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

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Module No.10
Lecture No.40
Explicit method
With PBC

Welcome we are looking at the explicit method with periodic boundary conditions and we are having some difficulties in getting the solution so I have noticed a couple of errors so I am going to go through the script.

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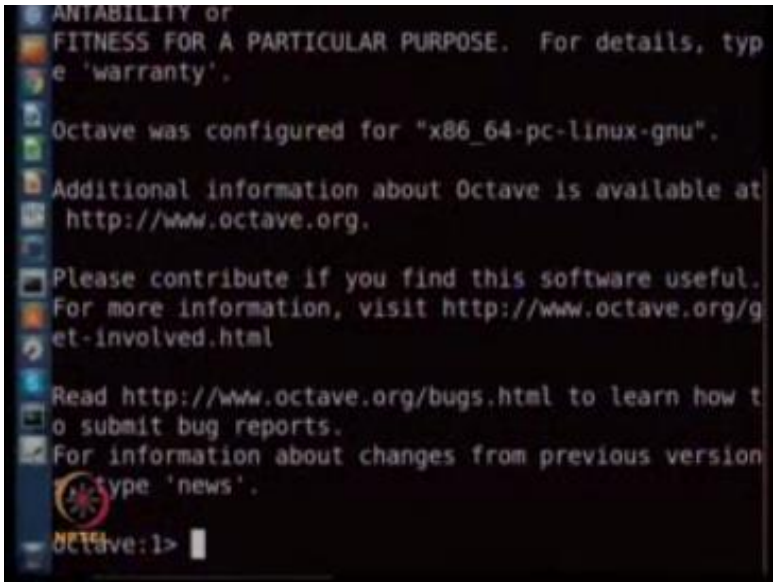

Once more and let.

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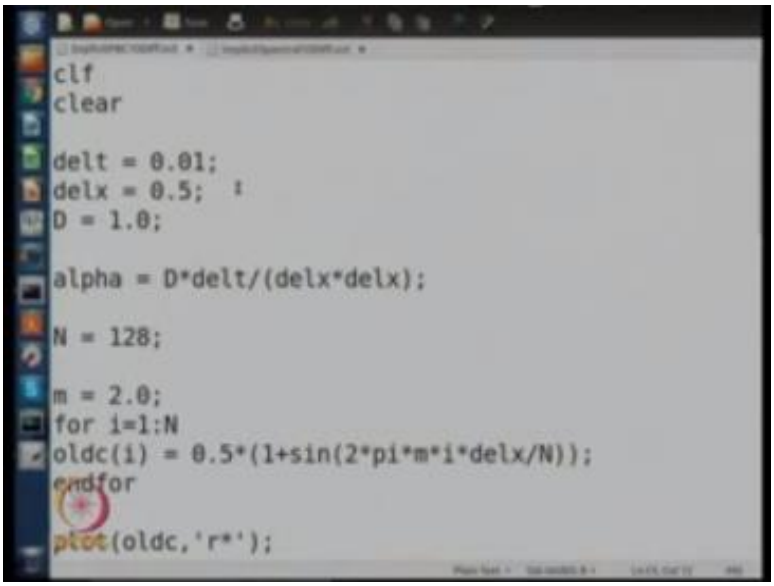

Us fix the errors and then run the code so we have the figure clear and then clear the all data that might be there and delta T is 0 point 0 1 and Delta X is point 5 d is 1 so alpha is defined as d times delta T by del x squared it is128 and because Del X is 0.5 m should be equal to 2 if you do not take e m to be equal to 2 because del x is 0 point 5you are getting just one half of the sine curve that we saw right.

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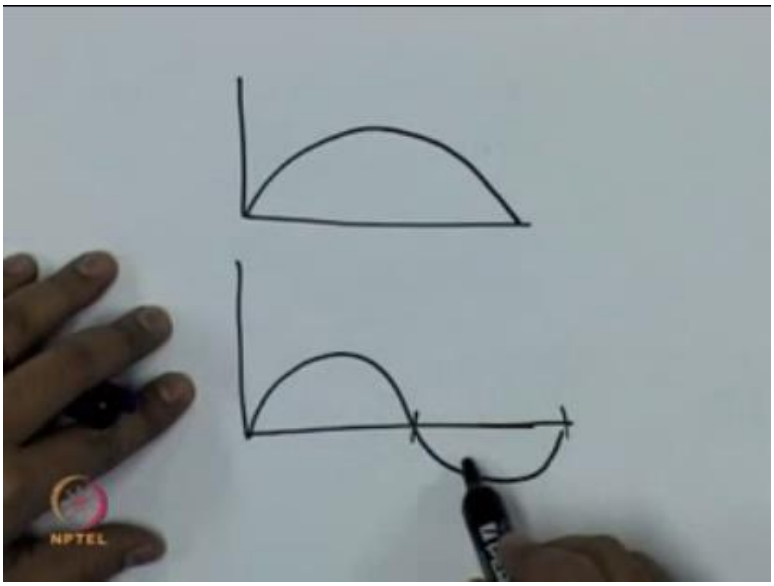

We are seeing that the composition profile looks like that instead of looking like that this half is missing because we are taking a delta t delta x.

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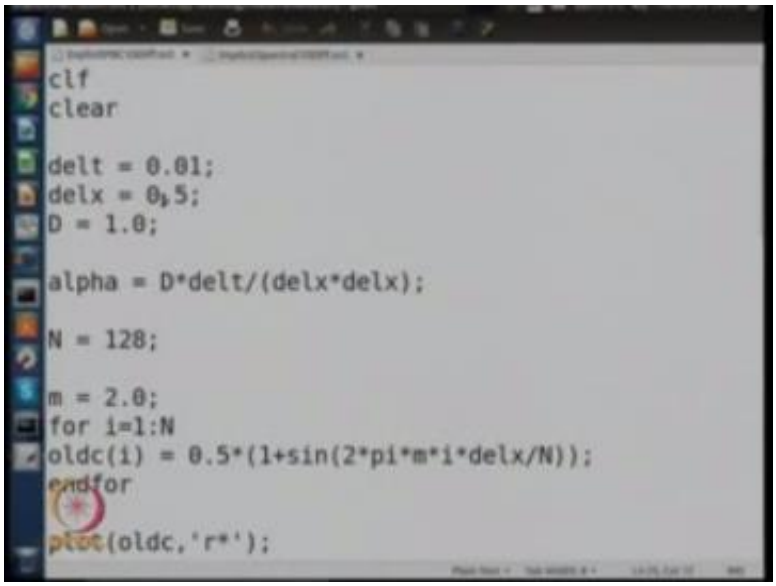

Of point five as we see here if you take Delta X of point five then the n becomes 64 and so we should take e m to be equal to 2 to get two waves okay so that is the first error that I noticed the rest are okay except for one small typo which is hard to catch it took some time for me to figure out so in this far I equal to one to n I just wrote I to n ok so that was an error and that is the reason why there was no evolution of the composition profile.

So I have corrected these two the rest of the script is as usual so we have the initial profile defined and then initial profile plotted with red stars then hold on and then this is the loop for plotting this is the loop for time evolution this is the loop for evolving in space and we define west and east point which is I minus 1 and I plus 1and the West there is no zero point so if you reach a zero point that is for the leftmost point the first point when you look at the west point we are going to assume that that is West plus N and if you are at the rightmost point and you are looking to the east point there is no east point.

So we are going to subtract 10 and take the first point to be the east point for the last point okay so this is periodic boundary condition then we evolve composition and we take the world to see the currency as the old sea and then we go through the loop and after that time loop is over then

we plot the composition and then end the plotting loop and then we take the figure as explicitly d0 DBS okay.

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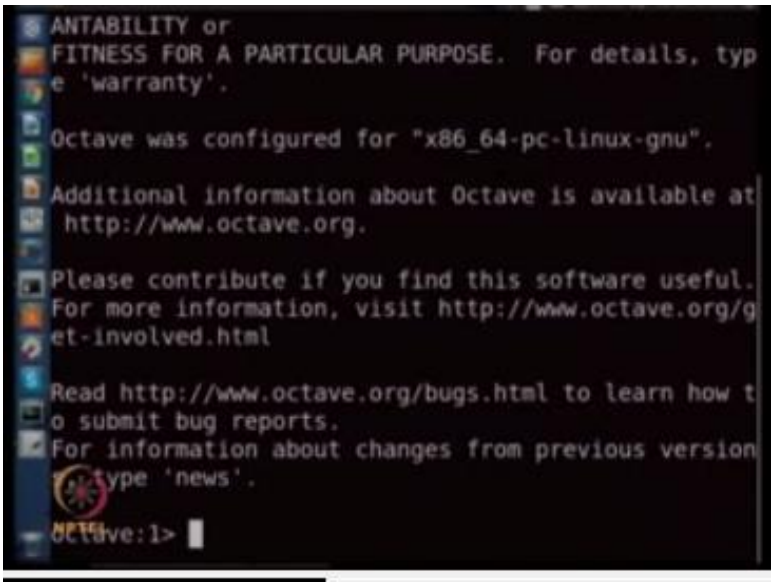

So let us run this code so I am in the right directory in which i have invoked octave that I can check so present working directory it says desktop or teaching phase field so and I can also list.

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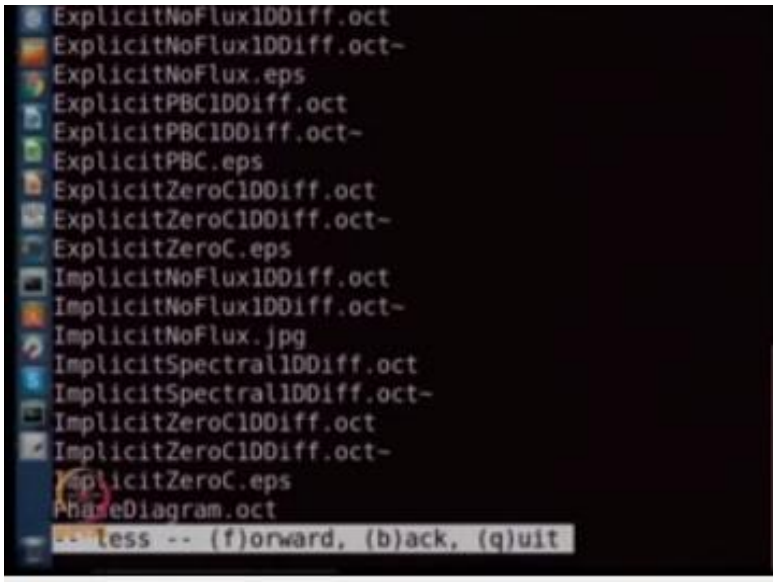

The files that are available so I can see that explicit periodic boundary conditions 1d diffusion dot octave is available ok so I am going to source that file.

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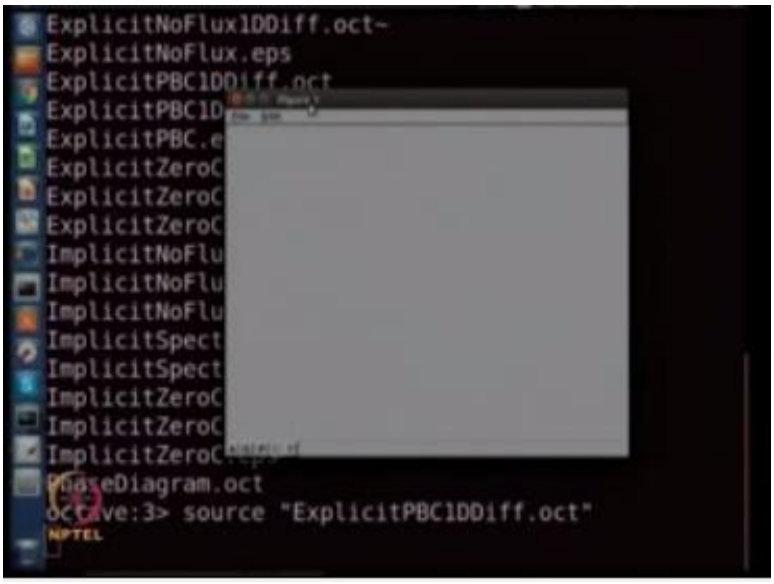

So what we are expecting is that because we have a sinusoidal profile like this.

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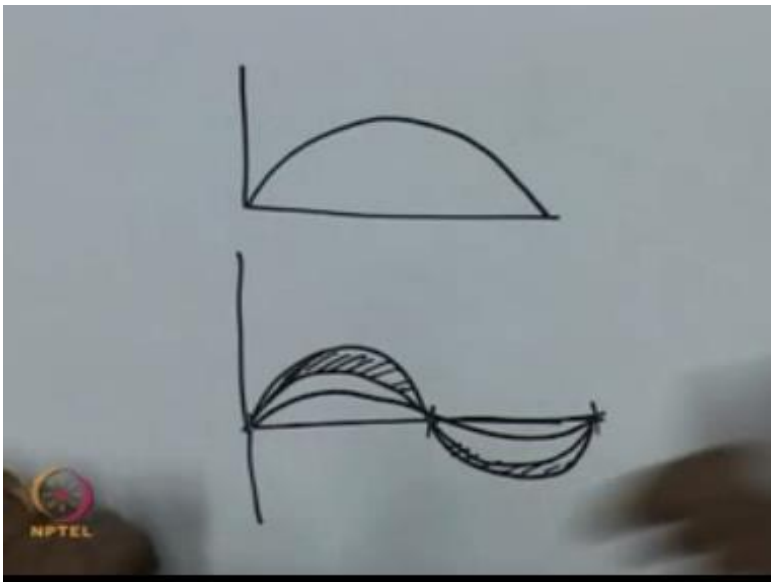

Alright so what we are expecting is that because this has a curvature like this at these points the composition should come down because this is zero curvature it should remain where it is and because this has a curvature which is positive I expect the composition profile to go up here so whatever extra material that is here should come here right and then it will go like that and then finally it will reach this point as you can see.

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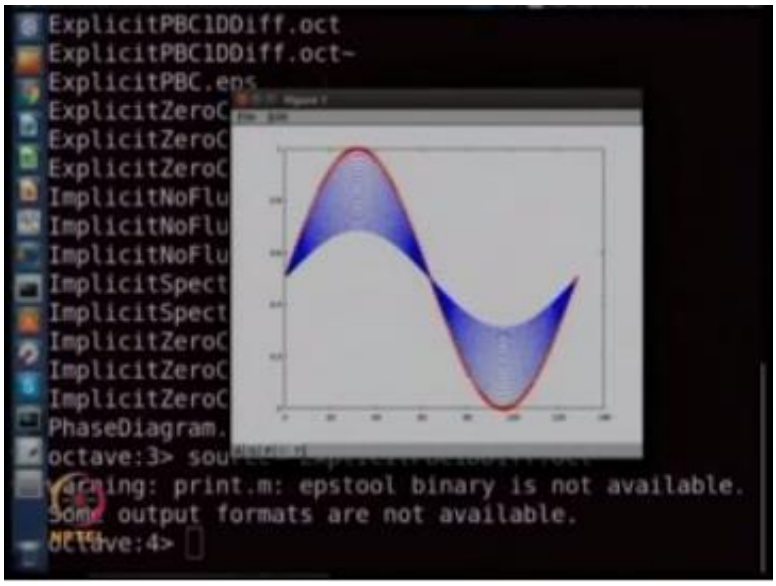

That is exactly what the solution of octave looks like so the red points or the initial profile that I had all the blue lines and there are 20 of them they are all corresponding to the composition profiles at different times and as us men of course this the point where there is no composition change because the curvature is 0 at that point so it is not going to change at all and near this point so wherever the gradients are high there is the composition changes larger and wherever gradients are smaller the composition changes are also much smaller.

So you see this nice curve that you get indicating that the Fick's second law says that compositional heterogeneities will be evened out this is the homogenization solution this is the meaning of Fick's second law second law says that the rate of change of composition at any point depends on the curvature of the composition profile if the composition profile has positive curvature in those points the composition is going to rise and if the curvature has is negative then in those regions the composition profile is going to go down.

So in the process any noise or any modulation you have can be thought of as to be consisting of positive and negative curvatures so they are all going to get evened out so this process is going to stop only when the curvature becomes zero everywhere so you have a flat light you have a

straight line parallel to x axis when composition is changing this position at all that is when this process is going to stop so this is the solution.

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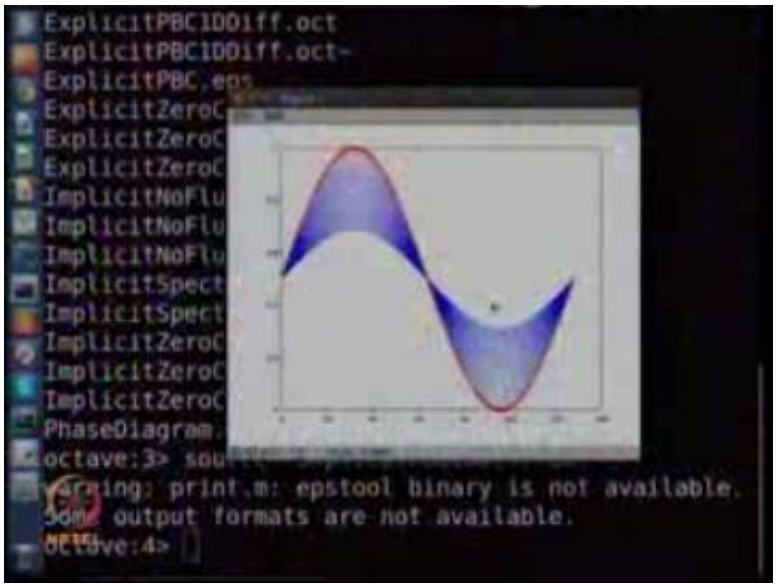

We had difficulty in producing this initially we had just one half like that and that did not evolve at all so that is because of the errors that I noticed and showed you now thank you.

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