Computational Techniques
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Module No. # 09
Lecture No. # 04
Partial Differential Equations

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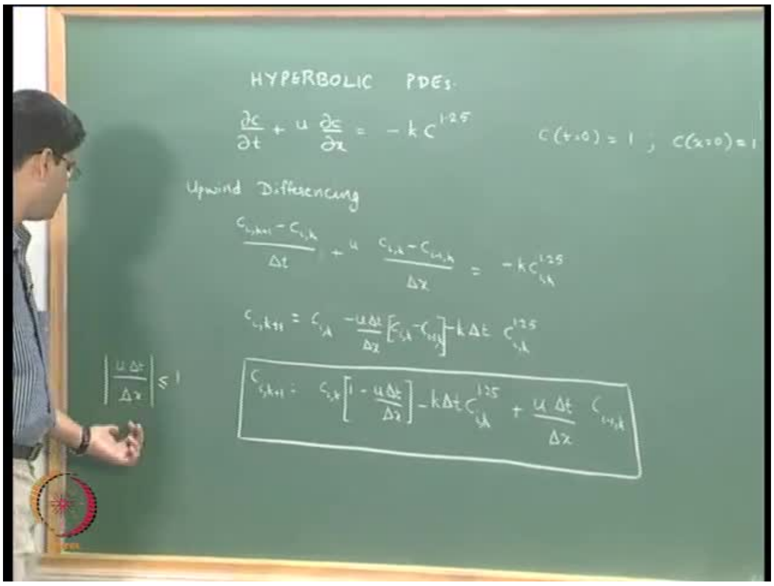

Hello and welcome to this last lecture in the PDE s module. In the previous lecture, we had we use microsoft excel to look at hyperbolic and parabolic PDE s and how to solve them using the forward in time central in space method. So, we were on hyperbolic PDE s and the example for hyperbolic PDE that we used was partial c by partial t plus u multiplied by partial c by partial x, equal to minus k c to the power 1.25. At the initial conditions c at t equal to zero equal to one and the initial condition c at x equal to zero also going to be equal to one.

So, this is the problem that we intended to solve and what we did was we use forward in time central in space differencing. We saw that for a small enough delta t of 0.1, still this particular method diverge, we got concentrations as negative values. So, next what we are going to do is we will use an upwind scheme because u is a positive value. What that means it is that it is going to be backward in sorry it is going to be forward in time and backward in space.

So, upwind differencing of the of this particular PDE is going to lead us to c i comma k plus one minus c i comma k, divided by delta t, is going to be equal to plus u multiplied by backward difference that is going to be equal to c i comma k minus c i minus one comma k, divided by delta x, is going to be equal to minus k c i comma k to the power 1.25. Then what we will do is we will multiply by delta t throughout, take these guys all on to the left hand side.

As a result of this, what we are going to get is c i comma k plus one is going to be equal to we have minus k delta t multiplied by c i comma k to the power 1.25. These guys taken to the left hand side will yield us minus u delta t by delta x multiplied by c i comma k minus c i minus one, comma k. This guy when we take that to the right hand side we will get this as c i comma k, which we can write this as c i comma k multiplied by one minus u delta t by delta x, minus k delta t c i comma k to the power 1.25 plus u delta t divided by delta x multiplied by c i minus one comma k. This is going to be our upwind differencing scheme.

Now, the stability of the upwind difference scheme actually depends on the value of u delta t by delta x and before as we had seen in the parabolic PDE s, with respect to alpha delta t by delta x squared. What we see in this particular expression also is that we need to satisfy the condition u delta t by delta x; the absolute value of that should be less than or equal to one.

So, that is the overall condition, u delta t by delta x should be less than or equal to one is the overall condition that needs to be satisfied. So, as we have done before, we will take the velocity u equal to one, delta x equal to one and delta t equal to 0.1. With this it satisfies that this particular value is less than or equal to one. Keep in mind, that the presence of this non-linear terms does complicate the stability results quite a bit, so the stability results are essentially derive as a without consideration of this non-linearity this non-linear term that comes in over here. So, if it was a homogeneous PDE we were guaranteed to have stability, if u delta t by delta x is less than or equal to one, else we will have the overall system to be unstable. So, let us try this particular example now with the upwind difference scheme, we will start off with what we had previously using the forward in time central in space method and then modified appropriately for the upwind difference method.

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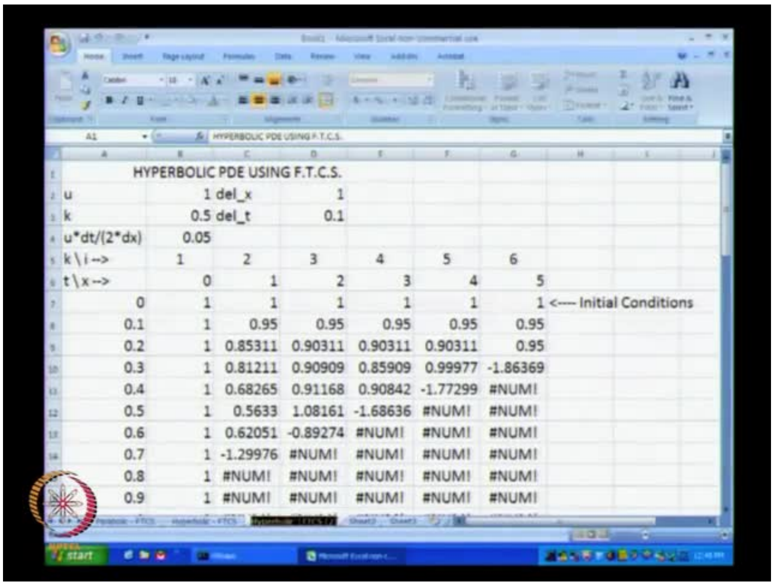

So, let us start where we had left off in the third lecture of this module. We will start off with the hyperbolic PDE s solving using the FTCS method. So, if we go to excel now. This was the excel sheet that we had obtain in the previous lecture using hyperbolic PDE solving using the FTCS method. What I will do is I will right click on this click on move and copy I will create a copy and what I want hyperbolic equation using upwind difference.

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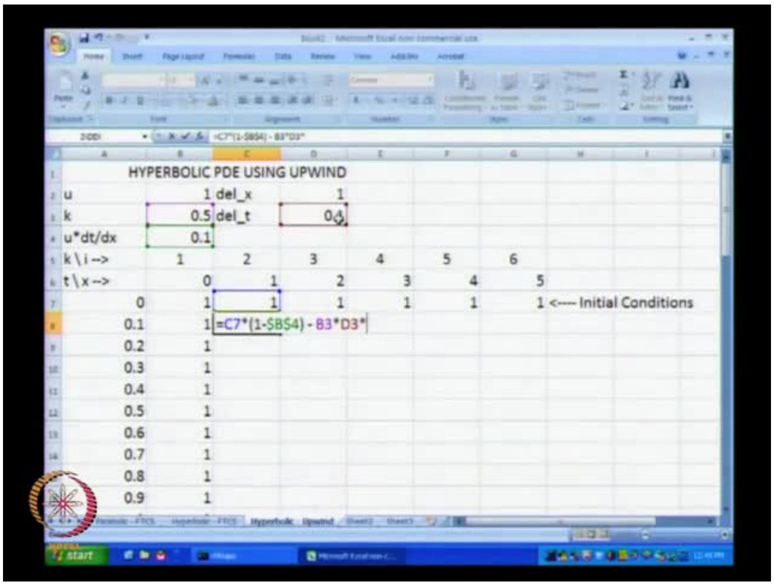

Nothing else actually is going to change over here in all these blocks. What is going to change is really everything from this point down. So, what I have done is I have deleted all these values, this point down, and these are the initial conditions. Our concentration was equal to one and these are our inlet conditions. Again at the inlet the concentration was also equal to one. Now, with the upwind difference scheme what we have is c i comma k plus one is going to be equal to, so what we will do in this case, now we require u delta t by delta x not by two delta x, so that is what we are going to compute. I will press F 2 and I will remove this part over here now what we have is u delta t by delta x.

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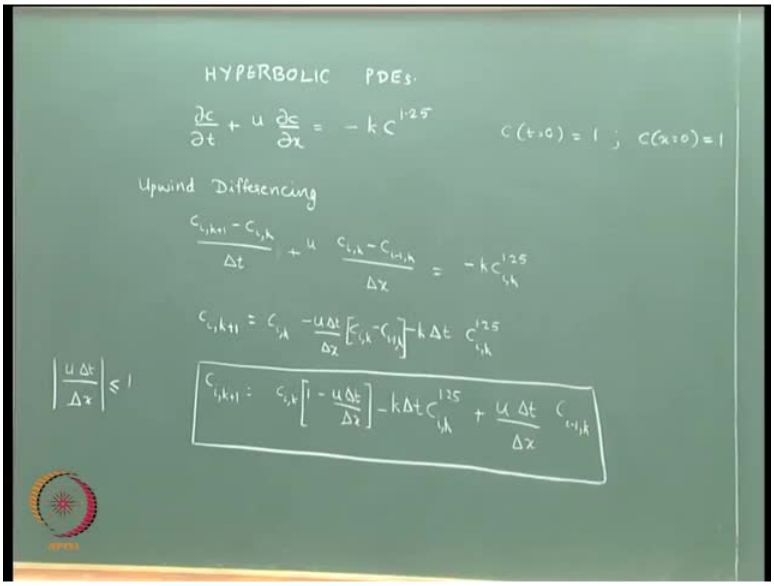

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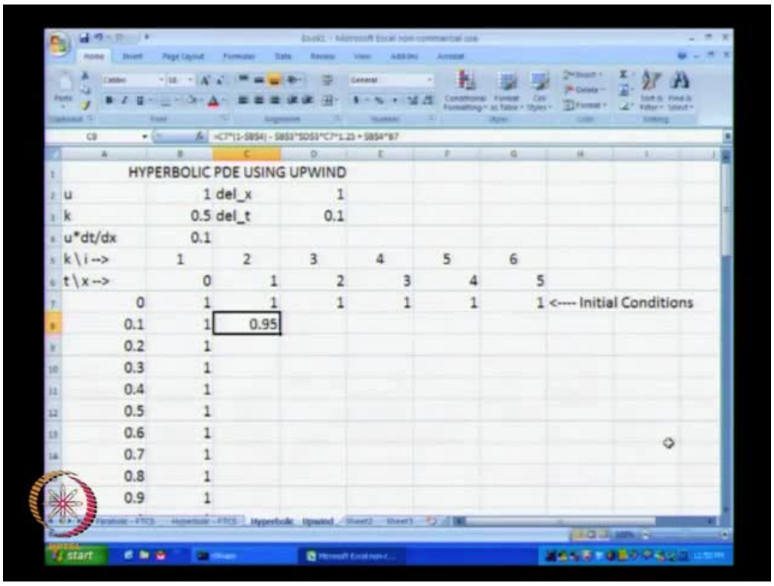

So, what we will do now is c i comma k plus one is going to be equal to c i comma k, which is this guy multiplied by one minus u delta t by delta x. I will put dollar signs. This guy minus k, multiplied by delta t, multiplied by c i comma k to the power 1.25. This is again c i comma k to the power 1.25. Now, because when i drag and drop, this k value and is delta t value is not going to change. I need to go back and put dollar signs at appropriate places, so we have k multiplied by delta t with the dollar signs there multiplied by concentration that is c i comma k to the power 1.25. The final term is going to be plus u delta t divided by delta x multiplied by c i minus one comma k; c i minus one comma k is this guy over here, c i minus one comma k, and i do need to put dollar signs for our u delta t by delta x term and that should do it.

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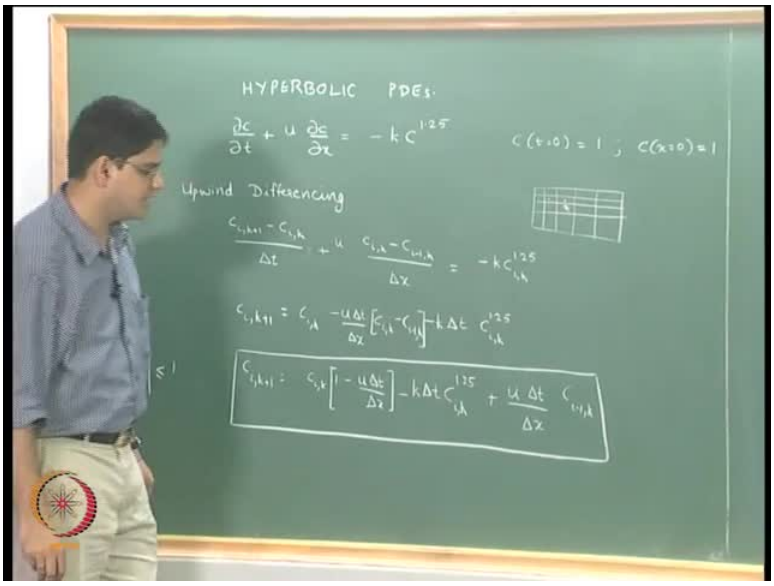

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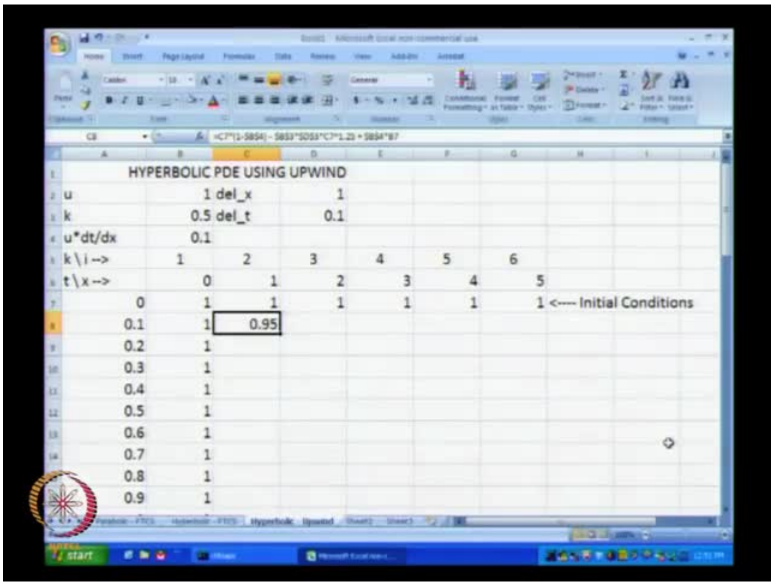

I will just quickly go on to the board and show what the expression once again. We just want to confirm that the overall scheme that we have obtain is indeed in the excel that we have written down is indeed what we had before. So, c i comma k plus one is c i comma k multiplied by one minus that u delta t by delta x term. This is what we have computed separately, minus k delta t multiplied by c i comma k to the power 1.25. So, if we are computing for one particular, so if this is a part of our excel sheet where we are computing for the various location and various times. If this is our c i comma k plus one, this guy is our c i comma k and this is c i minus one comma k, so we have c i comma k multiplied by one minus that particular coefficient minus k delta t multiplied by c i comma k to the power 1.25 plus that coefficient multiplied by c i minus one comma. So, let us go back to excel and check that this is indeed what we have obtained.

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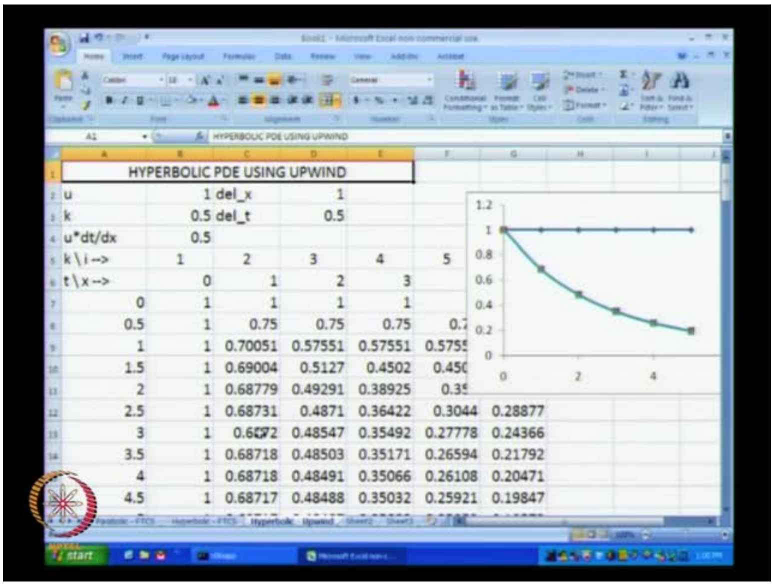

So, let us press F2 again and check that that is indeed what we have obtained. So, we are you trying to compute the value for this particular cell using values at these two cells. I will press F2 now, and we have the concentration in the upper cell multiplied by one minus that constant, which is over here, minus k delta t that is the k value that is the delta t value, multiplied by the concentration in the upper cell to the power 1.25, plus we had that particular coefficient. That coefficient again comes with dollar b, dollar b dollar four signs, that is over here multiplied by concentration in the upper cell but, one cell to the left and that is what we have over here.

So, this is essentially what we are going to get and I will just press enter and I will drag it along this particular row. Now, what I will do is I will highlight this entire thing, and then double click, and I will see that our solution indeed is stable. This particular solution is indeed not unstable and our concentration is decreasing both with length as well as with time. So, I think, we will need to go a little bit beyond time five. Maybe, we will go up to say time ten, so this is the overall concentration along the length of the reactor at time ten. We have started along the length of the reactor, the initial conditions, at all the concentrations equal to one, as before. Let us go and make a plot, insert for plotting this particular guys, we will highlight these two rows and this one scatter.

So, as the length changes, our initial condition is that the concentration is all going to be equal to one. I will delete this and I will as before increase the fonts, so that everything is readable. I will delete this grid lines and I will just make this particular guy little bit shorter. Now, select data and we will add data at time one, two, five and ten, let say or one, two, three and ten, maybe, and I will select the concentrations along the length of the reactor.

I will select the concentrations along the length of the reactors as the y axis. This is the x axis, the concentration along the length of the reactor are going to be the y axis, and that is at time one. I will add one more series and that is going to be at time two, the x axis data remains the same the location along the reactor. The y axis data will be the data at time two this and this is going to be how the concentration changes in the reactor with time and space.

So, this is the concentration at the initial time, t equal to zero. This is the concentrations profile that we get at t equal to two; this is the concentration profile- sorry t equal to one. This is the concentration profile we get at t equal to two, this is the profile at t equal to three and this is what we get at t equal to 10. It has converged and this is essentially going to be our steady state concentration profiles in our PFR, transient PFR.

Now, let us go and change our delta t from say 0.1. We will change this 0.2 and when we change this to 0.2, again, we find that the solution has still converged that is because u delta t by delta x is still going to be less than one. Now, let us change our delta t equal to two, and when we change our delta t equal to two, what we see is really what we are getting over here, if you see over here is that it is the concentration at time six has become negative and in indeed the concentration at location four at time 10 has minus 50 this is minus 150 and minus 400.

So, what we can see over here is that when the delta t is fairly high, at that time our overall solution is going to diverge. Likewise, the solution will diverge, for another value of delta t; say if we take delta t as 1.5. If we take delta t as 1.2, again we are having our solution diverge; solution is diverging a little more slowly, when our delta t values are closer to one. But, when our delta t values are further away from one, our overall scheme diverges very quickly. Now, when our delta t values, we take less than one again say 0.5, finally, will get our system to converge.

So, the overall take home message over here is that upwind scheme indeed is able to solve the hyperbolic PDE s. The upwind scheme is not globally stable scheme. We have a range of delta x values and delta t values for which the overall upwind scheme is going to be stable. So, let us now go and recap what we have done so for and the overall methods of solving hyperbolic parabolic and as well as elliptic PDE s. We will just recap all these methods and finish off this particular module.

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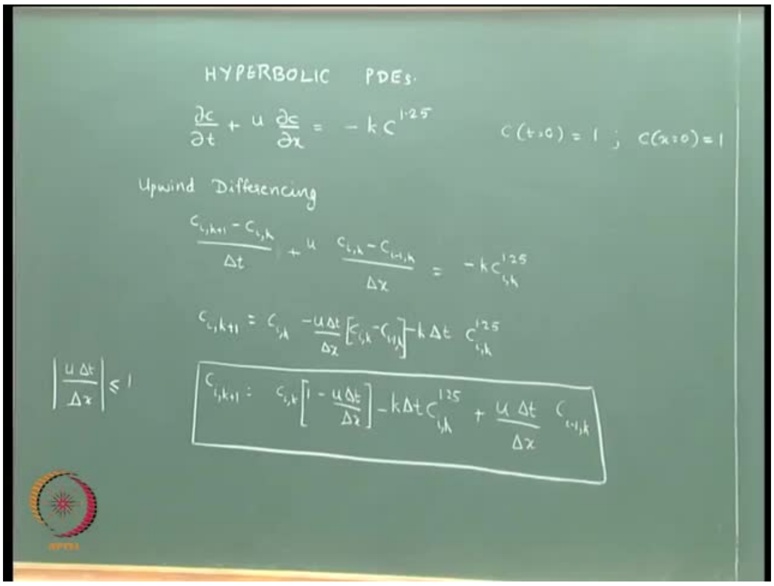

So, what we have done in today's lecture is taken a look at hyperbolic PDE s, but instead of using a central difference scheme for d c by d x, we have use a backward difference scheme for d c by d x. We use the backward difference scheme, because u value was positive. If u is negative we will use a forward difference scheme for d c by d x. when we did that and when we substituted all these guy in this overall equation. This is the final expression that we obtained. This is the expression using the upwind difference scheme for hyperbolic PDE s. Exactly, in the same way for parabolic PDE s, we can indeed use central difference scheme for d square c by d x squared and the reason for that is that indeed hyperbolic PDE s are going to be unstable for FTCS method, whereas, parabolic PDE s are going to be stable for FTCS method under certain conditions.

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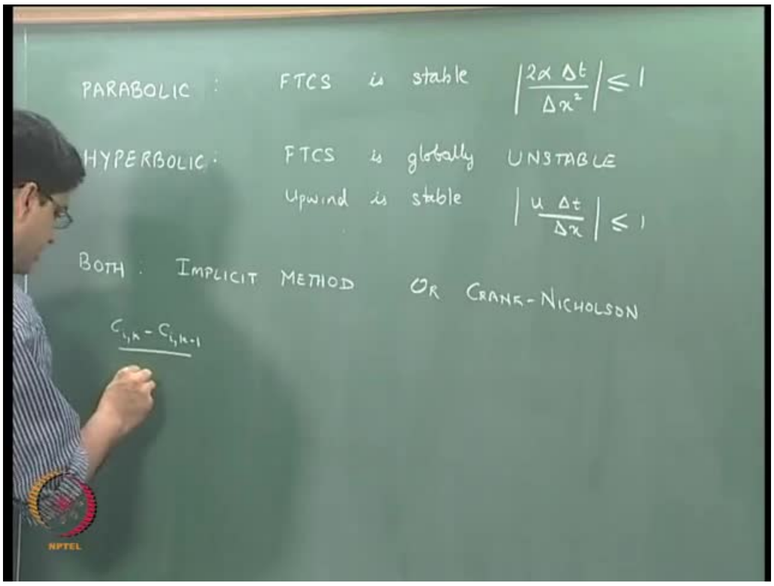

Conditions that we had obtained FTCS method is stable if 2 alpha delta t by delta x squared is going to be less than one. For parabolic, FTCS is globally unstable, which means that you cannot use the FTCS method. Whereas, the upwind scheme is stable if u delta t by delta x value is going to be less than or equal to one.

So, these were the conditions that we obtained for the I am sorry I have exchange hyperbolic and parabolic over here. (No volume between: 19:20-19:29) Parabolic, hyperbolic, and for both the schemes, sorry, both the parabolic and hyperbolic systems, we can use either implicit method or Crank-Nicholson method, the implicit and the Crank-Nicholson methods are going to be globally stable methods. What I will just show you is what expression we will get if we were to use implicit method, for the same hyperbolic PDE that we have over here. In case of an implicit method, instead of c i comma k plus one minus c i comma k, we are going to use c i comma k minus c i comma k minus one divided by delta t.

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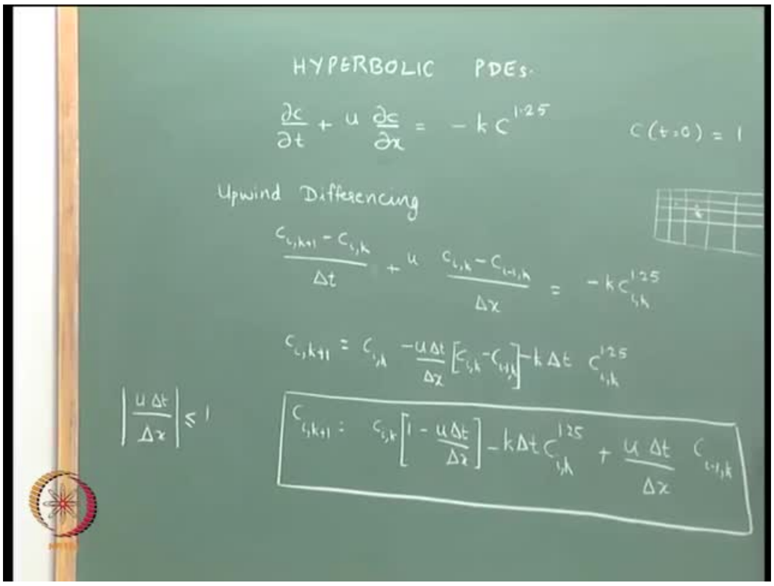

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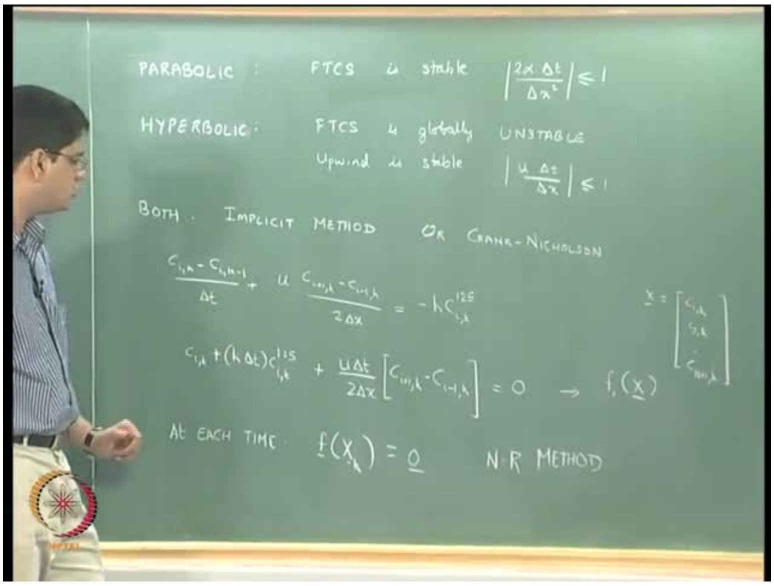

So, that is the only change that is going to happen. So, c i comma k minus c i comma k minus one divided by delta t plus, we can we will retain central difference in space, so we will have u c i plus one comma k minus c i minus one comma k divided by two delta x, equal to minus k c i comma k to the power 1.25. What we then need to do we will multiply by delta t throughout by n and bring this guy on to the left hand side. That will actually yield us c i comma k plus k delta t, we will move to the left hand side. So, we will have plus k delta t multiplied by c i comma k to the power 1.25, plus u delta t divided by two delta x, multiplied by c i plus one, comma k minus c i comma, sorry c i minus one comma k is going to be equal to zero.

Now, this is an implicit expression. It is an implicit non-linear expression or non-linear equation, in c i comma k, where i goes from one to n plus one. So, we will have n plus one equation in n plus one unknown, which we need to solve simultaneously. So, this particular equation becomes the ith equation f i in X bar where and I will use a capital x bar over here rather than small x bar, where X bar is going to be equal to c one comma k c two comma k and so on up to c n plus one comma k.

So, what happens is that at each time, we will have, if we were going to use either an implicit or a Crank-Nicolson method. At each time, we have to solve f bar of X bar k going to be equal to zero bar. We can solve this using say the Newton Raphson's method and we can keep repeating this, at every iteration, at every time step, in order to finally, get the overall solution for the various concentration c, as a function of time and space. At each time, when we solve this equation, we will get concentration c along the length of the reactor at that particular time. Then we go on to the next time we get concentrations along the length of the reactor at the next time so on and so forth.

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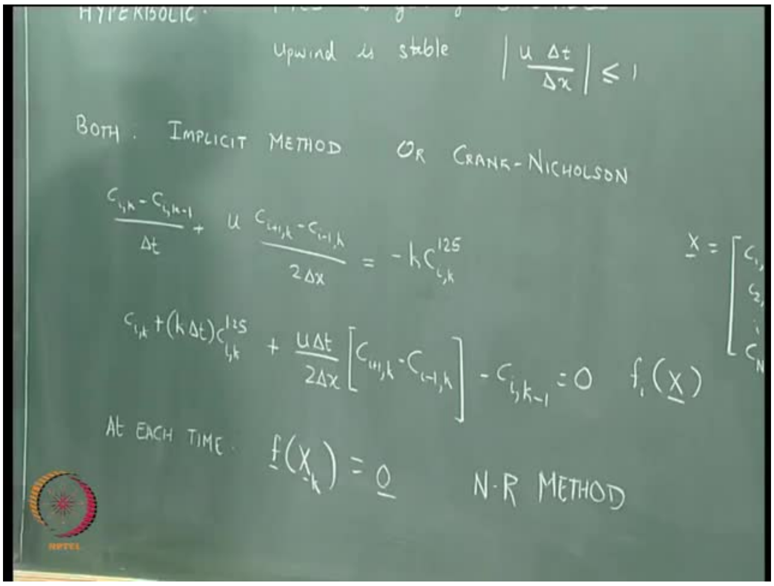

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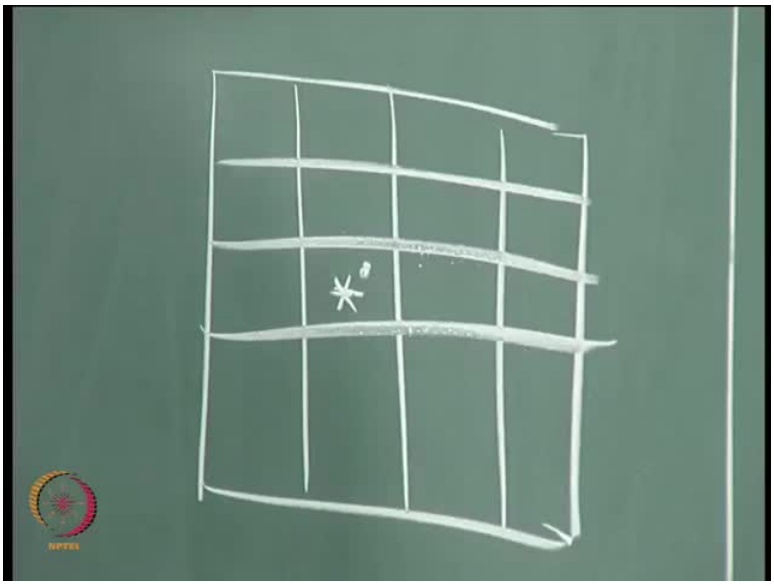

So, that is essentially what we are going to get by solving this particular equation using implicit method. So, this is the term c i comma k over here, c i comma k multiplied by k delta t, we have moved on to the left hand side. This is a term that I have missed out actually. So, this particular thing is little bit incorrect. I do have to in cooperate that term also, minus c i comma k minus one equal to zero. So, this is how the overall expression is going to look like.

Now, if we go over to look at our map in microsoft excel that this is the kind of map we had obtained where this starts species or sorry the start value, we were getting it from the two values above. But, instead if we are going to make the same kind of a block for this system over here and this is the star is the value that we are interested in finding that is c i comma k.

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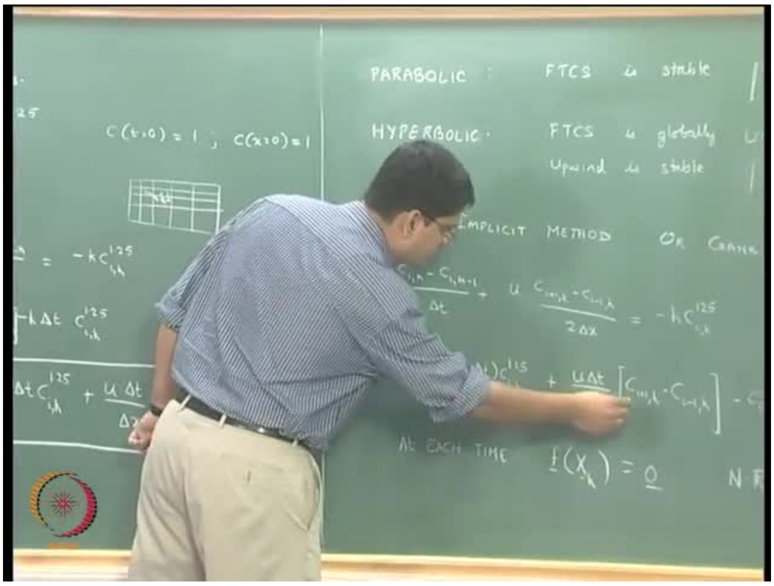

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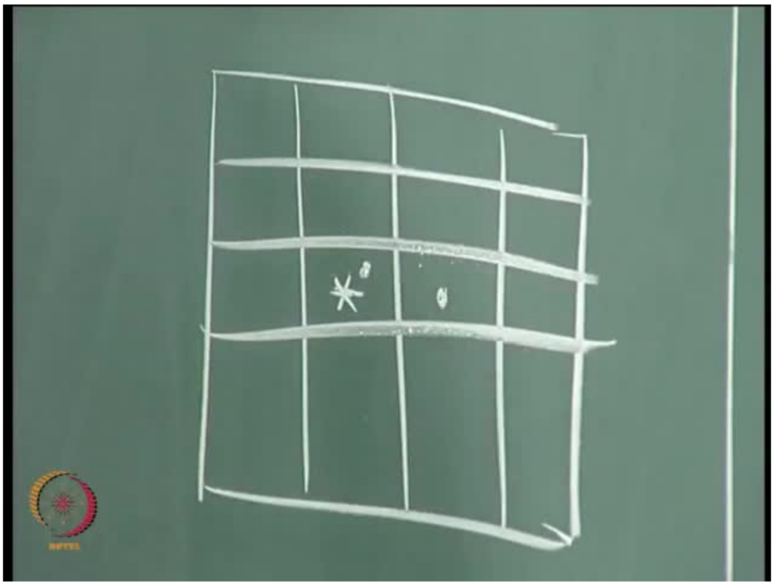

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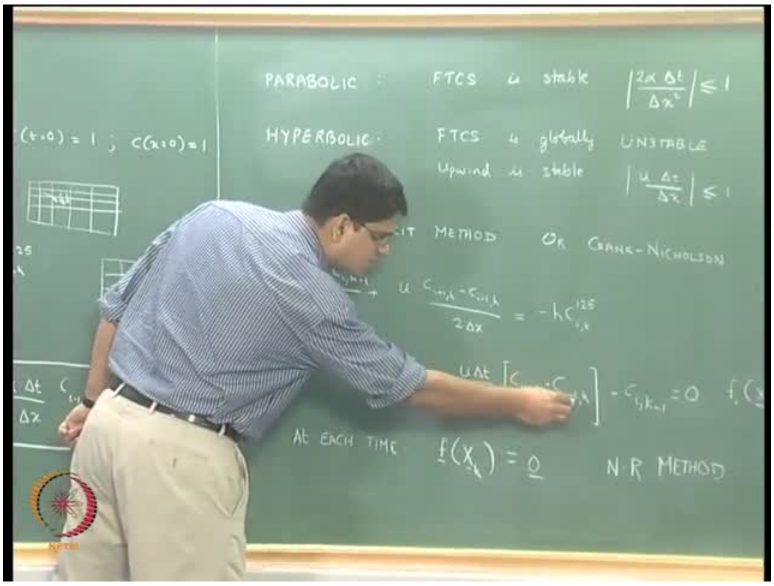

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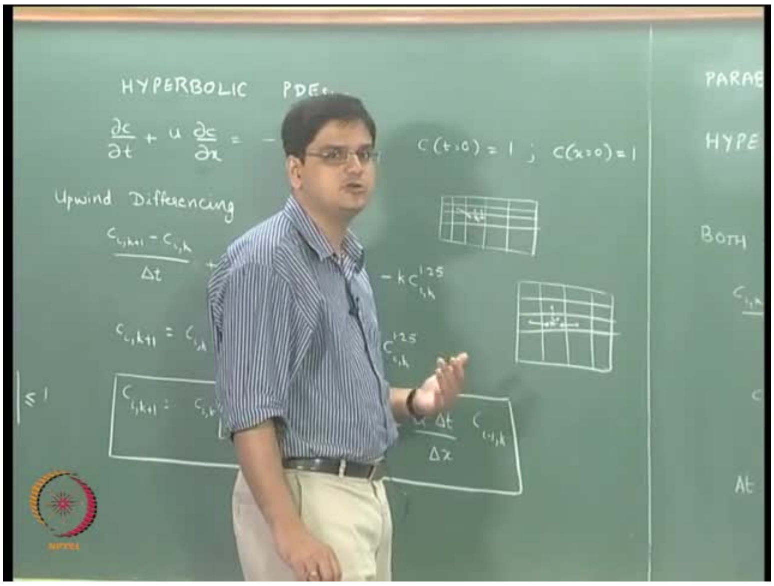

Now, c i comma k depends on c i comma k itself, so I will put a dot in this particular block, as well as it depends on c i plus one comma k, so it depends on this guy. It depends on c i minus one comma k, which basically means that it depends on this guy. As well as it depends on c i comma k minus one, which means it depends on this guy. So, when we are using central difference scheme in a space and we are using and fully implicit method, the value of star depends essentially on the values, at the same time, and the values at the previous time as well.

So, this is the overall linkage of any cell in the microsoft excel is what we are going to get, whereas, in an explicit method the values at this cell are only link to the values at previous cell, which values we already know. As a result, the explicit methods are much easier into solve using any of this standard techniques. The implicit methods are that much more difficult to solve. The advantage we get within a implicit method that is that that implicit methods are going to be globally stable.

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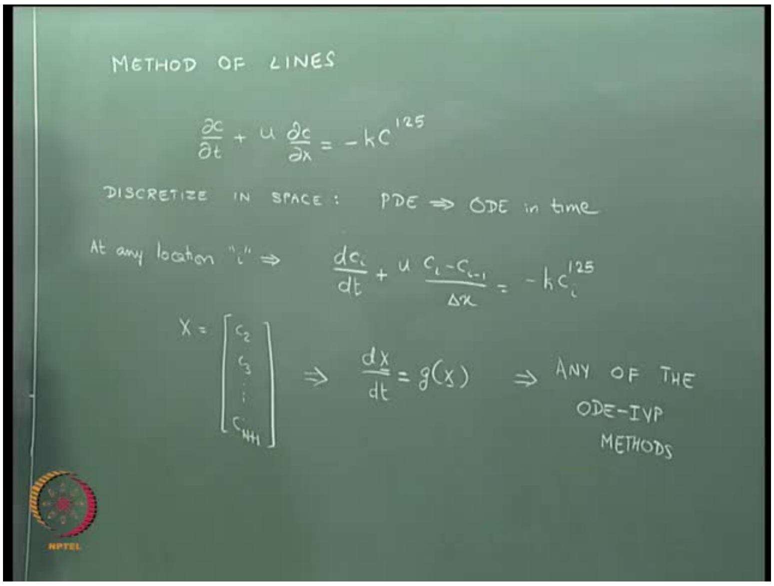

Now, we will go on to one finally, aspect of solving PDE s using what is known as the method of lines. I will mention that just for the sake of completeness, method of lines, is applicable for hyperbolic as well as parabolic PDE s. it is not applicable for elliptic PDEs and the idea behind method of lines is that you have for example, dou c by dou t, plus u dou c by dou x equal to minus k c to the power 1.25. The idea behind method of lines is discretize in space only. When you discretize in space our PDE gets converted to ODE in time. What I mean by that as before we just discretize c in terms of c one, c two, c three up to c n plus one, we do not discretize this in time.

So, when we discretize this in space for at any location i; at any location i, what we are going to get is d c i by d t is plus u multiplied by c i minus c i minus one divided by delta x, is going to be equal to minus k c i to the power 1.25. We will be able to write this for all of the locations. In case of location two, we will have c i minus c one, sorry we have c i minus c two minus c one and c one is going to be give in to us as c one was equal to one.

So, we would not actually use n plus one equation in n plus one unknown; we will actually use n ODE's and n unknowns. We can then solve the n ODE's in n unknowns. So, what we will define our x as; x we will define as c two c three and so on up to c n plus one. Keep in mind, c one is going to be equal to one, so c one equal to one is not an ODE. It is an algebraic equation, so we would not involve c one in this particular equation, in this particular scheme. When we define this we are going to get d x by d t is going to be equal to some g of x bar.

This d x d c by d t depends on c i and c i minus one only as a result this g of x bar. In each of those g of x bars c, c i is going to depend only on those two components. So, this is the overall ODE that we are getting. So, from the PDE we have finally, gone to ODE and this ODE, (no audio between: 29:45-30:01) we can solve it using any of the ODE-IVP methods for example. We can use fourth order a Rungakutta method, so that we get a lot of accuracy with respect to time. Then all we need to worry about is essentially the accuracy in the x direction, the small x direction, the accuracy in the spatial direction.

So, this is the final method again we are not going to solve a problem using the method of lines; however, I want to state this because important method for solving over PDE s. All that we have done is using the same ideas as before the concepts from numerical differentiation, we have implemented that over here. Using that we have converted our overall PDE into ODE and then we can use any of our ODE solving techniques.

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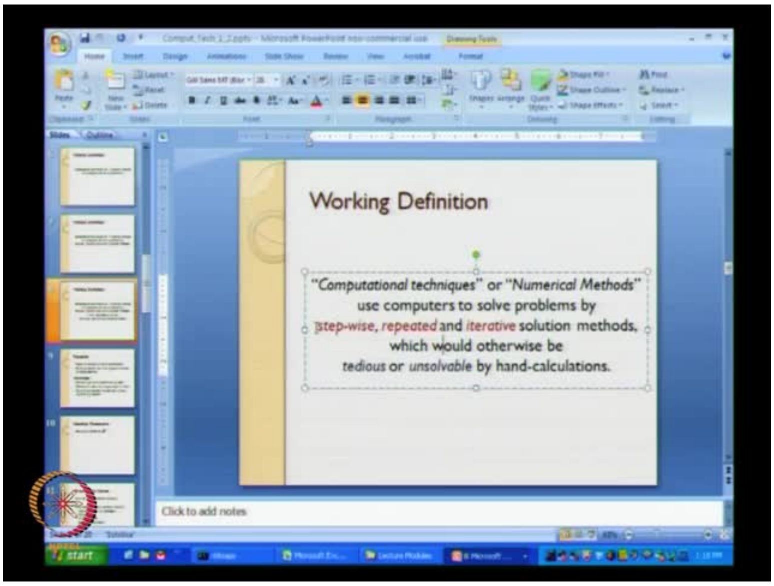

So, what I just wanted to spend the next fifteen minutes or so on is just to give an over view of everything that we have covered in this particular lecture series module one. We had just looked at introduction and basically what we did was the definition of the computational techniques that we use was the computational techniques or the numerical methods. We are going to solve the problems using stepwise repeated or iterative methods. As you have seen, for example, when we talked about PDE s in today's lecture what we saw over there is be found out how to get values from initial time zero to time delta t. The solution at time delta t, the same expressions we used to go from delta t to two delta t, same expressions we used to go from two delta t to three delta t, so on and so forth.

That method was a step wise method. It was a repetitive or an iterative method that means we use the same set of equations, in this particular case, it was a repetitive method that means we use the same expressions, in order to get the values of temperature or the values of concentration at the new time, along the length of the reactor or along the length of the rod. Now, these particular problems, for example, the linear example that was the heat loss from the rod is very much solvable by hand, because analytical solution exits.

It is a linear equation, but the problem of the nature that we saw in today's lecture, they are quite difficult to solve by hand, because of the nonlinearity associated with c to the power 1.25. You can indeed solve this problem still by hand, but for example, if you had to solve this coupled with the energy balance equation, we get the Arrhenius term e to the power minus e by r t that becomes extremely difficult to solve by hand.

If you were to use a calculator and do all this punching in the calculators is going to be very tedious, in order to use the calculator, and it is going to be unsolvable by using some of the analytical techniques. So, what these computational techniques allow us to do is use the step wise and repetitive procedures, in order to get the final solution that we desire.

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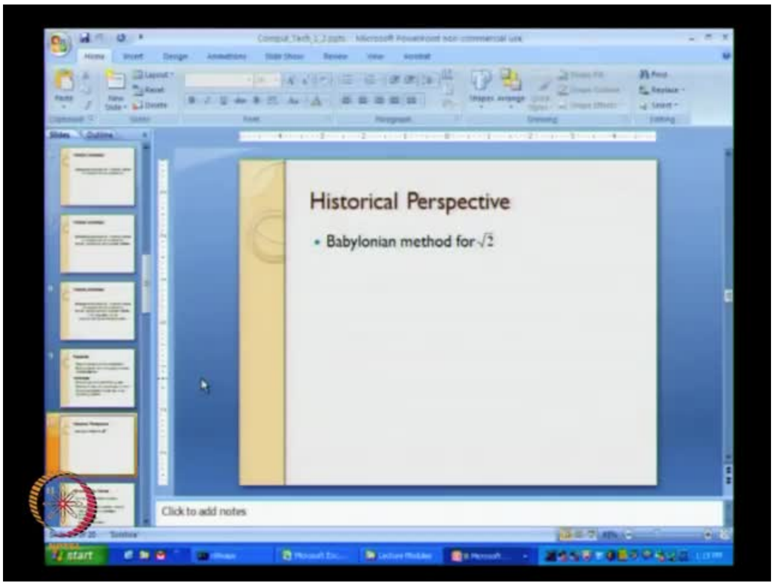

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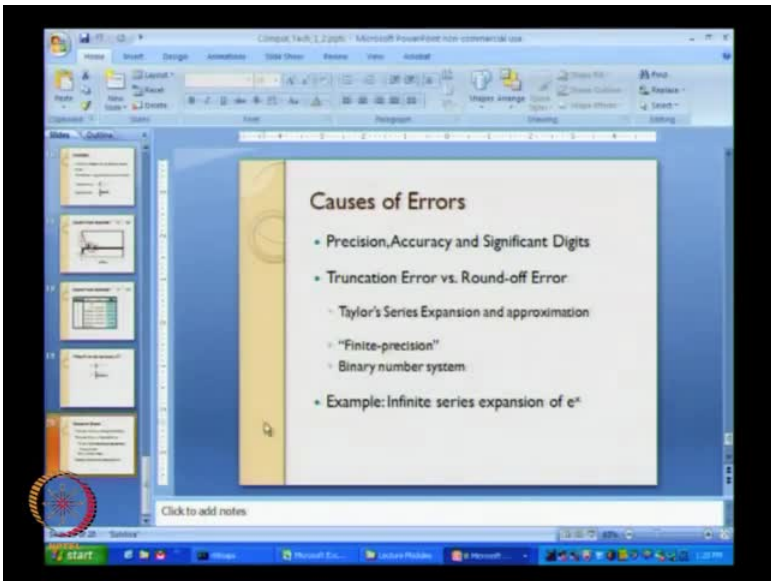

We went to the historical prescriptive using the Babylonian methods for solving the problem of getting square root of 2 and that is what we did. Finally, we talked about errors and in case of errors; we talked about precision, accuracy and the number of significant digits. The most important thing, basically, we talked about the difference between the truncation errors, round off errors and where exactly this truncation and round off errors appear, because of and we talked about the finite precision algebra and the binary number systems and that is essentially what we covered in the second module of this particular lecture series.

Taylor series expansions is essentially is, if we have gone through all the lectures you will realize the Taylor's series expansion is something the that appeared again and again in most of our derivations, either in the derivations or in finding out the error analysis for that particular system.

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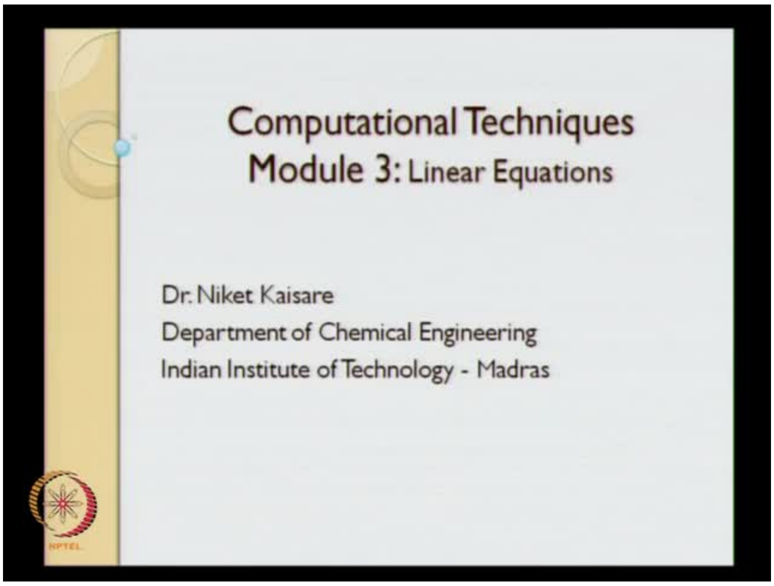

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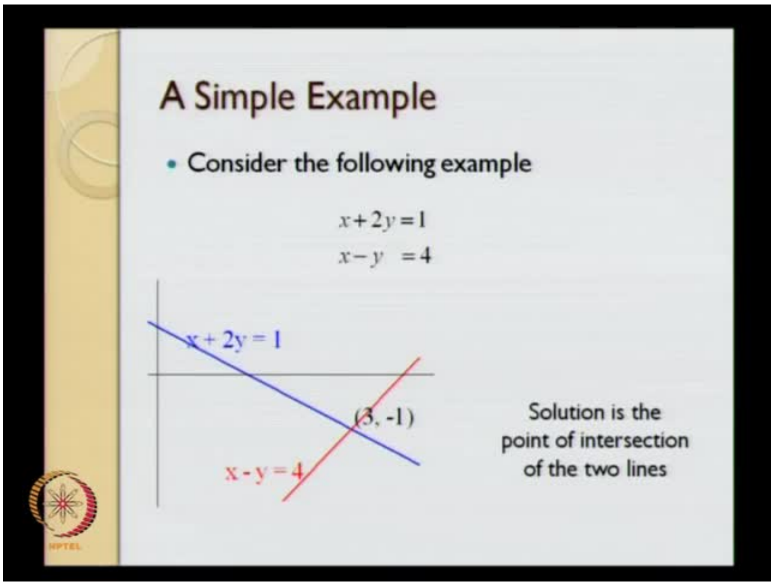

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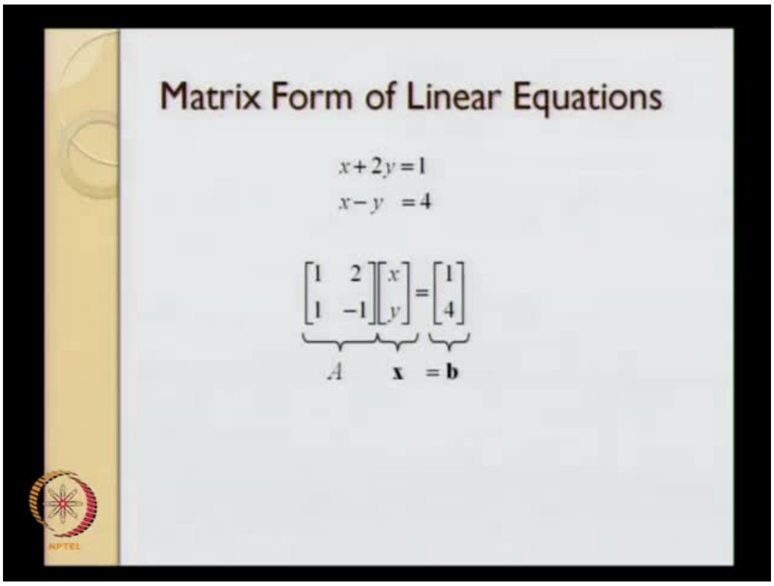

That is what we did in modules one and two and in module three; basically, we talked about the linear equations. Linear equations, we before going to that we did a quick recap of linear algebra and linear equations, we get a geometric interpretations saying that the linear equations involve nothing, but intersection of two lines. We put the linear equations in the matrix form, as we have shown over here and then we use various numerical schemes to solve the equations a x equal to b. And the reason to put it in this general form a x equal to b is so that we can come up with a numerical scheme, which is going to be independent of the number of equations, the number of unknowns so on and so forth.

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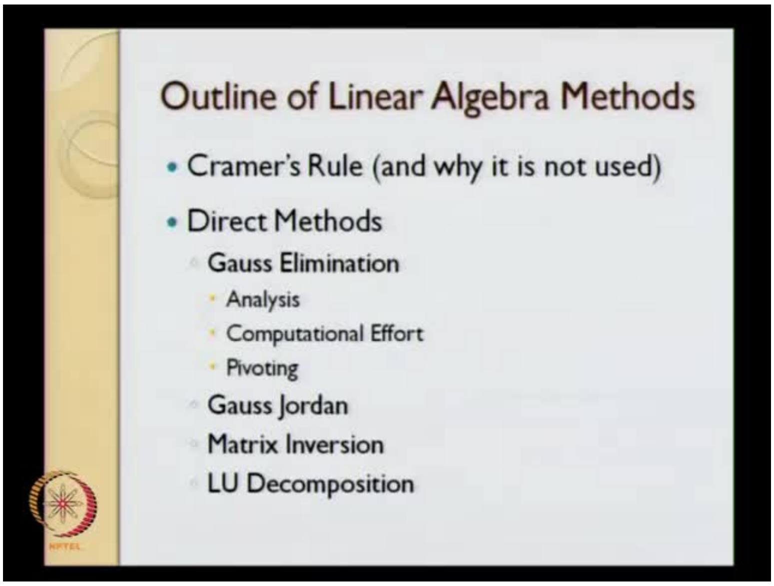

The methods that we saw in this particular module are basically the Gauss elimination method and we analyze this Gauss elimination method and said that the computation effort is of the order of n cubed. We talked about the Gauss-Jordan method and Gauss Jordan method; we said was a very useful method if we want we were interested in finding out the matrix inverse.

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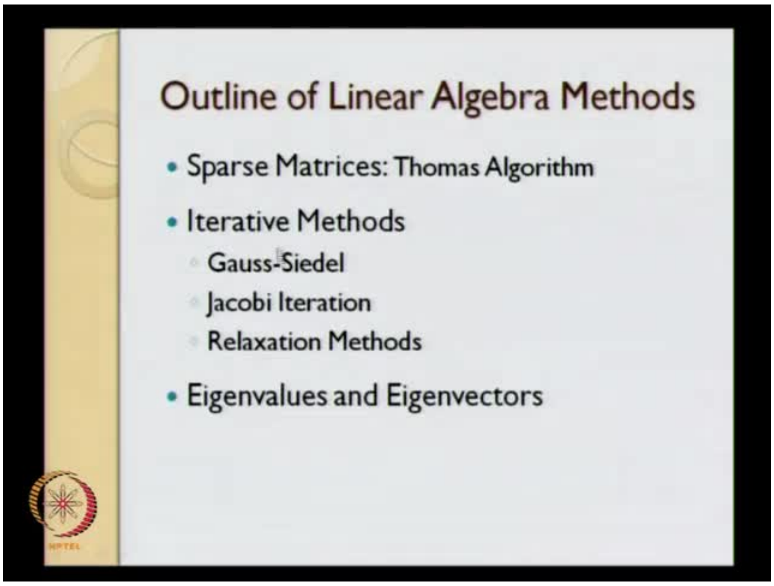

So, Gauss-Jordan method is very useful for the matrix inversion. LU decomposition method is another method that we talked about and then we went to the iterative methods for solving linear equations, the Gauss-Siedel iteration, the Jacobi iteration then we talked about under relaxation and over relaxation methods. Eigen values and eigenvectors, we did not cover numerical methods to get eigen values and eigenvectors, but we went to over to the physical meaning of the eigen values and eigenvectors was.

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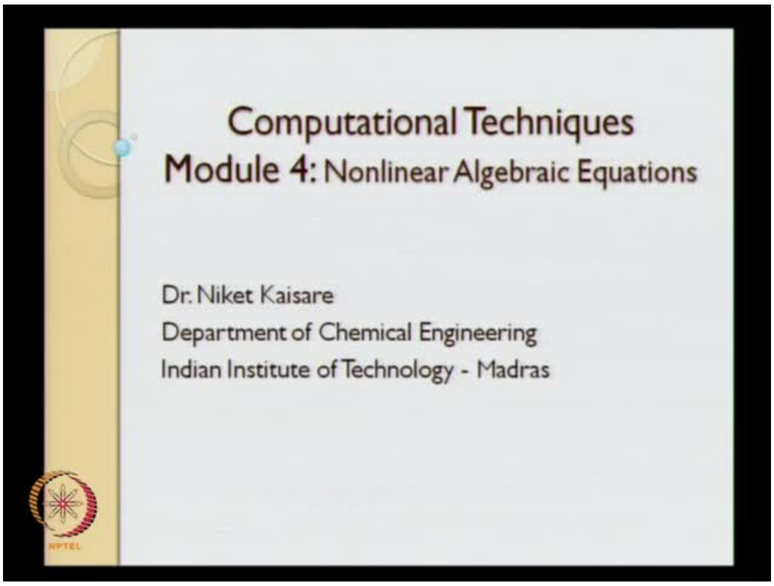

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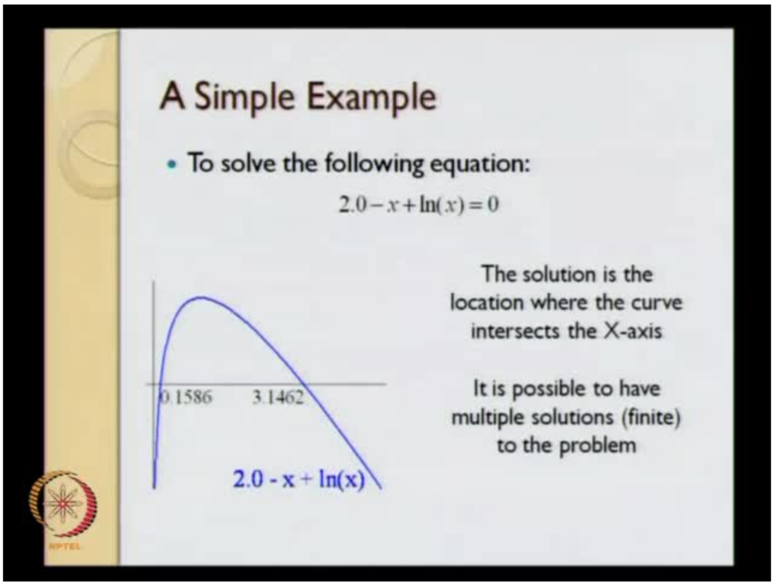

And after that we went to solving non-linear algebraic equations and the idea of non-linear algebraic equations is given a function f x equal to zero. We want to find out the values of x that is satisfies the equation f x equal to zero. The procedure that we used are for example, in this particular example, these are the two points at which this curve intersects the x axis. These two points are the solutions of f x equal to zero. We saw various methods to solve the problem f x equal to zero. All these methods would obtain one solution at a time; we will not get both these solutions simultaneously using any of the methods that we spoke about.

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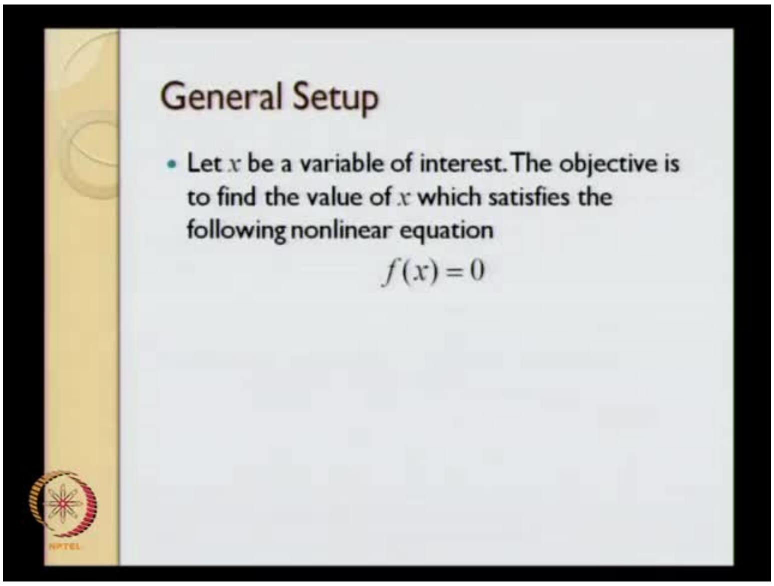

The general strategy we used for solving the non-linear equations is we started with some kind of an initial guess. We either started with one or two, initial guesses, based on the method we used for solving. Based on this method for solving, we use a chosen strategy in order to move hopefully in the direction of the solution. So, we will move from this initial spot to this new spot, using our chosen strategy. If this spot, this new solution is close enough to the true solution, we can find that out by couple of methods seeing how much the new solution has deviated from the previous solution. If the stopping criterion is satisfied we say that this is going to be our solution. If the stopping criteria is not satisfied, we repeat this particular procedure iteratively till the stopping side criterion satisfied and that is when we have obtain the solution.

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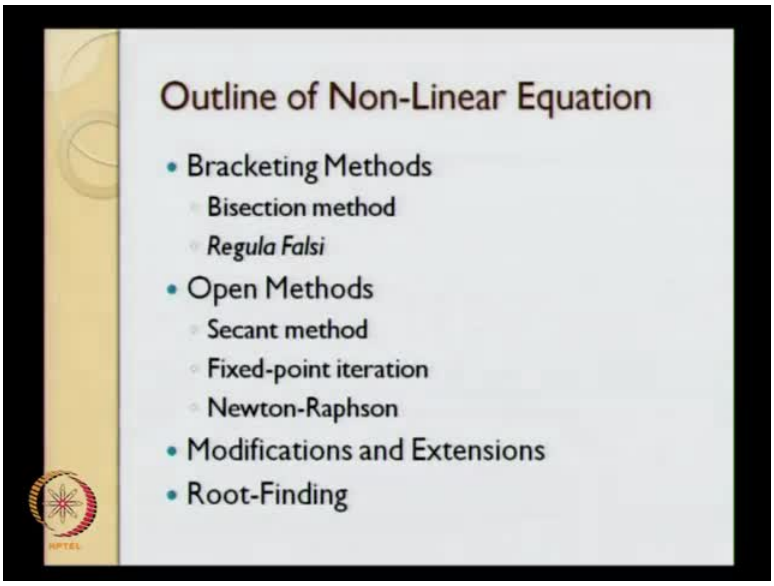

The methods that we have used were categorized into two types of methods. One was the Bracketing method and we saw two methods for Bracketing method, one was the Bisection and the other was Regula Falsi method. The bisection method, we saw was a linearly convergent method that means error in i eth iteration depends linearly on the error in i minus one th iteration.

The Regula Falsi method was super linear, which means the error in ith iteration dependent on error in i minus oneth iteration to the power 1.5 or 1.6. Then we looked at various open method; the Secant method is also a super linear method, the Fixed-point iteration is a linearly convergent method and the Newton-Raphson's; Newton-Raphson's, we saw was the reasons for Newton-Raphson's to be the most popular method and specifically the reasons are its a second order convergent method is the first reason, and the second reason for popularity is that it is very easily extendable to multiple equations in multiple unknowns.

Then we discussed modifications and extensions to the Newton-Raphson's methods particularly, but also to the other methods and finally, we talked about the Bairstow's method for finding out the roots of a polynomial. So, if you have an nth order polynomial the nth order polynomial has n roots, which we can find using method various method and a popular method is Bairstow's method.

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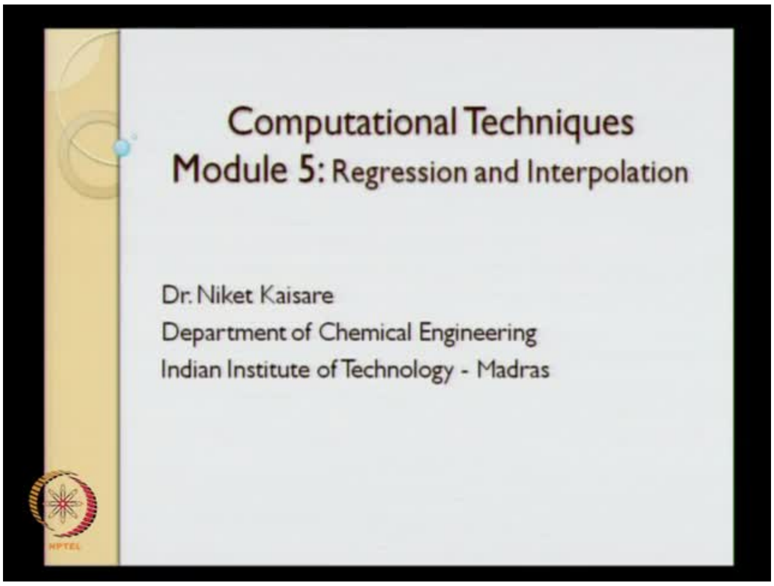

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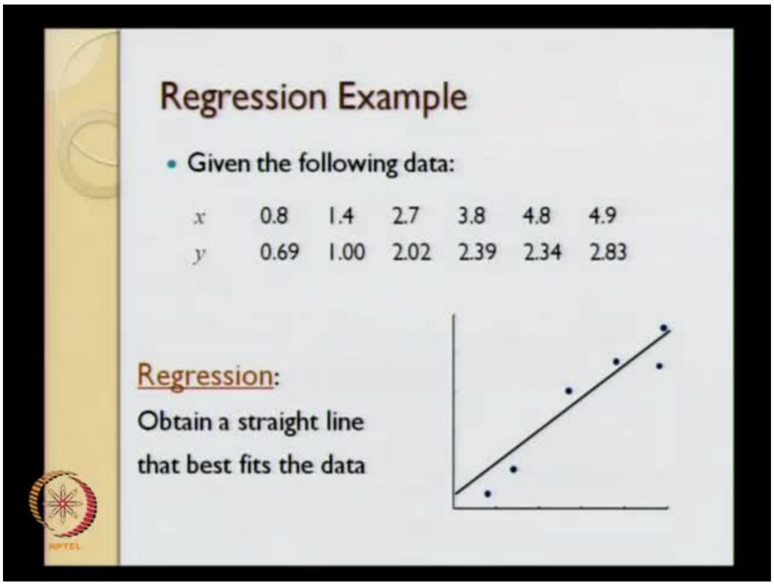

After that we talked about regression and interpolation; the idea behind regression is that given x and y data, so this is one sample data. The idea behind regression is to fit a line or second order curve in order, which best fits the data. So, we decide the kind of functional form that this curve is going to have, and then we are going to use various techniques in order to find the best fit curve. That is the idea behind regression.

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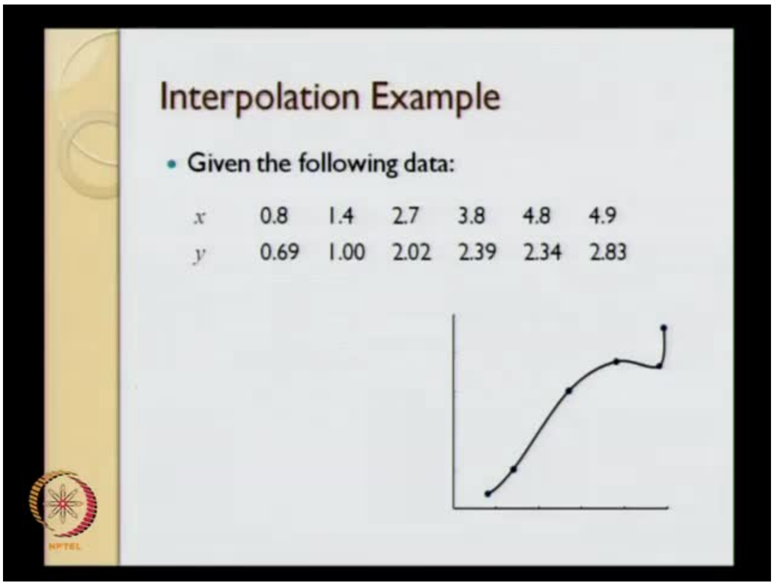

The idea behind interpolation is to find a smooth curve that can pass through all the points, all the data points that we have. The difference between regression and interpolation is that the regression is trying to fit a function to the various data and it is ok if there is an error between the function and the data. The objective is to minimize this particular error. The objective in interpolation is that the curve should pass exactly through all the points that we have been given, so that we can find out the values at any of the intermediate points. For example, if we were to find the value at x equal to two point five, we can get this particular functional curve and then just read the value of y at this particular point, so that is the idea behind interpolation.

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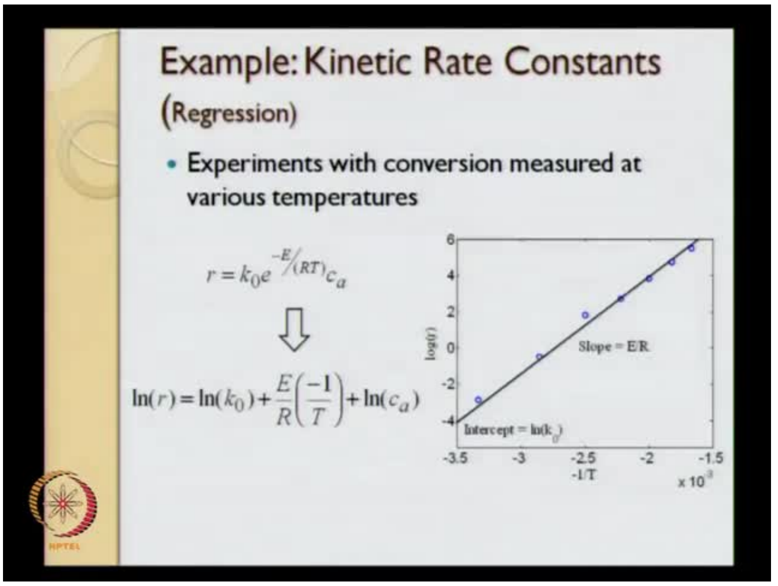

Then after that we took a couple of examples for regression. We said that for example, if we were to find the kinetic rate constants, our k zero and the activation energy and concentration to the power, if it is concentration to power alpha, then that alpha value also. In that case, we can take algorithm and converted into a linear regression problem and this becomes our y this becomes our, a naught, and this becomes our x and this becomes our, a one. And then we can solve this particular linear regression problem in order to get an approximate straight line fit as we have shown over here. So, this we could, we termed this as a functional regression we get a functional form and convert that particular function in such a way that we can use a linear regression technique.

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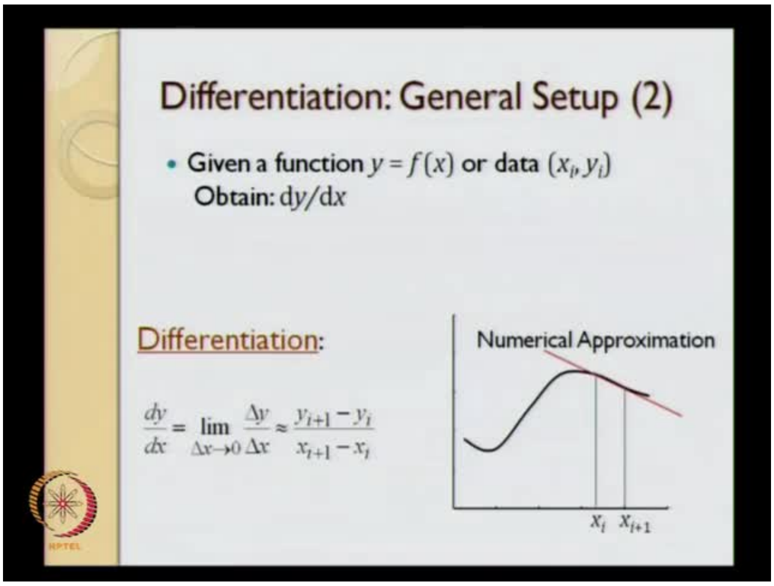

After regression we went on to differentiation and integration; numerical differentiation and integration, we interpreted the numerical differentiation as nothing but finding slope of a tangent and then we said that the differentiation d y by d x, can be approximately written as y i plus one minus y i minus one divided by x i plus one minus x i minus one.

This is exactly what we have used in the forward difference scheme in today's lecture. we did not use the forward difference indeed we use the backward difference scheme in case of a spatial derivatives. So, we had y i minus y i minus one, divided by delta x. In case of time derivatives, we use y i plus y k plus one minus y k divided by delta x and the idea behind this is that we need to choose our delta x or our delta t values, small enough such that delta a delta y by delta x, represents as closely as possible the true numerical derivative. So, these were the concepts from numerical differentiation that we actually imported into the PDE solution techniques using the finite difference method.

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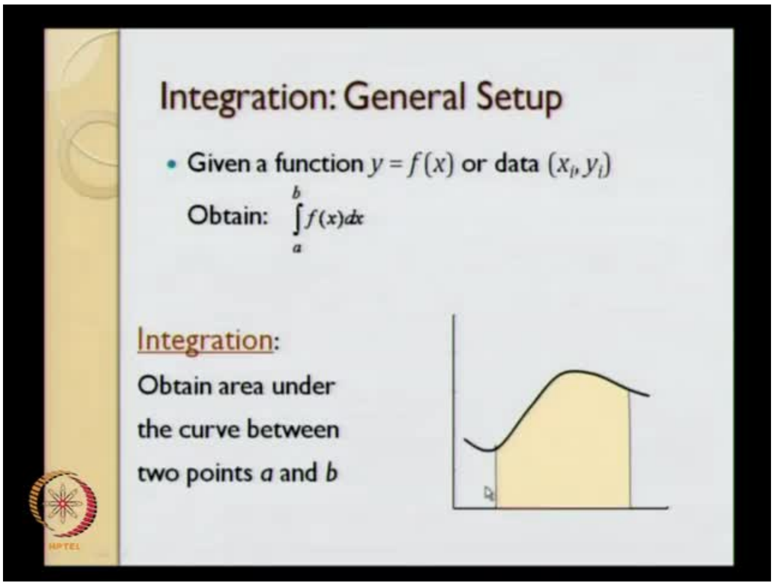

In the integration, the idea is that given a curve f of x d x, we want to find the area under the curve, which basically is integral from a to b, f of x d x. So, the shaded area is really the area under the curve and the solution to that integration problem.

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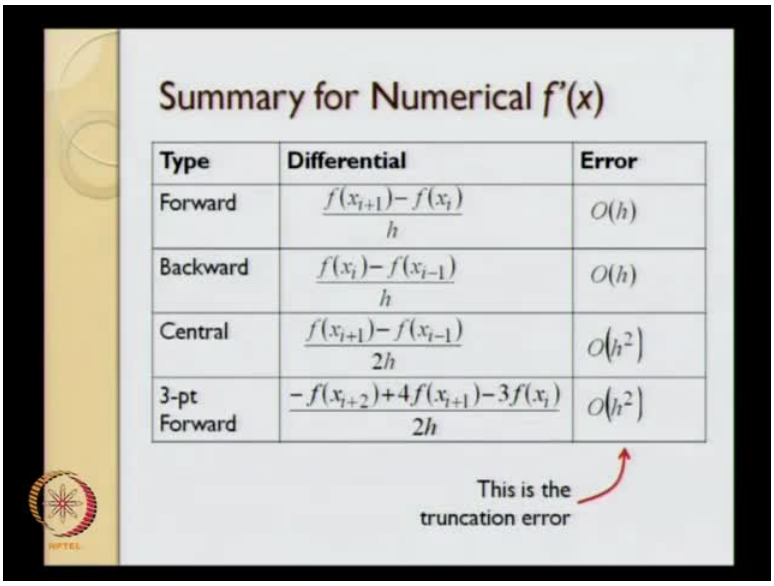

Then talking about the numerical differentiation, we looked at the forward difference the backward difference, the central difference scheme. We saw that the forward and the backward difference schemes for finding d f by d x were order h accurate, whereas, the central difference scheme was order h squared accurate. We saw what that means when we were talking about the partial differential equations, solution to the partial differential equations. And then we talked about a three point forward difference, three point backward difference formulae, as well, where instead of using x i plus one x i and x i minus one instead we use x i plus two, x i plus one, and x i. Likewise, in backward difference we will use x I, x i minus one and x i minus two, and those methods were h squared accurate.

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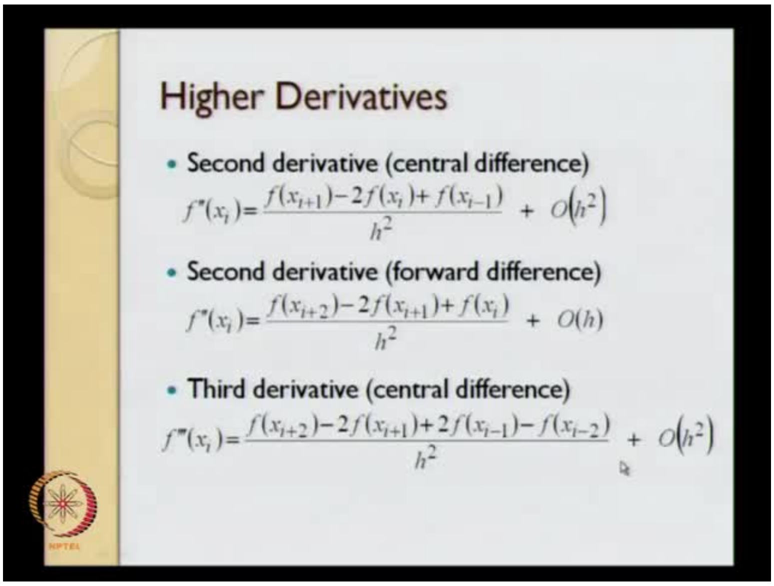

We then also looked at the various ways of getting the higher derivatives, the second derivatives using the central difference scheme and indeed central difference scheme for second derivatives, was something that we used in the previous lecture, for solving parabolic PDE s in a single variable.

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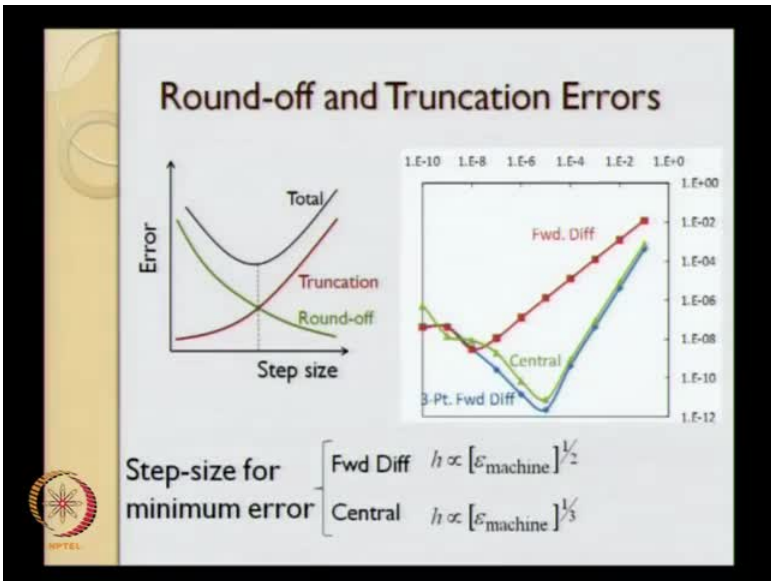

And what we also covered was how the round off and truncation errors change with the step size and here is was the plot of the actual total error using forward central and three point forward difference scheme. Then we say sort of saw that epsilon to the power one by two was the best values of delta x that you can take for a forward difference scheme. The best value of delta x to take for a central difference scheme is epsilon to the power one third and that is what this particular curve shows over here; the trade of between round off and truncation errors.

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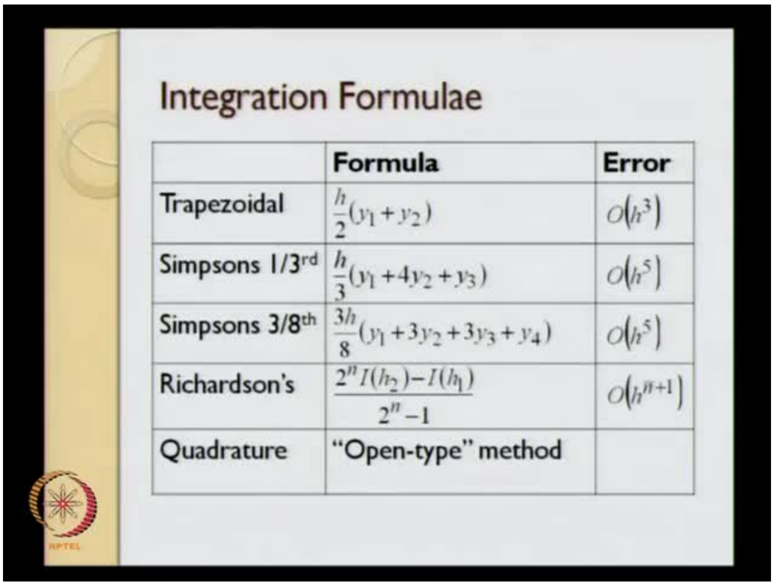

And then when we went on to integration we looked at the various integration formulae and the integration formulae was the trapezoidal, Simpson’s one-third and Simpson’s three-eighth rule. A trapezoidal is very popular, because it is a very simple way of applying the numerical integration scheme. It is order h cube accurate, so the accuracy is not bad at all for the trapezoidal rule. After trapezoidal rule, the next very popular method is Simpson’s one-third rule, because it is h to the power five accurate, but it uses only two intervals. Simpson’s three-eighth rule uses three intervals but, it is still h to the power five accurate. As a result of this, we did not use the Simpson’s one-third rule or Simpson’s one-third rule uses not as popular as the trapezoidal and Simpson’s one-third r the three eighth rule sorry is not as popular.

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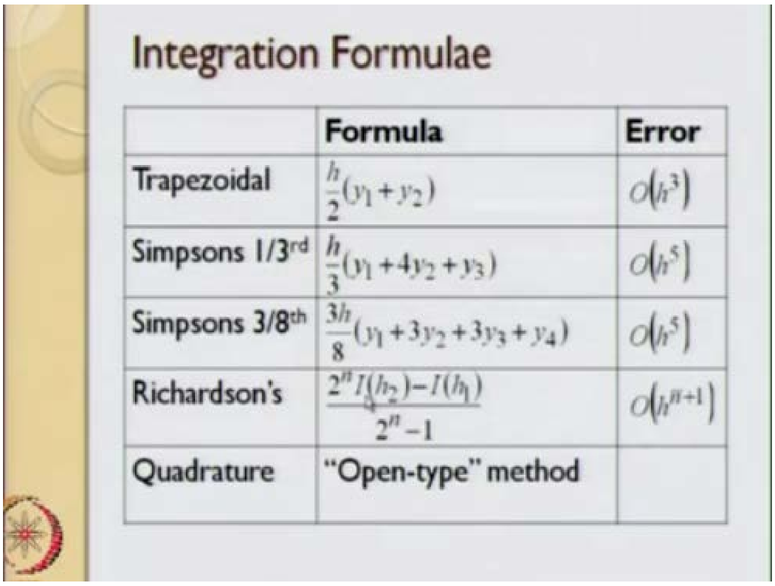

Integration Formulae

	Formula	Error
Trapezoidal	$\frac{h}{2}(y_1+y_2)$	$O(h^3)$
Simpsons 1/3rd	$\frac{h}{3}(y_1+4y_2+y_3)$	$O(h^5)$
Simpsons 3/8th	$\frac{3h}{8}(y_1+3y_2+3y_3+y_4)$	$O(h^5)$
Richardson's	$\frac{2^n I(h_2)-I(h_1)}{2^n-1}$	$O(h^{n+1})$
Quadrature	“Open-type” method	

And then we talked about the Richardson’s extrapolation and the Richardson’s extrapolation is that you use two techniques using two different values of h. Based on this particular equation, you can get a slightly higher accuracy method using the Richardson’s extrapolation.

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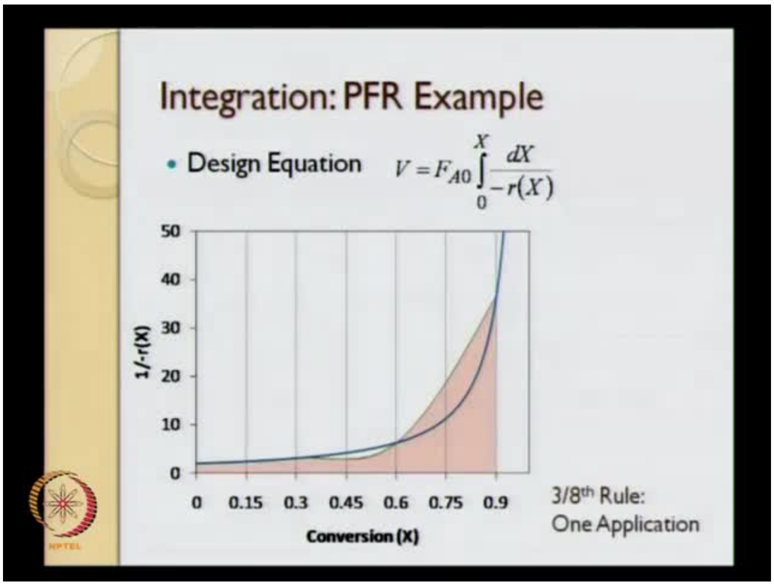

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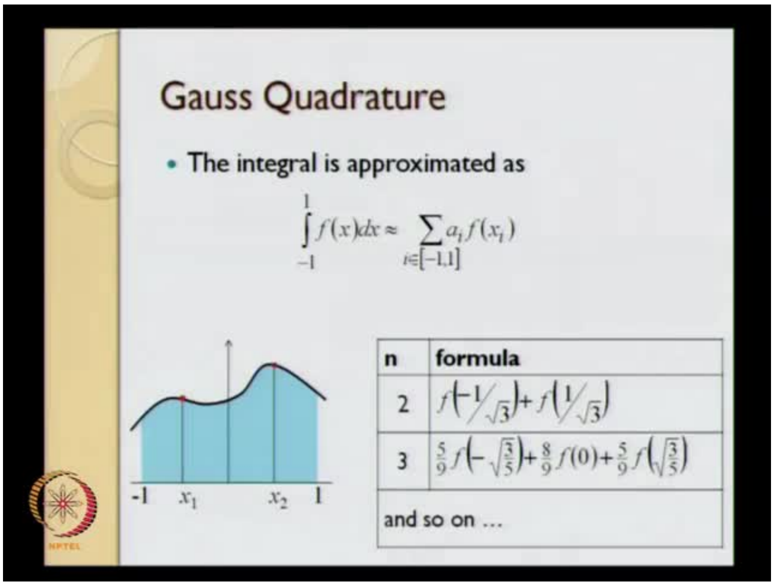

Finally, we covered Gauss-Quadrature method, which is an open type of method. And the idea behind the gauss quadrature method is that given this particular curve and you want to find the area, the shaded area and the integral from minus one to one, which is going to be a weighted sum of the function values at specifically chosen location.

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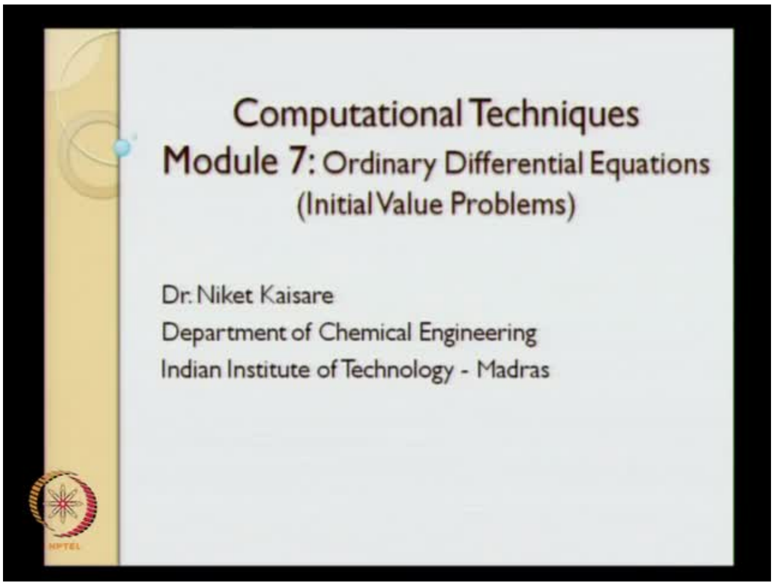

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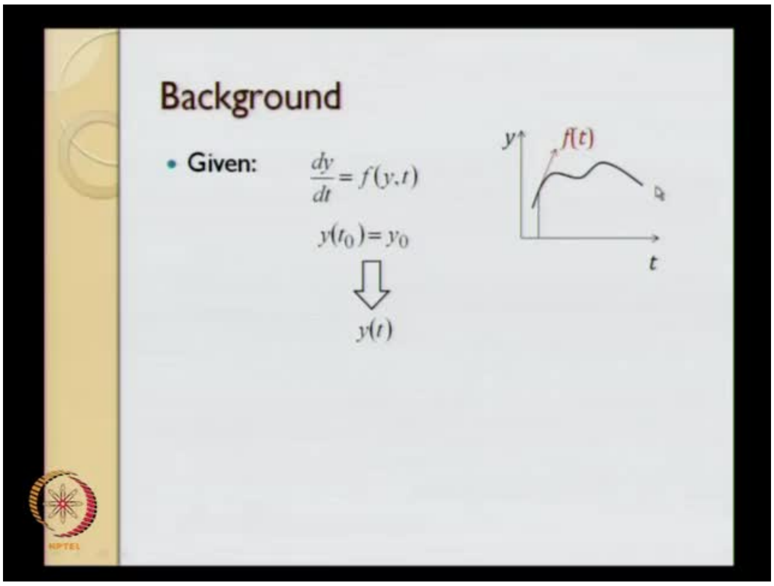

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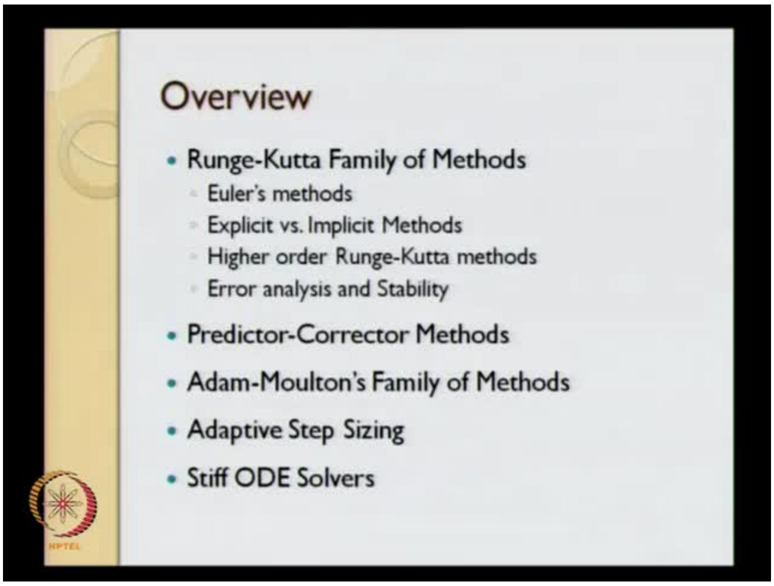

Module seven and eight were ODE's solving techniques and the idea behind ODE's was that given f of x, f of y comma t as the slope of the curve y versus t, we want to find the values of y, how the values of y change as the time t increases. This was all that we covered in ODE initial value problems. We covered the Runge-kutta family of methods, we talked about explicit versus implicit method, we use higher order Rungekutta method. We spend of fair amount of time on R-K two methods, specifically the midpoint method and the Heun’s method, looked at error analysis and stability of these methods, we said essentially that the implicit methods are going to be globally stable, whereas, explicit methods are not going to be globally stable. They have a range of delta t values for which the explicit methods are going to be stable.

After that we went to the predictor corrector family of methods. We took the Heun’s method which was a second order accurate method and modified this in a predictor corrector form. Finally, talked about the Adam Moulton's family of methods, these were the three different classes of methods for solving ODE-IVP. And then we took, we specifically in the last two lectures of this module, I think lecture eighth and ninth of this particular module, we covered adaptive step sizing and solving multiple ODE's using stiff ODE solvers. The whole idea behind this was to give you an introduction to some of the various advanced techniques that are covered in ODE-IVP methods.

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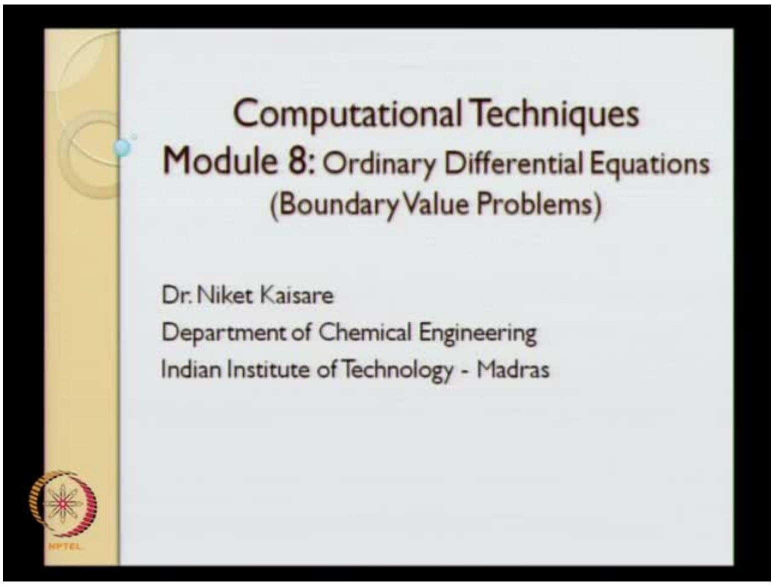

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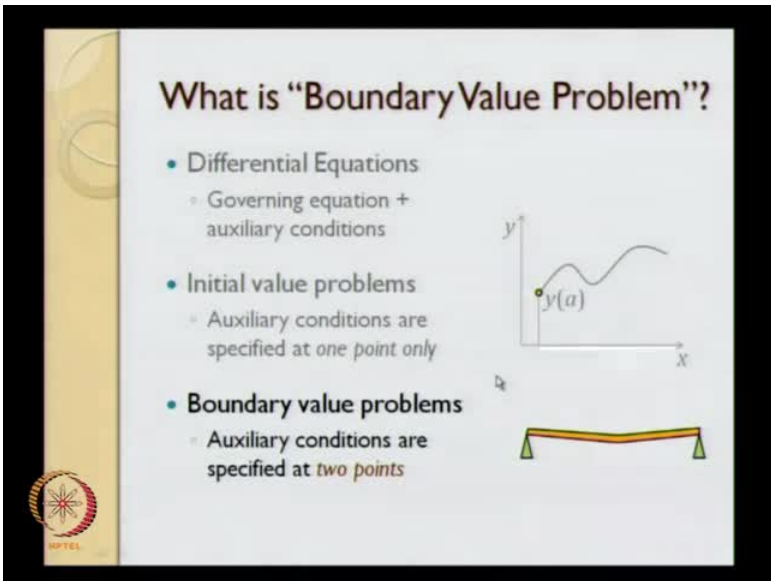

So, what we did in the ODE boundary value problem was to cover what is the difference between the initial value problem, which is hinged only at one initial condition, whereas a boundary value problem which as hinged at both the boundaries. That is how we motivated our boundary value problem and then we solve the boundary value problem using two different methods; one was the shouting method and the other was the finite difference method.

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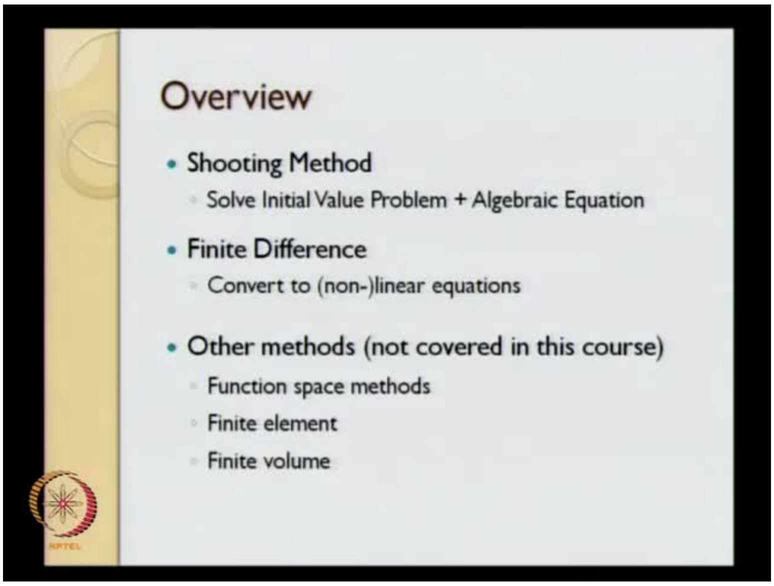

And in the shouting method what we did was we covered the boundary value problem into an initial value problem and solve the initial value problem along with a Newton Raphson's type of a technique in order to get the final solution.

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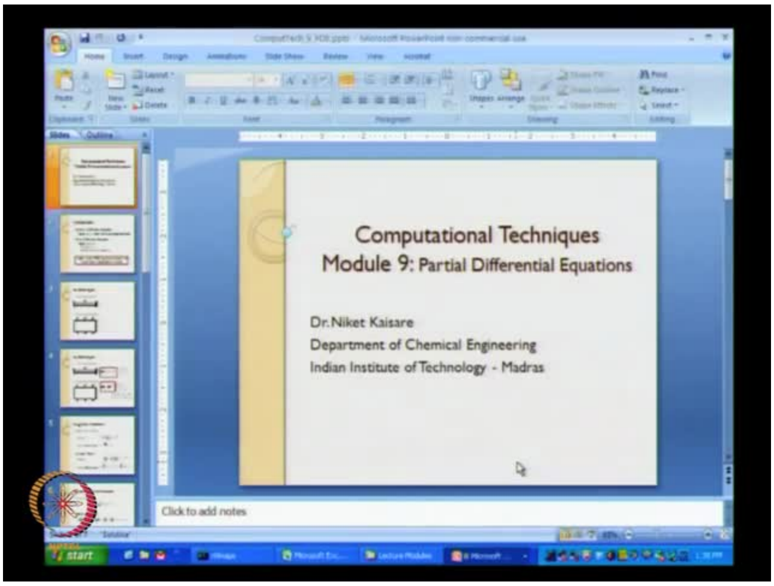

And in finite difference method we converted the boundary value problem into linear or non-linear equations. Finally, in this particular current module, we have covered how to solve partial differential equations specifically classified PDE s into hyperbolic, parabolic and elliptic equations and saw the various methods of solving this PDE s.

So, that is really the overview of what we have done in the last 40 lectures and this particular lecture in our computational techniques lecture series. What I invite you to do essentially is go over and solve the various problems that we have solved using the microsoft excel, solve them yourselves, so that you can get acquainted with the various numerical techniques. The really the only way to get acquainted and get comfortable with numerical techniques is through solving the problems.

We will have several problem sheets and problems are there, good problems are there, in the various textbooks and the various sources that I have recommended specifically the text book by Chapra and Canal, on Numerical Methods for Engineers and book by Professor S.K Gupta again on numerical methods for engineers. Specifically, professor Gupta's book is written by a chemical engineer for chemical engineers, although it has various other problems also.

So, hopefully you have gained a fair amount of initial knowledge about computational techniques in this particular lecture series and that will hopefully give you the confidence to look at the more advanced techniques that you will be using either in your research or in your job, wherever your job takes you.

Thank you and thank you for listening to these lectures.