Introduction to Computational Fluid Dynamics

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Lecture – 08
Finite differences, Laplace Equation

So, today's class what we will do is; we look at a one sided; we look at a one sided derivative for the first derivative representation, right and then we look at again, we will go back look at the second derivative and if we have time, we will go on to applying it to a set of simple problems because by the time we are finished here, we will know how to represent functions, we know how to represent derivatives.

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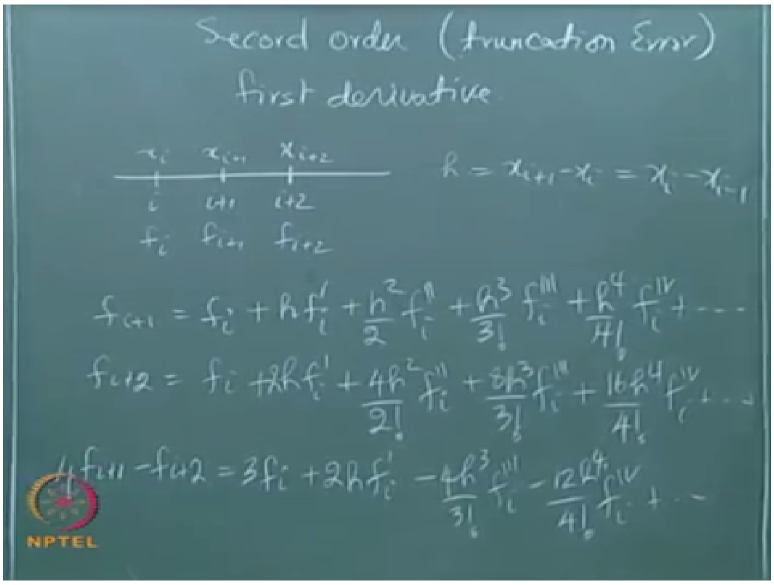

So, we might as well try out a few simple problems to see if we are able to solve differential equations that are of interest to us, okay fine, is that okay right. So, if you want second order meaning, truncation error is a second order, first derivative, is that what we want, right. The last class as I said I have already done a higher order, let us look at for a; look for the second order, so if I have the points i, i + 1, i + 2, these are located at xi, xi + 1, xi + 2.

The function values there are fi, fi + 1, fi + 2 and right now, first what we will do is; we will assume that h is like it is in fact equals xi + 1 - xi which equals xi - xi -1, you will assume that they are equivalent rules right now okay, later we will do unequal intervals because an unequal intervals are of interest to us though except here, you will see it here in this class and then you will never see me use unequal intervals again.

So, this class is important in that sense and unequal intervals are important but for this course, I am not going to do unequal intervals outside this class, okay, is that fine, okay. So, it is a simple game now, so now we are going to do it right clean from the start, simple game now, you want to find the derivative at i and I am going to use the points i + 1 and i + 2, you will use Taylor series.

So, f at i + 1 is f at i + h times f prime at i, the prime indicates differentiation with respect to x + h squared/ 2 factorial f double prime at i + h cube/ 3 factorial f triple prime at i + h to the 4th/ 4 factorial, f 4th derivative at i and then so on, okay. In a similar fashion, fi + 2 is fi - h times f prime at i; I am sorry, + 2h times f prime at i, you can see in my mind I have written 9 -1, it is okay, you have to be very careful, okay, fine.

Plus 4h squared/ 2 factorial f double prime at i + 8h cube/ 3 factorial f triple prime at i, the reason why I do not succumb to the temptation to expand this out and cancel and so on is because I know I am going to combine these 2 terms right, so I leave whatever is common between them I leave them as they are, okay, there is a temptation when you are writing this to cancel terms and so on, do not do it; +16h to the fourth/ 4 factorial, the fourth derivative and so on.

So, we look at these 2, our objective is to extract out the f prime at i, so what do I need to do? If I multiply the first equation by 4, I will get a 4h squared here and then I will get a 4h squared here, so if I multiply the first equation by 4 and subtract the second equation and knock out the h square term. So, 4 fi + 1 - fi + 2 is 4 fi - fi which is 3fi, 4h f prime, right - 2 that is +2h f prime at i, this will cancel that is the whole point of multiplying by 4.

And this gives me -4h h cubed/ 3 factorial, the third derivative -12h cube/ 4 factorial, fourth derivative, did I make a mistake; h power 4 and so on, okay, so it is very clear, it is very easy to make mistakes, you have to be really careful when you are doing this, fine.

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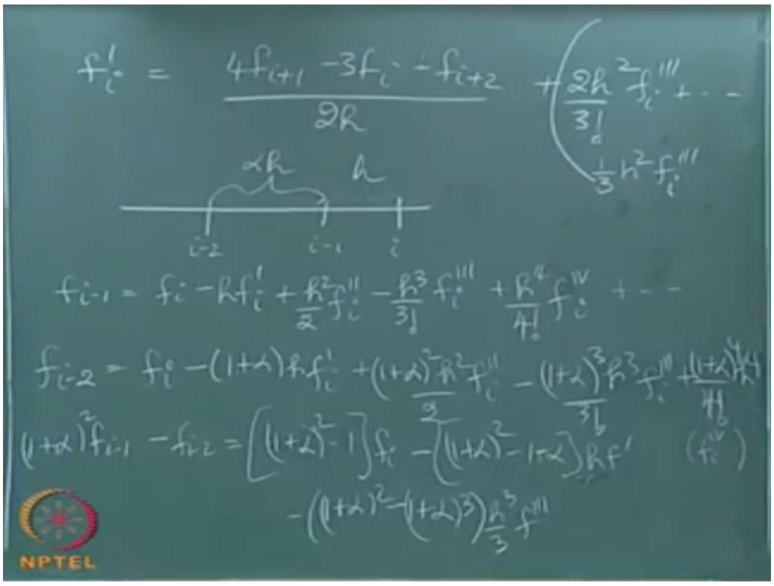

So, let us solve for f prime at i, so if you come here and you solve for f prime at i that derivative is 4fi + 1 - 3fi - fi + 2/ 2h, what does that leave me, 2h square/ 3 factorial f double prime + higher order terms, f triple prime + higher order terms, so if I throw this out, I say this is the representation for the derivative, I throw this out, right, so this is the truncation error; truncation error is of the order of h squared.

So, it is 1/ 3h squared f triple prime at i, is that fine, truncation error is of that order and again like I did last time, I make a quick check add 4 – 3 - 1 that is 0. Why do I say that, you ask yourself the question, why do I test even last time I test it by adding up all the coefficients to make sure they added up to 0, why do I do that? Constant function it should work yes; constant function it should work.

Constant function should give me a; should give me a 0, right, constant function should give me 0 and of course, in the limiting process, the numerator is supposed to go to f at i if I actually take the limit, remember this is a finite difference, if I go back to the infinite process which means I take the limit h going to 0, right, the numerator is supposed to independently go to 0 and then denominator goes independently to 0.

It is a ratio that gives me the derivative, you understand, right, so from a; how should I put it; from an operational point of view yes, I have a derivative; I have a representation for the derivative and the constant function should give me a 0 derivative, right that is one operational point. The other processes of course, I have an infinite process for which I have replaced by a finite one.

I stop, I do not divide by, I do not take the limit h going to 0 but if I do both take h going to 0, this should go to the derivative, it has to converge to the derivative right, we want it to converge to the derivative, is that clear okay, so the summation; so that is one sanity check that you can always do add, make sure that they all add up to 0, okay, this is fine. Now, what if they were unequal intervals; what is they were unequal intervals?

So, we have these weights, we have seen this is very nice, we have the truncation error but what if the intervals are unequal intervals; what if the intervals are unequal intervals and just for the fun of it; just for the fun of it, we can do a; we can still do a comparison but just for the fun of it, we will do i, i– 1 and i -2, okay and in this case, this length happens to be h and to keep or algebra simple, I will call this some alpha times h, is that fine.

Just to keep our algebra simple and this kind of a relationship you may actually get in future applications, so I leave this as alpha times h and we will just quickly repeat this process, okay, we will just quickly repeat this process, so what do we have? F at i – 1, yes f at i - h times f prime at i + h squared/ 2 factorial, second derivative right at i - h cubed/ 3 factorial f triple prime at i + h to the 4th/ 4 factorial, the fourth derivative at i and so on.

F at i - 2 is f at i -; I am sorry; 1 + alpha times h f prime at i + 1 + alpha squared; 1 + alpha whole squared h squared/ 2 factorial f at second derivative i, right, so it is very clear, it is not that bad plus so on, right, 1 + alpha power 4, 4 factorial h to the 4th and that will be multiplying the fourth derivative and you have all the other terms, what do I do now? So, if I multiply the first equation by 1 + alpha squared, I should be able to cancel out the second derivative term, okay.

So, 1 + alpha squared fi – 1- ; I am going to subtract out this term, fi - 2 equals, so you should be happy if alpha over 1+ alpha squared is 2 squared which is 4, which is what we did earlier right, so that is not bad, fi - 2 equals, you have 1 + alpha squared, so I keep doing that - 1 fi, what happens to this term, so you get a 1 + alpha squared - 1 + alpha h f prime, then what else; minus alpha, no by 2 that is the first derivative term.

Then, what is the third term? Third term goes away, so and then you get – 1 + alpha squared – 1 + alpha cubed h cube/ 3 factorial f triple prime and I would not bother with the fourth term, right the fourth term something that you can work out because normally, when I do it, when I am sitting alone I sort of simplify this a little faster than this, right so but it is fine, we will let us see what we get here.

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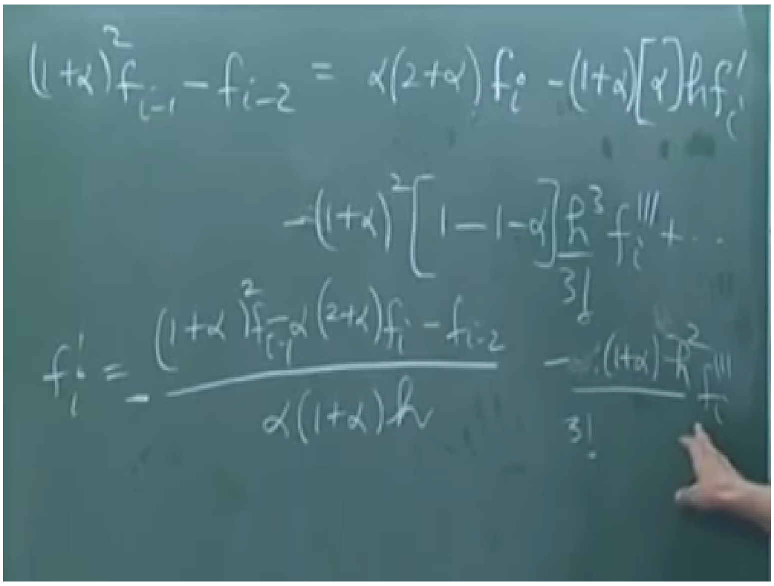

So, you have 1 + alpha squared fi - 1 - fi - 2 equals, alpha * 2 + alpha, is that fine, in that alpha equals 1 that gives you 3, so we are happy, it is working out, so it is fi, okay and what is the next term, I can factor out 1 + alpha, so that gives me a -1 + alpha * alpha h f prime at i in the alpha equals 1 that is 2, okay that also works, + or -; -1 + alpha squared * 1 – 1 - alpha h cubed/ 3 factorial f triple prime i and so on, okay.

Actually, I made a mistake here, there is a 3 factorial at that point, it is okay, is that okay, so what does it give me for a f prime at i; 1 + alpha squared - alpha 2 + alpha fi, fi – 1, fi – fi – 2/ alpha * 1 + alpha, do you have a sign problem? There should be a negative sign here okay, in this what is the truncation error now; - alpha * 1 + alpha squared h squared/ 3 factorial and I have to divide by alpha times 1 + alpha, so it gives you an 1 + alpha f triple prime at i.

It has to be a plus, no it is right, there is a negative sign here, there is a negative sign here, there is a negative sign here, there is a negative sign here and there is one more negative sign, it will turn out, right. See, I have another way; I have another way by which I checked if you notice I glanced at the other board, what was the truncation error for the 4 difference that was positive, so this will be negative, right.

There are some simple sanity checks that you can do fine, okay, so and you can see if you set alpha equals 1, whether it works out, so clearly if they are unequal; clearly if they are unequal, it is going to become very messy yes, "**Professor – student conversation starts**" We use i but you would not able to use i -1, I am not sure that I am understand the question. No, no you have; it is the same thing, you have 3 points, they are unequal, there are equal distances.

But I can still eliminate, I can still eliminate the second derivative term and get an expression for the first derivative leaving a truncation error which has only a third derivative, do you want to calculate the derivative at the next point and that could be; it could be you know some beta h or something of that, so that could be something else altogether, you would still have unequal intervals, you could still have unequal intervals.

No, no it need not always be alpha, there is a process called geometric stretching, where it is always alpha, right it is a constant that is a nice situation but if it is not; it need not always be the same, okay so the point next to it could be a sum ratio, is that fine, right it need not be h/ alpha or something of that sort, it need not be that way okay, right. So, the idea is that the adjacent intervals are not of equal size, fine.

So, and as you can see from the fact that the expression is so messy, it is possible for us to calculate it but clearly from a; thank you, clearly from a classroom point of view, right it does not add anything, I just want you to have an awareness, I will do one more in this class with unequal intervals as I said but it does not add anything to my class as such, right, so if you take uneven intervals, which you very often will be forced for other reasons right to take uneven intervals then you are forced to take uneven intervals, you will get messy expressions.

And this error seems to be slightly large I mean, if alphas depending on the value of alpha, the magnitude of this error term is going to change, okay so you may; you should have a reason, so you will be changing these h values because you have maybe possibly some knowledge and how the function is varying, right and then that is reason why you are trying to compensate, if you know that the triple prime is large, then you may be changing your alpha in order to compensate for that, it is possible, okay.

There are many reasons, you will see that when you run into it at a later date in a more advanced course, you will see why you change take unequal intervals, in this class as I said I will do it one more time but the reason why I will not persist, I will always assume equivalent rules is because it just makes life easier and the derivations are always possible, whatever I do with unequal intervals you can repeat as I have indicated with unequal intervals, is that fine, okay. “**Professor – student conversation ends.**”

So, let us look at the second derivative right, so far we looked at the first derivative, you have a first order forward difference representation, backward difference representation second order forward difference backward difference right, you have one third order representation that I did in the last class, so you can work out other higher order, I would suggest I would strongly recommend that you work, other higher order representations for the first derivative, okay, for the first derivative.

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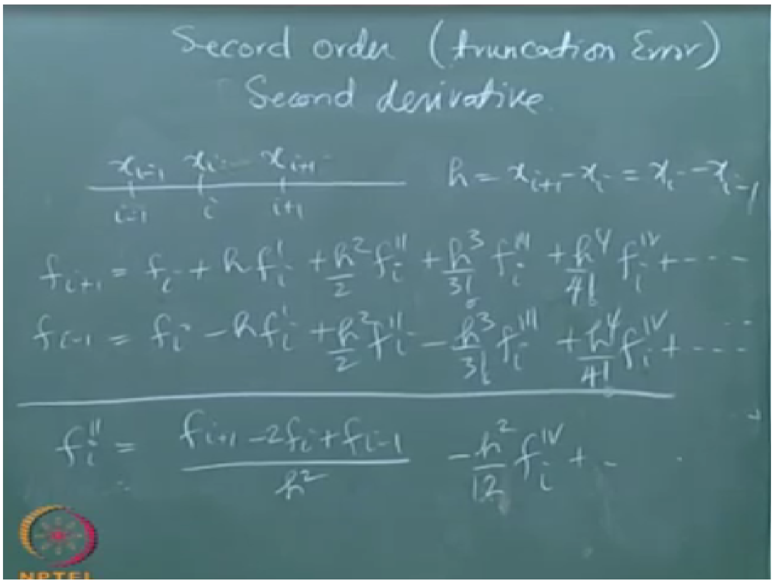

Now, let us look at the second derivative again, I will repeat the second derivative, I quickly repeat the second derivative, right that we did last time, so it is second order second derivative just because I am going to do it, I am going to do it twice one which we did last class and then I am going to repeat it again with unequal intervals. So, like I did I have xi, xi + 1, sorry; xi – 1, xi + 1, i – 1, i, i + 1, of course you can also see whether you can get one sided derivatives, right for the second derivative one sided representations, I leave that to you.

So, what we have is simple expansion again using Taylor series about the point i fi + h times f prime at i. And again h equals xi + 1 – xi equals xi - xi – 1, okay, this case they are equal, + h squared/ 2 factorial second derivative of i + h cube/ 3 factorial third derivative i + h to the 4th / 4 factorial and so on, please remember so we are using Taylor series to expand about the point i;

xi, okay you could as well use Taylor series to expand about any other point which was expand about the point i because we want the representation at the point i right.

We want the representation of the derivative at point i therefore we choose i, if you want the representation elsewhere then you have to expand about that point, is that fine, is that okay. So, f at i - 1 is f at i - h times f prime at i + h squared/ 2 factorial f double prime at i - h cube/ 3 factorial, so this is sort of a jury process unfortunately, you have to get it, right okay, it does not work, details very important.

So, if I just add the 2, this cancels that cancels, so it gives me for my first derivative and expression we derived in the last class, the second I am sorry the second derivative and expression we derived in the last class that is f double prime at i is fi + 1 - 2 fi + fi – 1/ h squared - h squared/ there are 2 of them, okay, this is the truncation error, we have seen this; we have seen this.

So, the question is what happens if we take on unequal intervals, okay, we look at that and then I will sort of; we will close the subject of what happens with unequal intervals, so what happens if you take unequal intervals for the representation of the second derivative, we have seen what happens for the first derivative; first derivative, we still got a second order representation, it is just that the coefficient of that truncation term change, we will see what happens here.

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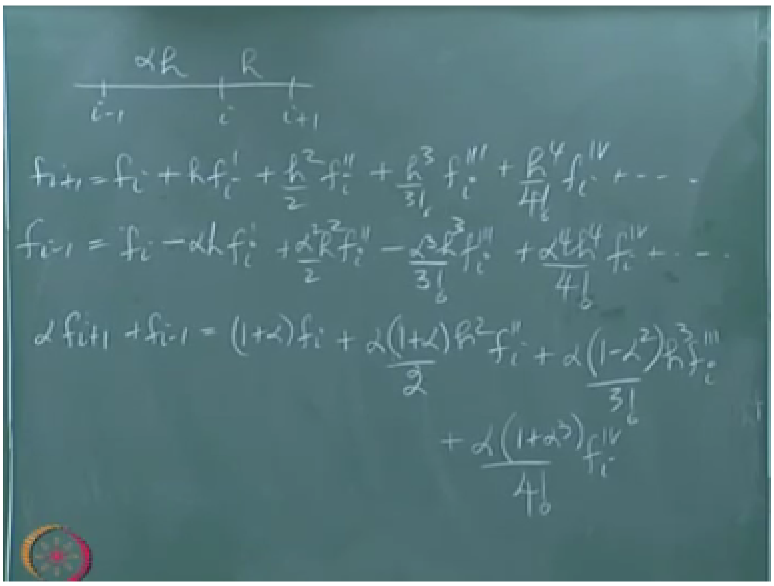

So, instead of h, instead of h so, okay we will just write it again, so we have i – 1, i, i + 1, this is h, this is alpha h, okay just to keep it clean, you just redo it quickly, so fi + 1 is fi + h times the first derivative + h squared time/ 2 second derivative, which is what you want, + h cube/ 3 factorial the third derivative + h to the fourth/ 4 factorial, 4th term and so on, okay. Normally, if you did not know how many, I would; you would take a lot of terms depending on what is it, what order you are going to take, right.

You cannot stop at fourth derivative if you want a much higher order I stop at fourth derivative because I know I am going to get something that is of the order of second order; fi - 1 one is fi - alpha h f prime at i + alpha square h/ 2 f double prime at i - alpha cubed h/ 3 factorial f triple prime at i + alpha to the fourth, this is not as bad as the first derivative, right h to the 4th, 4 factorial 4th derivative i and so on, is that fine.

H squared, H cubed being a little careless today, so if I multiply by the; so now, I am a little desperate I want to get rid of that, I have to get rid of that first derivative that is my need, I want the second derivative, so I multiply the first equation by alpha to get rid of that okay. So, I get alpha fi + 1 and to that I add the second equation fi - 1 equals 1 + alpha times fi, I get an alpha fi + 1 fi, the second term cancels.

What happens here; + alpha, 1 + alpha * 1 + alpha h squared/ 2 f double prime at i that is a term that I want, + alpha * and what happens to the last one, now this looks very different, this looks very different, so if I do; if I try to evaluate it maybe write it here, pardon me; **"Professor – student conversation starts"** no, no I think you can verify, you can check get it out, it is okay, I get it out to the way, we will stick with this material, what we are doing right now. **"Professor – student conversation ends."**

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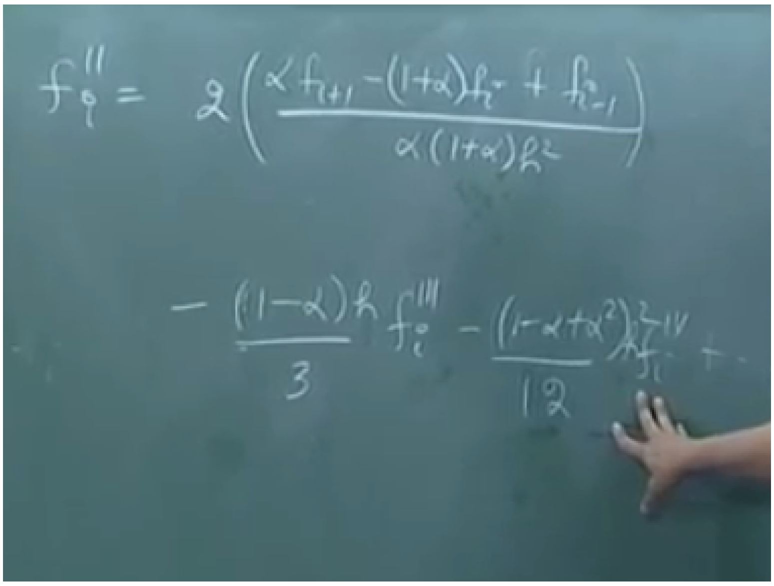

So, f double prime and i is alpha fi + 1 - 1 + alpha fi + fi – 1/ alpha * 1 + alpha h squared to 2, right so if alpha equals 1 that 2 and this 1 + alpha will cancel that is the idea, okay and alpha equals 1, this will be 1, that is 2, that is 1, it goes back to the standard expression. What about the truncation error? So, you have a third derivative term right, so you have a minus, this is a truncation error, so I have divided by alpha, 1 + alpha.

So, it gives me a 1 - alpha h/ 3 at i and this gives me a – 1- alpha + alpha squared, a little algebraic 4th derivative at i and there is an h squared here and this is the difference, so for the second derivative term, if you take unequal grids, the convergence rate drops, the representation of the derivative suddenly became; the truncation error became first and the convergence is linear, it is not quadratic, it goes to 0 as h, not as h squared.

This is very important to remember and it introduces a third derivative term, this will have significance later in the semester, I will remind you about this okay, later in the semester I will remind you about this, it adds so if you have unequal grids, if you have unequal grids, it introduces a third derivative term, is that fine, okay and it introduces a convergence, which is first order and not something that a second order.

Of course, if alpha equals 1, this goes away rate and we retrieve what we had for equal intervals, is that fine okay, so as I said it is always possible for us with unequal intervals to calculate derivatives, it is always possible, so when you encounter it you know how to do it but we are not going to do anymore because it is just a mess and it does not add anything else, okay but I do want you to remember.

This is very important that if you go for unequal intervals, you cannot be sure that the order that you get is the same order, you have to recalculate, you have to rework okay, right. Now, let us apply this now that we have all these derivatives that we can represent and functions that we can represent, let us apply these; let us apply what we have got, right to differential equations some differential equations, we will choose a simple one right now.

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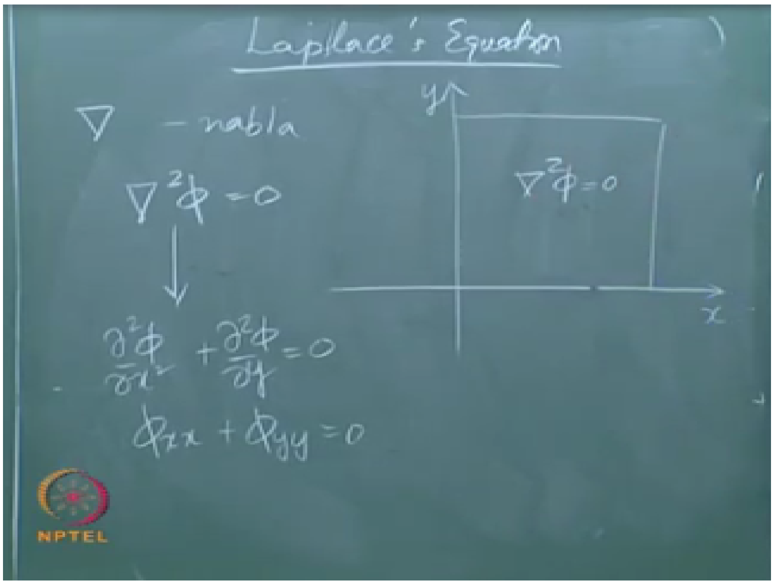

We will use; we will look at Laplace equation; we look at Laplace's equation, is that fine okay, so we look at Laplace's equation in 2 dimensions, I am going to stick to 2 dimensions here, so this symbol is called nabla, right you are used to calling it del but it is called nabla, so this would be nabla squared phi 0, okay, fine and we could choose to solve this problem in a very simple region.

We can choose a region that is in the first quadrant maybe a unit square and in this unit square, you have this equation that is valid and on the boundary possibly we provide boundary conditions, so you know of many ways by which you can solve this equation possibly, in PD you studied variable separable and so on, right there are many ways by which you can solve it. Here, we look at see whether we can represent the derivatives on a mesh.

And whether we can use that in for the solution, okay, so to obtain that solution, so we know that in 2 dimensions, this would be dou squared phi dou x squared + dou squared phi dou y squared equals 0, I will use an alternative notation, I may switch between them depending on convenience, so if there is no confusion you may occasionally see me write that it is much more compact notation, okay both of them represent Laplace's equation in 2 dimensions.

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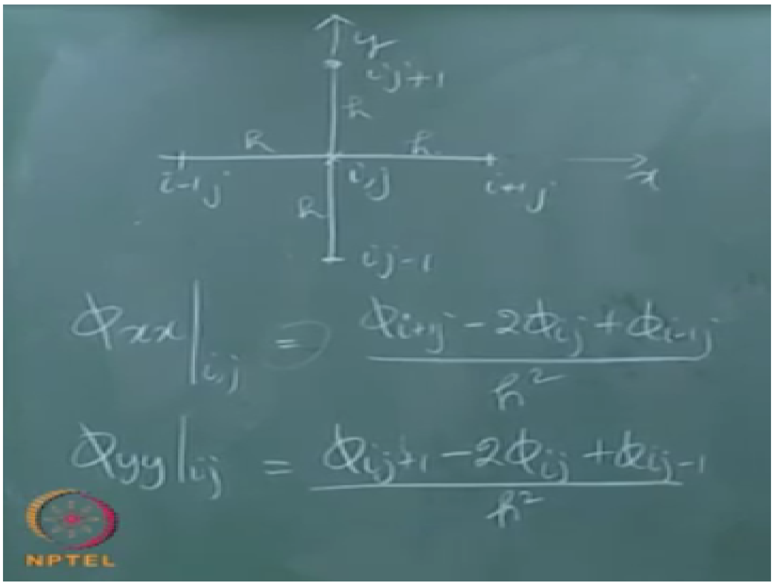

And this is an expansion of that nabla squared, so what is the typical mesh point that I am going to take, just like we said i, i + 1, i – 1, how are we going to do it in 2 dimensions. In 2 dimensions, in Cartesian coordinates, I am going to take equivalent rules, right so this would have now 2 indices; one for going traversing along in the x direction and one for traversing along in the y direction.

So, that would be i + 1 j that would be i – 1j that would be ij - 1 and that would be ij + 1, okay I will take all of these intervals for the sake of convenience to be h, I think you can figure out what will happen if you change the values, you could there are so many different things that could happen, it could be h here and it could be some different value in the y direction, each one of them can be different there is so many possibility, you can work it out.

So, what is the first derivative; what is the first term at the point ij using the expression that we have just derived, it is phi i + 1j - 2 phi ij + phi i – 1j/ h squared, okay. So, at the nodal points if I have the function phi given by i + 1j, ij, i - 1j, phi of the appropriate points, I can estimate the derivative okay and we have a truncation error associated with it, I say equals at this point but we know already that I say equals but we know it is an approximation, it is a representation, right.

But I will write equals ij in a similar fashion is phi ij + 1 - 2 phi ij + phi ij – 1/ h squared clearly, if they were delta x and delta y, it would be delta x squared and delta y squared, okay that is not a big deal, fine. So, now to represent Laplace equation at that point, so now I am talking about representation, so far we talk about derivatives, now I am going to actually represent the equation, I will add these 2, okay.

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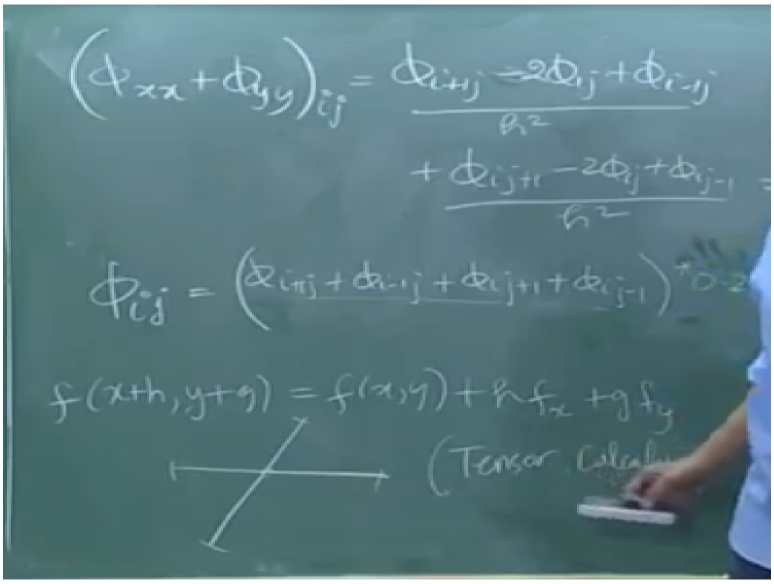

I will add the 2 and I can actually represent Laplace's equation, xx + phi yy at the point ij gives me phi ij, phi i + 1j – 2phi ij + phi i – 1j/ h squared + phi ij + 1, not a big deal means – 2phi ij + phi ij - 1 h squared and this is supposed to be 0, this at that point supposed to be 0 at that point okay, so now i say this represents the Laplace's equation at that point; at the point ij and it is actually possible for us, it is actually possible for us to solve for phi at ij.

After all that is really what we want, we want the phi at ij in fact, turns out, so if you multiply through by h squared, the right hand side is 0, so the h squared will go away, okay this turns out to be phi i + 1j + phi i – 1j + phi ij + 1 + phi ij – 1/ 4, right you could write by 4 just to encourage you to multiply instead of divide, I will write times 0.25, so now change to a programming notation, multiplied by 0.25, okay that is fine.

But by the 4 is important, it is the average of this; of the neighbour that is the key, so solution to this equation is the average of solution to this equation at this point, the value at this point is the average of the values at the neighbouring point, okay is that fine, okay. So, now we have some mechanism by which we can take represent Laplace’s equation at a given point, we will see what we can do with this.

"Professor – student conversation starts" Yeah, do you have question, oh, well in this case it does not matter because we are taking derivatives only with x and y but you can actually write Taylor series in 2 dimensions, there is a Taylor series expansion for 2 dimensions, so if you say, you may have seen it in multivariate calculus, you can actually write it, you can actually expand about the point f(x, y), right. **"Professor – student conversation ends."**

And then it will turn out to be; I am just writing this fx, fy, where fx is derivative with respect to x, fy is derivative with respect to y and you can go on, so you will get a h squared fxx, g squared fyy, 2hg fxy, you understand and you can add, you can keep on adding terms right, so there is a from your multivariate calculus, you go back you look, you will see that you will actually pick up, okay.

So and you would need that you would need that if these grids were not orthogonal to each other that is if you had grids that were not only unequal but they are not along the coordinate lines, so not only are there it could be equal or unequal but they are not along coordinate lines, right and then you can run into this problem that you would have to do it in, you would have to do it this way.

But trust me there are better ways by which one can do this, right, so we will see, if we will see may, I do not know whether you need to look up a little tensor calculus, I usually do something on tensor calculus we will see whether we get there or not at least I will give you a motivation for why you should learn tensor calculus as we go along, okay let us get back here, what do we have?

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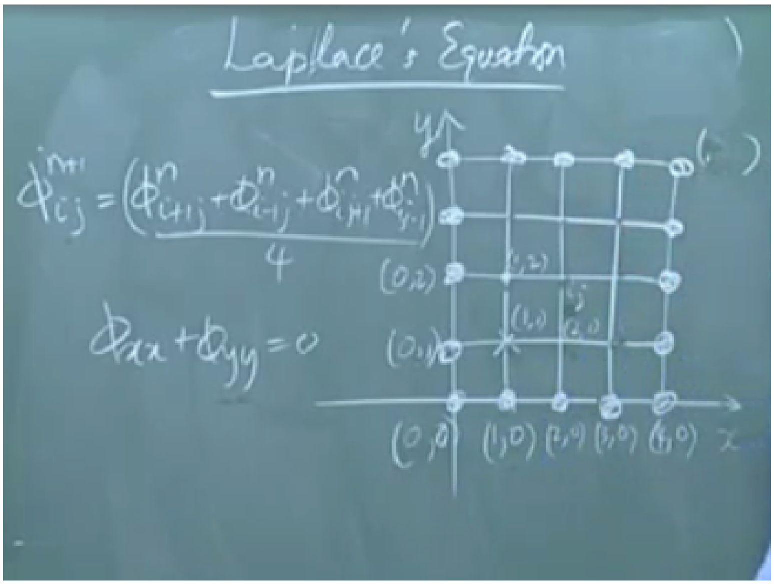

So, this is a problem that we want to solve, we will make up a problem and we will see how we would go about solving using what we have just derived, so what we do is again to keep life easy, we will break this up, we will break up our problem domain using a mesh and you will notice that in this case of course, there are 1, 2, 3, 4, 5 at the 3 interior points, right, so this would be; so that would be at some point ij that I was talking about okay.

And how would the problem be normally prescribed, how would you normally prescribe the problem? So, just say this is a unit square, so this is the point 0, 0 which is the origin, this is a point 1, 1, right so unit square located at the origin; unit square located the origin and what we want to do is; we want to see whether we can solve Laplace's equation, so given some boundary condition we will figure out how to get those boundary conditions, given some boundary conditions.

So, I prescribe some boundary conditions which means that the values at these points are known, so if I prescribe some boundary conditions, the values at these points are known and if we are able to find the values at the interior points, right then we have phi ij's at the interior points and using possibly hat functions or something of that sort we may be able to interpolate, it actually we use hat functions in 2D but I have not defined hat functions in 2D.

But you can use hat functions and actually use linear interpolants to find a value anywhere in between okay, is that fine. So, what you can do now is at any given point ij, you just repeat this, so phi ij is phi i + 1j, phi i – 1j, phi ij + 1, phi ij – 1, then say divided by 4 here but you know you have to multiply by 0.25, you just repeat this process for every interior; every interior node, the conditions on the boundary are given okay.

So, when you are trying to figure out what is the value at that node, this is known that is known, right let us number these, so let us say this point is 0, 0, this is 1, 0, 2, 0, 3, 0, 4, 0 okay, so this is 0, 1 and this would be 1, 1 get rid of that 2, 1 and so on and this point is of interest, this is 0, 2, this is 1, 2, so if you want to find the value at 1, 1 you need the values at 1, 2; 2, 1; 0, 1; 1, 0 from the boundary conditions you have the values at 1, 0 and 0, 1 okay.

You do not have the values at 1, 2 and 2, 1 so if you not only do not have the value at 1, 1 we do not have the values anywhere in between, so in order to get this working, the process that we will start doing is we will make an assumption about the interior values, just make an assumption let us start with the guess, right a good guess would be 0, we have nothing to go with right now.

There are many possible guesses right now, I have not even told you about the boundary conditions, so good guess is 0, so let us just assume that all the interior values are 0 and your given boundary conditions okay, so you can find phi ij at any given point by taking the values of the neighbouring point, then you can go to the adjacent point, take the values of the neighbouring point, you understand.

And you can do this for all the interior points, you do not touch the boundary points because the boundary points are known already, so if you keep repeating this process for all the interior points as time progresses, we hope that the phi ij of all that you are generating a sequence of phi ij’s, so this is the generating a sequence of phi ij’s right, n equals 1, n equals 2, n equals 3, n equals 4 that you generate a sequence of phi ij's.

And you hope that sequence converges right now, we hope that sequence converges and if that sequence converges you will have a set of few values at every grid point okay, is that fine, okay, so I i's better if you just try it out and work a problem and I think then it will work out. If you go through that sequence and it has converged, how do you know the answer that you have got is the right answer?

Well, you have points at these values, you have grid points, so when you say something is the solution to a differential equation what do you do you substitute into the differential equation and verify whether it is true or not right, so you could substitute into the original differential equation phi xx + phi yy equals 0 but in this case, you just have points at various nodes, okay right.

And if you substitute in the difference equation, you can find out what is it that the difference equation gives you, okay but the differential equation itself requires that you take derivatives and you have only discrete nodes okay, is that fine right. So, I think what you do is you can try this out just give some arbitrary boundary conditions will work out maybe a more specific problem in the next class, just try to give it some arbitrary boundary conditions and see what it works, what happens, right.

Professor – student conversation starts" yeah, right, in this, what I have drawn have 9 unknowns, right. We have 9 conditions, right so we can solve linear set of equation, yeah there are issues so that we will get to that right, so we will see what it is that we are doing that is actually what we are doing, right we will actually figure out what is it exactly; what exactly are you doing okay, right. **Professor – student conversation ends".** So, we will get back to this on Monday, thank you.