# Tools in Scientific Computing Prof. Aditya Bandopadhyay Department of Mechanical Engineering Indian Institute of Technology, Kharagpur

Lecture - 24 Boundary Value Problems

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Hello everyone in this particular week we are going to study about Boundary Value Problems. So, far we have considered equations which evolved in time and they are classified as initial value problems; because the initial conditions are known and then the system state and things such as plotting the state in the phase diagram, they are the evolution of the parameters in accordance to how they are governed and their initial value problems.

But in a different category of problems we can have a domain such as a string and then you can impose certain conditions. For example, we can have a displacement of the string like this and this end of the string is left free things like that. So, things which we are familiar with things pertaining to vibrations and all these things or displacements and they all fall within the purview of boundary value problems.

So, without any delay let us look at a particular very simple boundary value problem  $\frac{d^2 f}{dx^2} = f$ . So, it is a linear ODE and we have to define over what domain is this

particular equation valid. So, let us take it over the domain 0 to 2 and at x = 0; let us say f(x) is equal to I mean directly right. The first boundary condition as f(0) = 1, second condition could be f'(2) = 0.

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So, this in a solid mechanics viewpoint this would be a prescribed displacement and this would be a free or unconstrained member. So, something which maintains a slope, but it does not define what the displacement will be ok.

So, it has to just maintain a slope it could go from something like this also I mean not this much, it could go something like this all it has to do is maintain this displacement there is no prescription for it. And maybe if we have to find that out as a part of the solution who knows.

So, these are the two conditions and this condition is known as the Dirichlet condition and this particular condition is known as the Neumann boundary condition. So, here the value of the function is specified at the end point one of the endpoints and over here the derivative is specified. And so, this is how you distinguish between a Dirichlet and a Neumann.

Alternately you could have the situation where you have a mixture of both that is something like f'(2) + 2f(2) = a, or something. So, it is a mixture of first derivative and

the specified value of the function and this kind of boundary condition is known as the Robin boundary condition ok.

So, how do we go over approaching this problem? Well, first thing we could do is obtain the analytical solution. So, what is the solution for this? So,  $f = A\cosh x + B\sinh x$  and that is the straightforward solution. I mean you could write the solution for this as  $f = Ae^x + Be^{-x}$ , that is a linear combination of  $e^x$  and  $e^{-x}$  where the constants A and B are determined using the boundary condition.

So in fact, let us use this hyperbolic form. So, we have  $f = A \cosh x + B \sinh x$  using the first boundary condition f(0) = 1. So, 1 so when once you substitute x = 0 this term will become 1; so, this will be A. And this particular term will become 0, because sin h of 0 is 0. So, A becomes equal to 1.

And similarly using the Neumann boundary condition so what do we have?  $0 = A \sinh x|_{x=2} + B \cosh x|_{x=2}$ ; this becomes  $A \sinh 2 + B \cosh 2 \operatorname{cand} A$  is already equal to 1 and this implies  $B = \frac{-\sinh 2}{\cosh 2}$ .

So, combining this so this is the solution ok where A is this and  $B = \frac{-\sinh 2}{\cosh 2}$ . So, we could write down the expression by substituting all this over here, but because we are going to plot it in python anyway or octave as you like. So, we are not going to bother much about that.

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So, let us go and create a new file. So, let me copy this bit of code alright. So, let me then create a linspace between 0 and 2. And let me in fact, let me call it xe this is for x exact and y exact is ye = A\*np.cosh(xe) + B\*np.sinh(xe) we can send this to the next line because we need to define the constants A and B.

So, A is 1 while B = -np.sinh(2)/np.cosh(2). Alternately you would have written it as - np.tanh(2), but anyway this is fine. So, with this let us do a plot.

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So, this is how the exact solution looks like and the value of the function at the other endpoint that is x = 2 appears to be something which is near to 0.3, but less than 0.3. So, this is what we have from the exact same, but now we are interested to solve this numerically. So, how do we go about solving it numerically? Let us see.

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So, the first thing that we do the first very first thing that we go over doing is to discretize the domain into a bunch of points. So, this is x = 0 and this is x = 2. This is

going to be so, we make a linspace out of this. So, this will be 0, 1, 2 all the way to N-1. So, if we have a linspace which has an elements. So, let us do that and see.



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So and let us keep this code over here and let us write this here. So, x = np.linspace(0,2,20) and let us say we take 20 points. And yeah so let us print x just for good measure. So, this is how x looks like the 0th point is 0. And the last point so 0 will be 0 whereas, 19 will be 2. So, it is going all the way from 0 to N - 1 alright.

So, now our task is to discretize this particular equation over on this grid. So, we have what  $\frac{d^2 f}{dx^2} = f$ . So, how do we discretize a function at a point? So, I must write the function in terms of the neighboring points. So, the very easy way of doing it is writing a central difference approximation alright.

So, I mean I whether or not it is clear how to do this I will just give you a gist of how it is done. So, we have  $f(x) = f(x_0) + \frac{df}{dx}|_{x_0} \Delta x + \frac{df^2}{dx^2}|_{x_0} \frac{\Delta x^2}{2!} + \dots$  So, now  $\frac{f(x) - f(x_0)}{\Delta x}$  gives us a good estimate of what  $\frac{df}{dx}|_{x_0}$  is going to be. But we have neglected the other terms, but the magnitude of the other term. So, I have divided everything by  $\Delta x$ . So, this will be  $+O(\Delta x)$ . Meaning whatever I am neglecting is going to be proportional to the  $\Delta x$  that I have over the grid, if  $\Delta x$  is small then this approximation is also good if  $\Delta x$  is large this approximation is not going to be good. So, how do you go about finding the central difference approximation? Well you have on one hand the approximation for f of near x<sub>0</sub>.

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And similarly, you can write an approximation of f. So, what we have? This is  $x_0$  this is I mean well. So, I just write an approximation for f(-x) that is the point on the other side.

So, 
$$f(-x) = f(x_0) - \frac{df}{dx}\Big|_{x_0} \Delta x + \frac{df^2}{dx^2}\Big|_{x_0} \frac{\Delta x^2}{2!} - \dots$$

So, as you can imagine if I add these 2 equations the odd terms will cancel out because  $\Delta x^3$  term will be there and here it will be  $-\Delta x^3$ . So, all these odd terms will cancel out. So, finally, we have  $f(x) + f(-x) = 2f(x_0) + \frac{df^2}{dx^2}|_{x_0} \Delta x^2 + O(\Delta x^4)$  and so on.

And so, this gives us a good measure of the second derivative as  $\frac{f(x) - 2f(x_0) + f(-x)}{\Delta x^2}$ . And so, the error will now be order  $\Delta x^2$  because I have divided everything by  $\Delta x^2$ . So, this also is gets divided by  $\Delta x$ .

So, such an approximation is said to be second order accurate because as  $\Delta x$  becomes small, by say a factor of half the error is expected to reduce by a factor of one-fourth

which is in stark contrast to the forward difference approximation for a single derivative. Well I have rub that now.

But similarly, I could so what we had earlier  $\frac{df}{dx}\Big|_{x_0} = \frac{f(x) - f(x_0)}{\Delta x} + O(\Delta x)$ . And now I can

choose whatever x and -x is to be a point coinciding with the neighboring grid. So, now x becomes  $x_1$  and -x becomes x-1. Because f(-x) is simply the - firsth node and this x will become the first node, if this node is the 0th node.

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So, this approximation was first order accurate, but you can actually evaluate a second order accurate derivative and the way to do it is; is going to be f (i+ 1). So, if I call

this 
$$\frac{df}{dx}|_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}$$

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Essentially it is saying and if this is a function if this is 1 point i. So, if you want to approximate the slope at this point which is something like this, I can discretize the grid over which it is defined. So, this is i this is i +1, this is i - 1. So, this point is  $f(x_{i-1})$  this point is  $f(x_{i+1})$ . So, I can approximate it by taking a difference between these two points that is the central difference I can approximate it between these two points this is the finite the forward difference.

I can in fact, approximately using these two points as well that is the backward difference. So, depending on the scheme that you use 1 will arrive at an approximation to that particular derivative which will have some order of accuracy. And as to what that accuracy will be is a matter of what your choice is alright.

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So, let us get rolling with this so yeah. So,  $\frac{d^2 f}{dX^2} = f$ . So, I can do a finite difference approximation at the ith node. So, what this will be? Will be  $\frac{f_{i-1} + 2f_i + f_{i+1}}{\Delta x^2} = f_i$ . So obviously, the left hand side is order  $\Delta x^2$  accurate. Now, let me collect the terms containing I mean let me segregate the terms  $f_{i-1}$ ,  $f_i$  and  $f_{i+1}$ .

So, I have  $f_{i-1}$  ok. So,  $f_{i-1}$  is obviously, referring to f at x i - 1 ok. So, this is just a small shorthand for writing  $f_{i-1} + f_i(-2 - \Delta x^2) + f_{i+1} = 0$ . So, you have many nodes and here is 0 and you have many nodes and here you have N - 1 ok here you have N - 1.

So, now this particular discretization let me call it as A. So, this is valid for the interior nodes because we must treat the boundary conditions a bit a bit differently. In the sense

that I know that f (0) is = 1 and  $\frac{df}{dx}\Big|_{x=2} = 0$ .

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Now, while we are added let us have sort of discretization for this fellow as well. So, this is quite trivial this is simply going to be f(0) is going to be 1 this is going to be. So, let me take a backward difference at the final node. So, backward difference at the final node will involve N -1 and N - 2 fine. So, this will be  $\frac{f_{N-1} - f_{N-2}}{\Delta x} = 0$ , alright.

So, this is for node number 0 this is for node number N - 1, but what about the inner nodes. Let me substitute i = 1 over here. So, what do I have? I have f (0) + f (1). So, let me call this as  $\alpha$  alpha because; it is not going to change over the equations because we will have a regular grid meaning  $\Delta x$  is not changing across various locations on the grid. So, that kind of a grid is called as a uniform grid or a regular grid no problem.

So, its going to be  $f_1\alpha + f_2 = 0$ . Now, what I can do is I can write it for i = 2, 3 and so on. So, this is for i = 1, i = 2 i will have  $f_1 + f_2\alpha + f_3 = 0$  and so on. Why = 0; obviously, i have f (0) = 1 and for f sorry or i =N - 1 i have  $f_{N-1} - f_{N-2} = 0$  because  $\Delta x$  can go on the right hand side and it will be; obviously, 0.

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Now, what I can do is write down these equations. So, for N equations I have N unknowns. The N unknowns are  $f_0$ ,  $f_1$ ,  $f_2$  all the way to  $f_{N-1}$ . And how many equations do we have? We do have an equation starting from 1 = 0 to i = N - 1.

So, its a set of linear algebraic equations. So, we have converted the ordinary differential equation into a set of linear equations alright. So, if I can go ahead and write this in a matrix form how will this particular set of equations look? So, over here I have  $f_0 f_1 f_2$  all the way to  $f_{N-1}$ . So,  $f_{N-2}$  comes on top and this will be equal to something.

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So, this kind of equation will always come out in the form Ax = b. Where a is like the mass matrix I mean it borrows its nomenclature from solid mechanics or structural mechanics its stiffness matrix ok. So, b this is the right hand side ok let us not alert to that no increase or not. So, we simply obtain this set of equations say Ax = b forgotten most of structural mechanics.

But yeah you do get an equation of this particular form over there as well alright. So, this is a matrix, this is a vector, this is a vector. So, let us populate those vectors. So, what do we have. So,  $f_0$  so for the first node  $f_0 = 1$ . So, this will be  $1 \ 0 \ 0 \ 0 \ 0 = 1$ . So, this is  $1 \times f_1 = 1$  over here we have  $1 \ \alpha \ 1$  then all 0s this is going to be equal to 0 over here we have.

So, there is no f<sub>0</sub> over here. So, this becomes 0 is  $\alpha$  this is 1 is  $\alpha$  1 and everything else is going to be 0. Again, 1 sorry this is 0 1  $\alpha$  1 0 so, this continues on. So, apart from the first row and the last row this keeps on continuing this tridiagonal set keeps on continuing up until the last node upon which we have a backward difference to take care of alright.

So, the backward difference in this case is quite simple it simply implies  $f_{N-1} = f_{N-2}$ . So, this is - 1 over here and this is going to be 1 and this is equal to 0. Why is it - 1? So, all these are going to be 0 is - 1 ×  $f_{N-2}$  + so, basically this particular term + 1 ×  $f_{N-1}$  is equal to 0 alright great.

So, now our task is to construct the matrix A and the vector b and then solve for x ok. So, solution x I mean over here I am writing it as x, but it will be really f great. So, let us go over here in fact, yeah. So, we do have an expression for x. So, now, what will be the size of the matrix A? So, A has to be A square matrix having the same size as x.

So, it will be np dot zeros and the size will be. So, let me soft code it as N; where N will be the number of points. So, N = 20 alright great. So, A has been initialized to 0s. Now what will be b? So, b will be np dot zeros. So, its N rows and 1 column alright. So, A has been initialized b has been initialized. Now it is a matter of constructing the appropriate structure for A. So, what we could do is run a loop from i = 0 to N - 1 and based on this particular logic we can assign all the different members of the matrix.

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So, we are not going to do it like that, but I am just going to outline how to do it in case you are doing it in c or something where vectorization is not possible this is how you would do it for i = 1 sorry for i in 1 np.arrange 0, N.

So, A so what do we have? So, if i = 0, then you will say A 0, 0 = 1 else; i = N - 1 or rather yeah = n - 1, then what will we do? We will say a N - 1, N - 2 = -1 A N - 1, N - 1 = -1 rather 1.

So, these two if else statements take care of the boundary conditions rather the boundary nodes; if they are not the boundary nodes then we continue as normal else A N or rather A i , i. Well I could have written this in terms of i as well i - 1, I think it is better to write it in terms of i.

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Because its already doing the check whether i is = N - 1. So, I do not need to write it in terms of N - 1 i can simply write it in terms of i yeah. I think that is much better. So, A i, i will be =  $\alpha$  A oops i, i - 1 is going to be 1 A i, i + 1 is also going to be 1. So, essentially it is assigning the three values and you can figure it out whether how this is going to work.

So, let me define what  $\alpha$  is. So, alpha we had defined as  $-2 - \Delta x^2$ . So,  $-2 \times -dx^2$ . So, what is going dx going to b?e dx is going to be x 1 - x 0 its simply the difference between 2 nodes alright. So, let me run this and let me show you how A looks like. In fact, let me reduce the number to something manageable like 5 alright. So, this is how A looks like.

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So, look its 1 over here and all 0s and 1 - 2.25 1, 1 - 2.25 1 and the boundary nodes are different, but everything else is like a tridiagonal matrix.

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And actually, boundary value problems where you are discretizing with the nearest neighbor it does resemble a tridiagonal matrix alright ok. So, yeah this is what you can do to construct A, but its actually looping over all the elements and doing and we can alternately take a great shortcut. Let me comment [FL] I cannot comment over here ok. But let me split cells and keep it for later. So, what we will do is we will use the np dot diag function. So, what is the np dot diag function?

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So, let me show you. So, let some small a be 1 2 3 right. So, A = np .diag a , 0. So, now, let me sorry let me show what A is. So, it will take a vector and it will push all the vector elements to the diagonal elements. So, I have to pass a vector which is having the same size as the length of the square matrix alright. So, over here it is 3 and so on. So, this gives us an idea. So, because all of them are going to be  $\alpha$  except the zeroth node and the N - 1 N node I can handle them easily ok.

So, let me write this. So, diagonal vector is going to be alpha times np dot ones the size is going to be N rows and its just a vector dv1 is the offset ok. So, dv1 is the offset meaning if b is = 5, 6 and I write B = np.diag b, 1 then let me print B its going to take the vectors and it is going to put the vectors in the shifted location to the diagonal.

The shift is specified by this. So, over it is inserting b the elements of b into the matrix capital B and having a shift of 1. So obviously, it has to have 1 less element the more you shift the lesser elements you should have great that gives us a different idea.

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So, this simply going to be np.ones N - 1, So, yeah that is it. So, now, a will be np.diag(dv) + np.diag(dv 1, 1) + np.diag(dv 1, -1). Where I have used the fact that the upper shifted diagonal and the lower shifted diagonal have the same value to be inserted ok.

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So, having done this let us print what A is. Let me reduce this to 5. So, great we have the tridiagonal matrix as we want. Now, I will unset the boundary nodes to be zeros.

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So, A 0, all is going to be 0; A N - 1, all is also going to be 0. Let me print and show that we have indeed unset these 0 and the last node great.

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So, now we can simply incorporate the boundary condition. So, A 0, 0 is going to be 1 and the other boundary condition is going to be A N - 2, N - 1 is going to be - 1 A N - 1, N or we do not need to write N - 1. I am just being silly over here.

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Because we can simply write A - 1, - 2 is = - 1 and A - 1, - 1 = 1. And we have seen this in the very beginning that - 1 is simply same as N - 1. Let me in fact, print A and convince you.

So, A 0 0 has been set to 1; A - 1 has been set to - 1 and N - 1 - 1 has been set to 1. So, now, I must also set the b matrix. So, b is going to b. So, b 0 is simply going to be 1 that is it. So, now, we do have the system of equations say A x = b and its just a matter of solving it.

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So, how do you solve? I mean because its a very trivial case we take an inverse of A and multiply it. So,  $A^{-1}A = A^{-1}$  b and but  $A^{-1}A$  is going to be the identity matrix. So,  $\overline{I}\vec{f} = A^{-1}b$  and  $\overline{I}\vec{f} = \vec{f}$ . So, the solution  $\vec{f} = A^{-1}b$ .

So in fact, let us do it I mean its not the most efficient way of doing it most way, but let us do it regardless. So, f is going to be np dot inv A and now we have to do a matrix multiplication.

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So, np.dot A \* b there is there appears to be an error np. inv. So, that the function inv actually lies inside the linalg sub module yeah.

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So, now that we have done this we can plot it. So, plt.plot x, f. Well let us try to superpose this with the earlier solution what was it xe and ye.

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e	A[i,i] = 1; elif i == N-1: A[i,i-1] = -1 else: A[i,i] = alph	l; A[i,i] = 1; na; A[i,i-1] = 1;	A[i,i+1] = 1;					
[19]: a = [ b = [	A[i,i] = 1; elif i == N-1: A[i,i-1] = -1 else: A[i,i] = alph [1, 2, 3]; A = np [5, 6]; B = np.di	l; A[i,i] = 1; na; A[i,i-1] = 1; o.diag(a,0); prin iag(b, 1); print(	A[i,i+1] = 1; t(A) B)					6

So, let me give this a label of approximate or numeric plt.plot(xe, ye, 'ok', label="Exact"); plt.legend(); plt.xlabel("\$x\$"); plt.ylabel("\$f(x)\$").

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So, there appears to be some error; I mean not some error, but it is exact at the end, but here there is a great deal of error. In fact, oh 1 reason could be the very ridiculously low number of grid point.

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+ %	<u>ت</u> )	■ C	➡ Code	~						Python	3 O
[30]:	<pre>N = 50; x = np.lins A = np.zero alpha = -2 dv = alpha" dv1 = np.on A = np.diag A[0,:] = 0; A[0,0] = 1; A[-1,-2] = b[0] = 1; f = np.dot( plt.plot(xx, plt.plot(xx))</pre>	<pre>pace(0,2,N s((N, N)); - dx**2; np.ones((N es((N-1,))) (dv) + np1; A[-1,1; A[-1,1; A[-1,- np.linalg. f, label= , ye, labe ); plt.xla</pre>	<pre>); dx = x[1 b = np.zer ,)); ; ; diag(dv1,1; = 0; 1] = 1; inv(A), b); "Numeric"); l="Exact"); bel("\$x\$");</pre>	<pre>!] - x[0]; ros((N,1)); + np.dia; I plt.ylab;</pre>	;(dv1,-1); 21("\$f(x)\$")						
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So, let me take 50 grid points maybe it makes things better it makes things much better the numeric and the exact solution do a does appear to match, but at the end point there is still something its not really matching exactly.

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[32]:	N = 100; x = np.lins A = np.zero alpha = -2	pace(0,2,N); s((N, N)); b - dx**2;	dx = x[1] - x = np.zeros((N	[0]; ,1));							
	dv = alpha* dv1 = np.on A = np.diag A[0,:] = 0;	np.ones((N,)) es((N-1,)); (dv) + np.dia A[N-1,:] = f	); ag(dv1,1) + np 0;	.diag(	dv1,-1);						
	A[0,0] = 1; A[-1,-2] = b[0] = 1;	-1; A[-1,-1]	= 1;			I					
	<pre>f = np.dot( plt.plot(x, plt.plot(xe plt.legend()</pre>	np.linalg.inv f, label="Nu , ye, label=" ); plt.xlabe!	v(A), b); umeric"); "Exact"); l("\$x\$"); plt.	ylabel	("\$f(x)\$'	.)					
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Well maybe if I make it a 100 points its much much much better, but well why is does it not match as good as the other points? So, over here for example, you can hardly discern that there is some error, but why is this I mean let us go back to our workout working. So, the backward difference this has a truncation error of delta x of order delta x.

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Whereas the central differencing that we have used for the interior nodes it is order  $\Delta x^2$  the truncation order is order  $\Delta x^2$ . So, we must now come up with an approximation

of the boundary condition at the end node at N - 1th node which is order  $\Delta x^2$  and the way to do it is again a central difference scheme.



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So, you have the N - 1th node, you have the N - 2th node. Now, we have to imagine a ghost node say the Nth node. So, this is actually not a part of the domain its a extended ghost node that you sort of have in order to do something with it. So, now, the boundary condition was df/dx at N - 1 or the N - 1th node is = 0.

So,  $\frac{f_N - f_{N-2}}{\Delta x} = 0$ , but because its using the Nth node Nth - second node its order  $\Delta x^2$  accurate alright. The truncation order is of order  $\Delta x^2$ , but what do I gain with this. I now have introduced an extra node. So, I can write down the equation that I had for the interior nodes for the boundary node as well.

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So, now I can have  $f_{N-2} + \alpha f_{N-1} + f_N = 0$ . So, I can do this, I can use the equation that I had formulated in the interior, because I have extended the domain by 1 ghost node. So, this sort of becomes the interior this is the ghost node very spooky.

So, now I have an equation in terms of  $f_N$ , but from this equation I have what?  $f_N = f_{N-2}$ . 2. So, substituting this over here I will have  $2f_N + \alpha f_{N-1} = 0$ . And now this is the last equation that I should modify everything to, alright.

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So, let me make a copy of this or in fact, let me change it to A1 and I will make the other thing as A2. So, that we can plot everything in N 1. So, everything is same for A1 and A2 up until the last point. In fact, we could have used np dot copy, but anyway we have doing we have done it the hard way no problem. We could have used np dot copy that is copy make a copy of A1 and assign it to A2 but anyway.

So, now what changes is over here. So, this does not change this is still 1; I mean 1, but over here now what do we have? So, this is  $\alpha$  alpha, and this is 2 ok; this is going to be alpha sorry this has to be written in terms of f<sub>N-2</sub>. So, I will have A2 - 1, -1 =  $\alpha$  and A2 - 1, -2 and that is going to be = 2 ok yeah that is pretty much it.

Now, let me make another solution let me call it g this will be the inverse of A2. And we expect the solution from A2 to be more accurate than A1 let me also plot, alright.

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Let us run it we have too many grid points let me make it 10 to highlight the difference perhaps the exact solution. (Refer Slide Time: 42:51)



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We can put as a marker and for the exact solution we can take maybe only 6 points. So, because it is an exact solution we know that the markers will be exactly at the correct point.

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So, look the second order solution is far more accurate than the first order solution. In fact, let me make it first order. So, just to say that its the boundary condition is of the first order ok, the second order boundary condition matches quite well.

So, what you can do is give a go of this technique that you learned the ghost node. You can do it for any you can open up a textbook and find out any equation that you have you can try to solve it using this technique ok.

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And I have shown it for a linear equation, but you can extend all this calculation for nonlinear as well. And you now know the tips and tricks to how to implement all of this in any language really. We are not dependent all we have used is the inverse finding trick over here. And actually, in the next class before beginning I will discuss a bit about various other algorithms.

So, you do not really go about finding an invoice these are direct methods. So, to say, but do it iteratively. I will just make a small note on what techniques do exist and what is being used because once you have large systems finding an inverse of a sparse matrix is not that easy ok.

So, go ahead and try different problems from your textbook you have analytical solutions as well; you can try to plot them to convince yourself everything works ok. So, with this we end this in the next class we will see how to use some of the inbuilt libraries in python to do all this thing in a very small I mean wrapped way ok. So, we will be using the solve BVP ,nd and I will discuss about some solvers. So, with this we conclude this lecture I will see you next time bye.