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

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Module No.16
Lecture No.67
Interfacial energy: numerical
Versus analytical value

Welcome back let us go back to the script that we wrote in the last lecture for solving the consulate equation and calculating the interfacial energy so I am going to take the same script and I am going to run it in octave and from there we will take up comparing it with the analytical solution that we have a ride right now okay.

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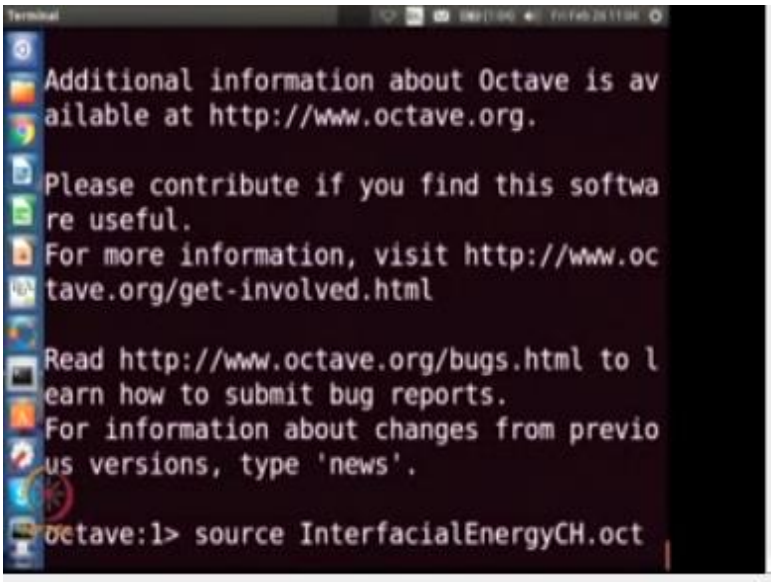

So as usual we go to octave so I am in the right directory and the code that we wrote was called interfacial free energy dot-com here dot OCT.

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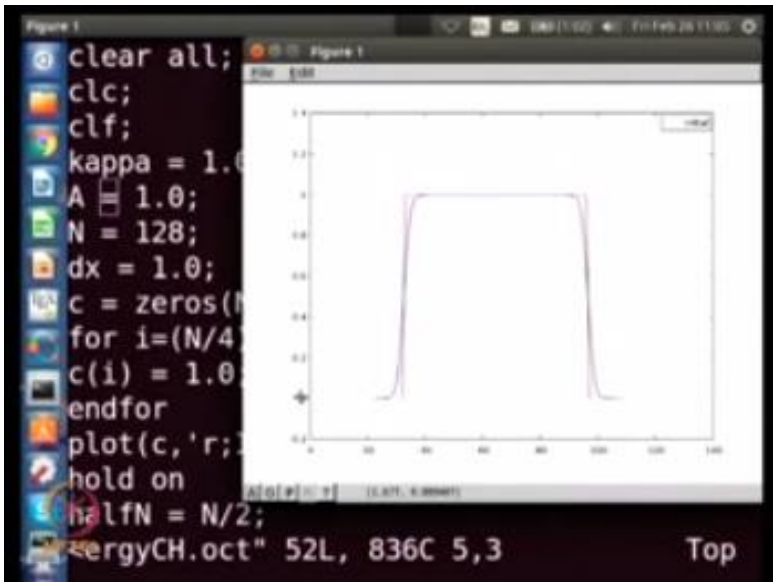

So let us run that and let me also show you that you so the PA the kappa value and a value that I am using or one that is for which I am trying to get the solution and there is a small difference between the analytical solution that we obtained and the numerical solution that we have obtained see the analytical solution was obtained assuming that as x goes to infinity the composition remains at 0 as X goes to plus infinity the composition remain at one.

However when we are solving it numerically because we are using the food a transform we have to use periodic boundary conditions so the other boundary condition that this remains at 0 that remains that one is possible if you use the finite-difference technique but as you will see later in too deep finite-difference becomes too problematic so we want to solve it using four transform four transform demands that you have periodic boundary conditions so to be consistent with this periodic boundary condition is why we have made two interfaces right that is the reason.

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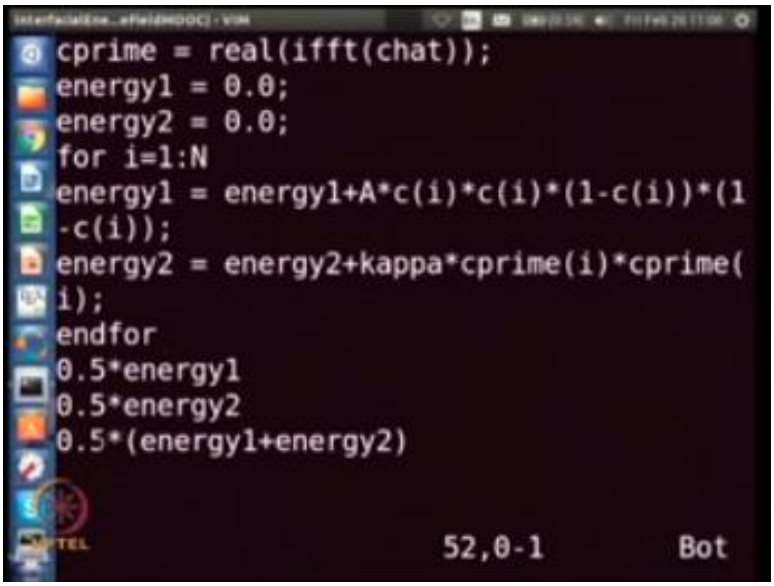

Why we actually calculated the interfacial energy and we divided it by two because instead of looking at one interface in this case we are actually looking at two interfaces ok now the solution for the continuity equation analytically was obtained assuming that at x equal to 0 is where the composition profile is point 5 so if i want to superimpose the analytical solution on this curve I need to know exactly where this is becoming point 5 okay so to do that let me look.

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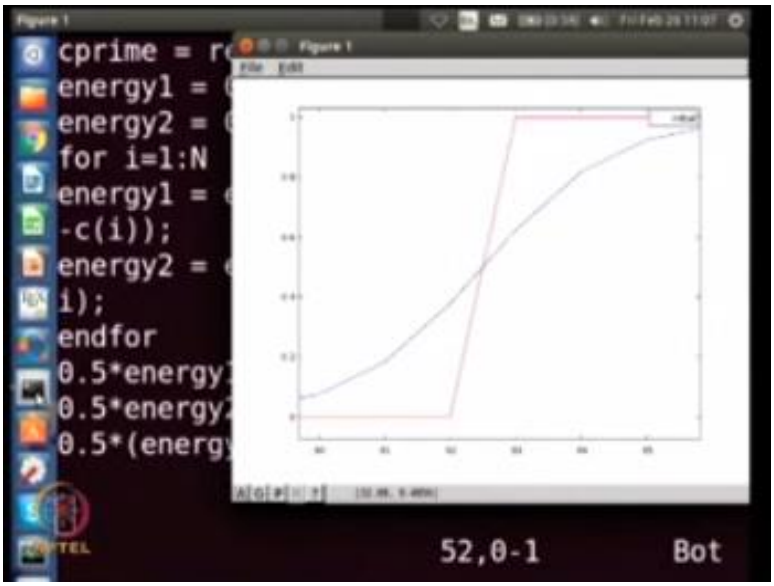

At this so I am just focusing on the area so where it becomes point 5 approximately 32.50 somewhere around 32.50 I can see that this is becoming point 5 so what I am going to do is that I am going to so let me get back to the figure let me make it go to be full form okay now I am going to take.

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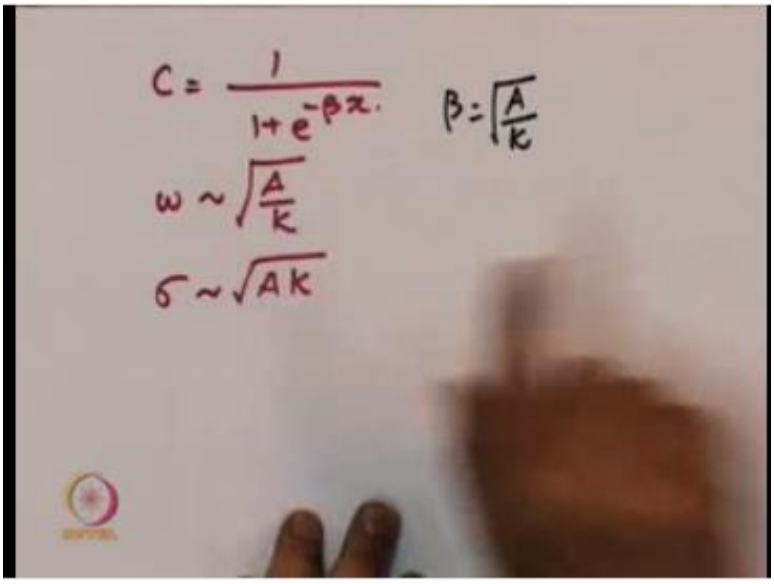

The octave window remember the solution n that we obtained is here so it is c is equal to 1 by 1 plus e power minus beta X that beta was a by Kappa okay and Kappa is one so beta is one our case 0 1 by 1 plus e power minus X is what we want so X let us take runs from0 to 32 sorry 64 okay so the elliptical solution that I want to plot so I want to say hold on.

So on the same plot I want I want to plot x comma 1 by 1 plus exponential minus beta is 1 X but X should be shifted to have its origin at two 32.50 so ex- 32.50 so that is the curve and I think that is one okay and I am going to plot it with a red open circles so that we will be able to easily identify that on the curve so let us go back to the curve.

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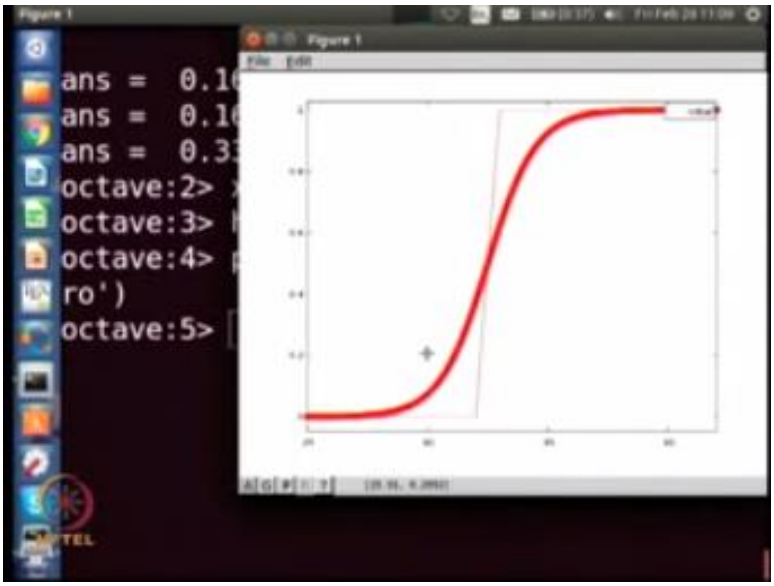

And see what has happened so as you can see the solution matches perfectly okay the points are too close let me clear the figure let me run the code once more so this time let us plot the few points so that we will be able to clearly see the interface okay and so I want to take but I do not want to take so many points let me take once every two points and I brought this.

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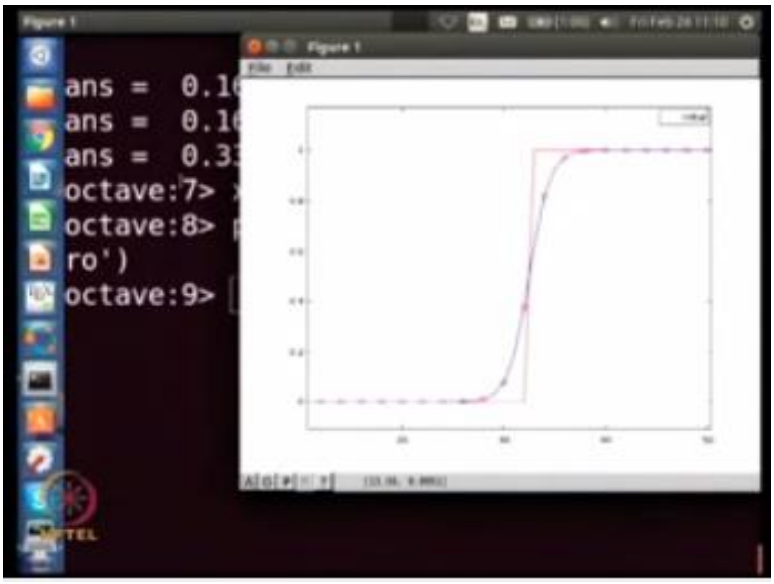

So you can see that the numerical solution is the line the analytical solution is the points and you can see that we are actually matching numerically the analytical solution okay now because beta is a by kappa and that is one the interfacial energy which is gamma by three and the gamma was root A and so that is one so you get 1 by 3 but the moment you change that.

For example let us go and make kappa to be four right what should happen to if I make up our to be for the beta should become half that means the interface should be come much wider and the interfacial energy should become twice so let us see if that is so okay so we run this and now the beta is half of the earlier beta so when we compared with the analytical solution I now need to change it.

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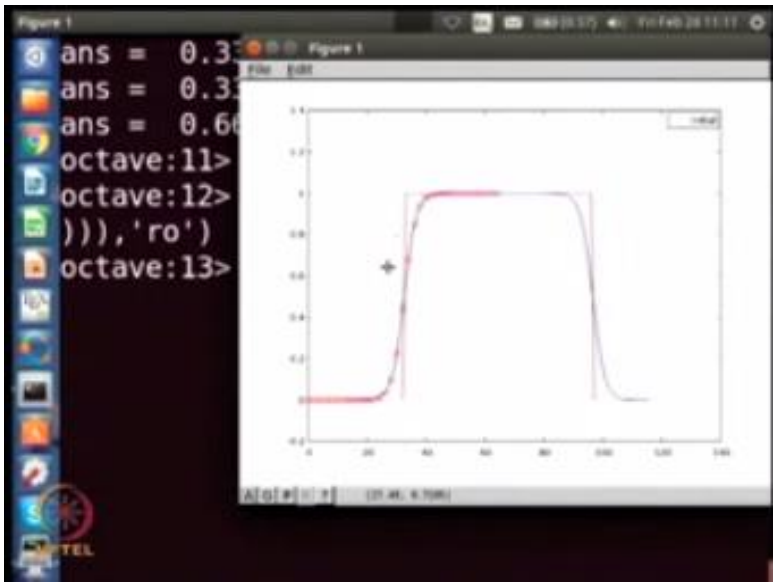

So let me go I define X now the solution so beta is half of what it was so it should be 0 point 5 into this okay so now let us go and see so you can see analytically the solution is matching and you can also see that the interfacial free energy has become double we can go back and make a to be four and copper to be one okay.

And again run the code okay and in this case now beta is twice so the solution will match if I take 1by E power minus 2x and the of something went wrong okay probably the I have done is not sufficient to take such huge a so let me take a 2 br2 and see if in which case it should be root yes so let us see a square root of 2 into1 by 3 okay so that is the point four seven one so that is the answer we are getting.

So it is scaling as a root a the interfacial energy and to get the plot so we will take X and we now have to change this Oh point 5 2 square root of two so that is one point for whatever so when now when we go see again we will see the match the reason why for it was not running is that interface now you can see has hardly let us look at that also.

So that is why it was giving n a n see interface now has one two three four points okay when you wake the a value still higher there will be hardly any points at the interface and hence numerically the DC by DX that you calculate blows up and that is the reason why we had any n so when you make a larger probably you have to decrease the distance okay so instead of taking b x to be one probably you have to take the x 2.5 or something so that you will have more points to capture the interface.

So that the much sharper variations can be captured then you will not have a problem okay so this is just to prove that the numerical solution that we obtained our taste in1d we are able to compare with the analytical solution that we are able to derive not just the solution we are able to compare the interfacial energies we know that they match we know that the interfacial wits also match because the profile is changing with the different alpha beta values and but that weal ready know from the parameters that we use and we are able to match.

So this shows that the numerical solution that we got is indeed correct it also shows something else that if you look at the error point four seven one the error in the energy that we are calculating is in the fourth decimal place okay it is very hard to get this Sakura see if you use a technique like finite difference. For example okay for it is very difficult to get to the interface profile which equilibrists sand matches with analytical solution because that will take much longer time and much computer resources for you to do.

But even after you do the error would still be higher than what we are getting this is because spectral techniques are probably the best techniques for obtaining these numerical solutions okay they are they are the most accurate that you can think of so that is the reason why we are getting very good accuracy for the interfacial energy also we saw that even in the case.

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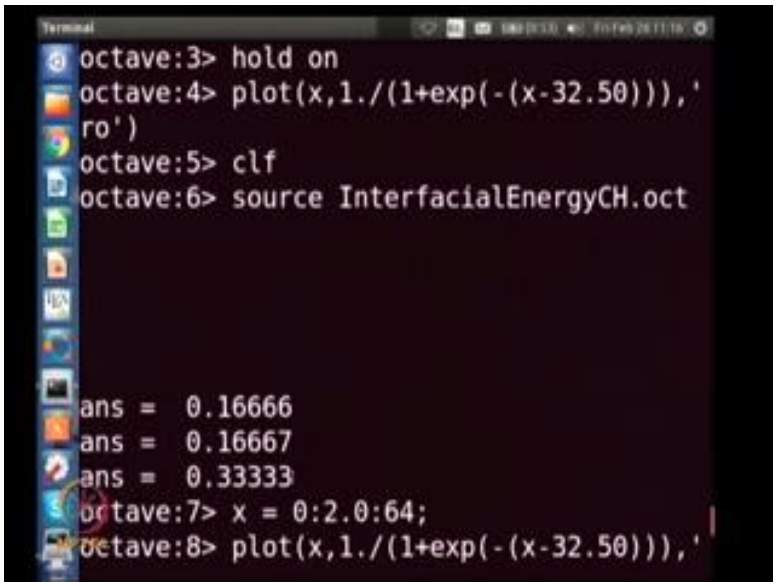

When we had the interfacial energy to be one-third you can see that one two three four five up to five decimal places I do not see any difference so it is 0 point 3 333 so that is one third case so the solution is and when we made it twice we gave we got a point six so point 68 so it is very accurate solution that we are able to manage with the spectral technique so that is another thing that I wanted to draw your attention too.

So in the next lecture we will look at another phase field equation which is known as alençon equation unlike the classical Cahn-Hilliard equation I am not going to spend too much of time in deriving it will do a short derivation and then we will try to solve it numerically and you will see that that equation also has at an hyperbolic kind of solution so that is what we will do in the next lecture thank you.

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