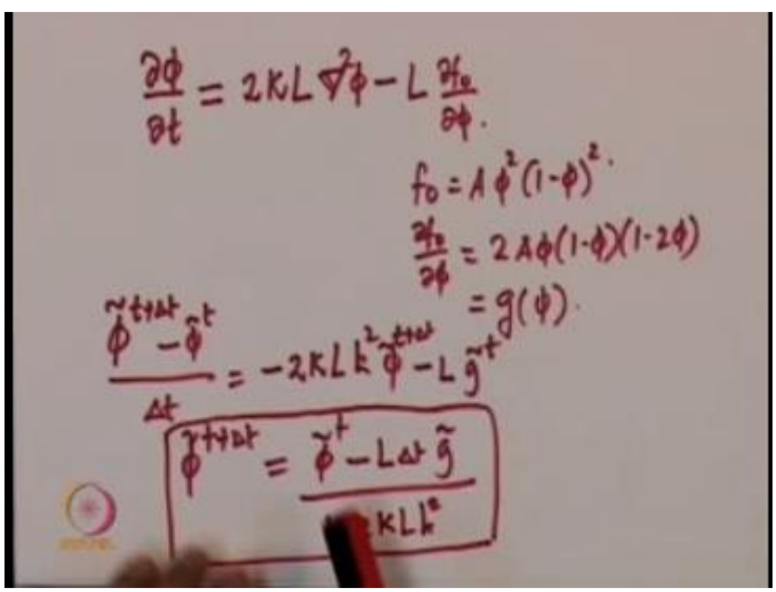

That is the rate of change of the order parameter fee which is a non-conserved variable is given by some2 kappa l ∂ squared V minus L ∂ f 0by ∂ fee where f 0 is equal to a p square into 1 minus c whole square let us called 0 of 0 by ∂ fee which is to a fee into 1 minus V into 1 minus 2 fee to be some function GFE okay.

This equation can also be solved using finite difference technique I am not going to do that we will leave it as an exercise assignment problem for you but I am going to solve this equation using Fourier transform and that is what we will do now and as usual we are going to assume non dimensional in such a way that k L a everything is one okay so in the in the implementation so let us do the Fourier transform.

This thing so it is feet tilde t plus delta t minus v tilde t by delta t is equal to minus 2kappa l k squared V minus L Jeter down now this fee I am going to take at T plus delta T and this G I am going to take at time T so this is semi implicit spectral technique okay so then fee V plus delta t is nothing but fetal dot t minus l delta T G tilde divided by1 plus 2 kappa l k squared so this is what the evolution equation. That we have to implement to solve so given a fee you can calculate G and then you can use this formula to get fee at a future time so let us go back to octave.

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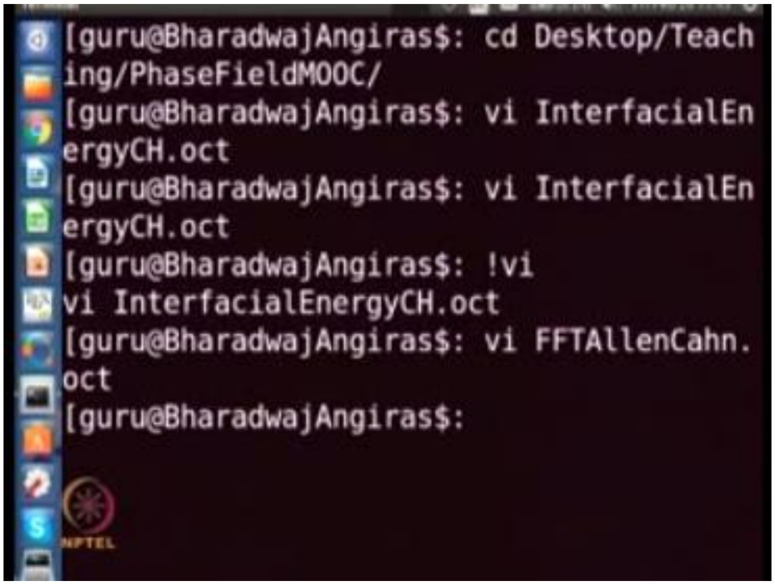

And write the code so let me call it as FF t ln con dot OCT ok so first we say clear all is LF so we clear everything and then I define kappa to be equal to 1 l to be equal to 1 and a 2 b equal to 1 right and we start with so let us take en to be equal to 1 28 and we are going to solve in the same scenario so I am going to take 0 for the first and the last water and one in the middle so v is equal to 0 comma 1 okay.

So let me also define the DX to be equal to1 it is not relevant unless you are taking some sinusoidal one but let us define it so I am going to say for is equal to n by 4 2 n by 4 plus 1 2 3 n by 4 if it is so then I am going to make the fee of I comma 1 to be equal to 1.0c of I to be 1.0and far okay so is taken to be 0everywhere and then the middle half I have made it one so this is the initial profile so let us plot p lot fee and with the red line and also write initial profile.

So that we are clear as to what this is then we hold on so that are the final profile when we plot it will be clear to us what it is I have to define half n which is n by 2 because that is what the periodic boundary condition implementation requires in this case so del k as usual this 2 pi by n ok and DT that is the time so let us take to be 0point 10 point 5 ok and this is the type loop for m equal to 1 to four hundred.

We want a ball how do we want a well first we want to calculate g is equal to 2into a dot star p dot star 1 dot minus V dot star 1 dot minus 2 dot star p right so this is the G and we take the Fourier transform G hat of is equal to f of T of G right Sophie hat is nothing but F of To f fee so now both are in fluid space and we calculate the for every point I equal to one to n we calculate if I minus 1 is less than or equal to half n.

So we say k is equal to I minus 1 into del k right end F if on the other hand if I minus 1 is greater than huff in we take it to be I minus 1 minus n 2 del k so this basically makes sure that k lies between minus PI by 2 pi by a to plus pie by a so it is it is the first blue one's own so this is the period boundary condition okay so we take K 2which is K squared as K into K we have now the evolution is Phi hat of I is nothing but Phi hat of I minus L into dt into G hat of I.

This whole thing should be divided by 1 plus 2 into Kappa into l into dt 2 kappa l dt into k square right so that is what we have okay so and end for so before in far so we have to the this is the for loop that is ending for I equal to one to n here so then we take the fourier transform back p is equal to real of inverse phosphor via transform of C hat this step is important because now we want a fee in real space before we go for the next step so that G can be calculated in real space and so the evolution is over.

Then we were to plot the field that is the final solution okay so this is the code which is very identical to what we wrote for the diffusion equation and the continuity equation so let us go and source this file and see what happens source f of T okay.

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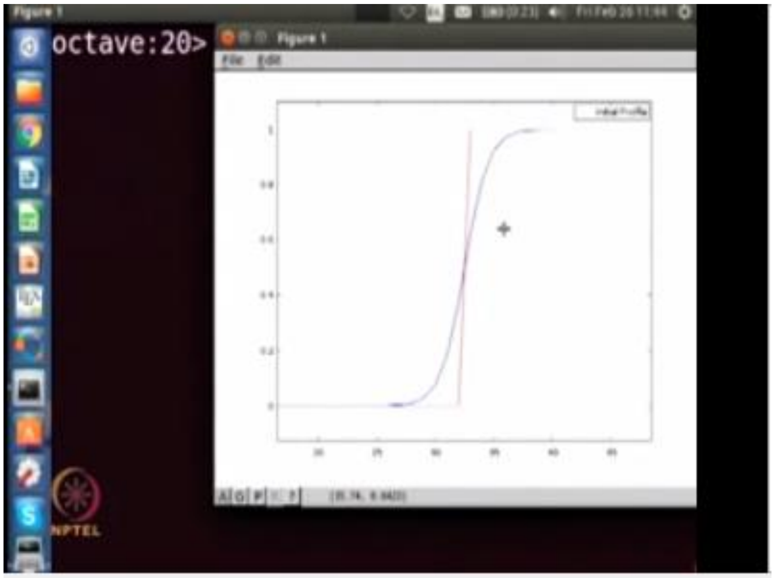

As you can see the initial profile is taken to be this half is one and it forms a nice tan hyperbolic interface in the case of alençon equation also so alençon equation in 2d if you try to solve. The same problem it is not stationary like this will move so in this case also you can show that the solution is tan hyperbolic and in the case of moving solution it is tan hyperbolic of x minus VT that is the velocity of this point if you take into account with time.

Then it will move with the same profile so basically this profile will shift to some other point after some time so that is how the evolution of the colonel alençon equation solution looks like okay. So this brings us to the end of this section alencon equation is fairly well-known it is also known as time-dependent Ginsburg land of equation because in the super conductivity literature it was Ginsburg and Landau who wrote an equation which is very similar to this it is also known as so there is this computer scientist called Alan Turing who wanted to understand the pattern formation on animals like zebras.

So he wrote a similar reaction diffusion equation for what he called as chemical morphogenesis so you will be able to look up Google for touring and chemical morphogenesis you can get his paper the equation is not very different so the equation is very similar to what we have written in fact when 2d we will look at the patterns that are formed by the alençon equation and you will see that it remains one of these patterns that one sees in nature.

So these equation even though we look at them from the material science metallurgy point of view or more well-known more widely use d equations they are basically I mean from a mathematical or numerical implementation point of view just diffusion equations nonlinear diffusion equations and in which way you introduce non-linearity makes them corn Elinor alençon equations and but from a physics point of view they are very different I mean the constitutive laws and the conservation laws.

That goes into deriving these equations are very different but from a purely mathematical point of view you can think of them as nonlinear partial differential equations which are like modification of classical diffusion equations which leads to interesting patterns and microstructures are patterns and they are interesting not only because they look nice but also because they determine.

The properties of any material and the processing besides microstructure which in turn besides property so the processing property correlation is through this bridge of microstructure so when we want to understand how I should process this material to get this particular property what we are basically looking at is how to I tune my micro structure so that is why these models are very important facial model ideal for micro structural evolution.

So we will look at some of these cases in the lectures to come so they will be like case study so we will take one by one spinodal decomposition then order disorder transformation then we will try to put them together and look at something like precipitate growth and then we will complicate things by putting more than one grain and looking at grain boundary going and things like that okay thank you.

NPTEL
Principal Investigator
IIT Bombay

Prof. R.K Shevgaonkar

Head CDEEP

Prof. V.M Gadre

Producer

Arun Kalwankar

Digital Video Cameraman

&Graphics Designer

Amin B Shaikh

Online Editor

&Digital Video Editor

Tushar Deshpande

Jr. Technical Assistant

Vijay Kedare

Teaching Assistants

Arijit Roy

G Kamalakshi

Sr. Web Designer

Bharati Sakpal

Research Assistant

Riya Surange

Sr. Web Designer

Bharati M. Sarang

Web Designer

Nisha Thakur

Project Attendant

Ravi Paswan

Vinayak Raut

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