Introduction to Computational Fluid Dynamics
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Lecture – 07
Representing Derivatives - finite differences

Okay, so today what we are going to do is; we are going to look at approximating derivatives right, so far we looked at approximating functions, right and we have seen there are lots of ways by which we can approximate functions. All I have done by way of either box functions, hard functions, hat functions right, all of cubics, quadratics cubic spline, quadratics and so on, it is just one class.

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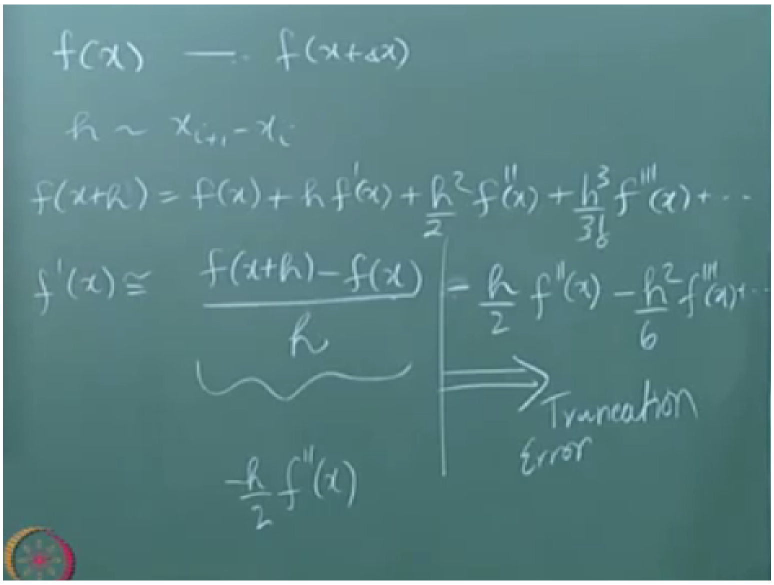

There are many, many ways by which you can write approximate functions and represent them on the computer which is the most important part that we are interested. Now, we saw in the last class that if you had a function f(x) and you wanted to find out what was its value at f(x + delta x). Let, we could use Taylor series, right we could use Taylor series to write f(x + delta x) in terms of f(x), okay.

So, for the sake of this discussion like I did earlier, I will say h is approximately xi + 1 – xi, I know I have introduced delta x because that is what you are used to seeing in your Taylor series formulas and so on, right so I will write this as f(x + h) is f(x) + h times the derivative f prime of x + h squared/ 2 factorial/ 2; second derivative of x and so on, 3 factorial, third derivative, is that fine.

So, I am just writing a Taylor series expansion of f at x + h expanded about the point x, right that is usually; that is usually what we call and it is possible for us one thing that we saw is it was possible for us to approximate f at x + h in terms of these terms, the more information that you have, the more terms that you can add. So, if you know the first derivative, you can get a representation whose error is of the order of h squared and so on, right.

The other possibility that we saw was that we can actually use this to extract are the first derivative that is f prime of x can be written as solving for f prime; f(x) + h - f(x)/ h, then we have to take all of these infinite number of terms to the other side and what will that give us? + excuse me; -h/2 f double prime of x – h squared/ 3 factorial which is 6; the third derivative of x and so on, okay.

If you go back, if you think about one of the definitions at least that you have seen of the; of getting the derivative of actually calculating the derivative, right from first principles using limits, you would have seen that f(x) + h - f(x)/ h, right limit h going to 0, it would be the definition of the derivative and all of these terms will go to 0 and you will get the derivative, so that is an infinite process, right.

It is a limiting process, it is an infinite process, we do not go through the infinite process, so we stay with a finite process and therefore this is called the finite difference, okay, so we have a finite difference approximation for the first derivative, I will truncate the series at that point; I will truncate that series at that point. This error that you see here all the terms that I have truncated called the truncation error.

And the order of the truncation error is indicated typically by the leading term, which is –h/ 2, the second derivative x, is that fine, okay. So, the representation that we have for the derivative f prime of x, right is f(x) + h - f(x)/h, if I am going to truncate it, then I have to replace this, it is really more of an approximation rather than right; rather than being exact.

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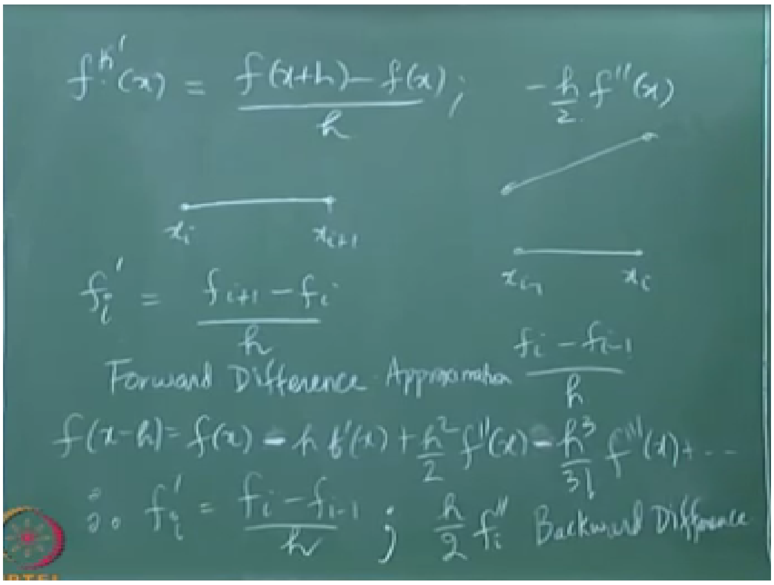

So, you could call it f prime, you could; we can indicate an H up there, prime of x, the h indicating that, right equals and as I told you earlier, I will use this h to indicate that it is an approximation and after a point maybe I will drop it where it is just clarity of that, I am actually talking about an approximation. So, this is f(x) + h - f(x)/ h and the truncation error is –h/ 2, second derivative of x.

What does the nature of the truncation error? In the limit h goes to 0, as h gets smaller and smaller, the truncation error is going to go to 0 in a linear fashion; in a linear fashion okay, so the convergence is basically first order convergence okay. For what polynomial; what degree polynomial is the truncation error 0? For a function that is linear, right for a function that is linear; for a function that is linear.

So, this sounds like the hat function, it sounds like the hat function, remember what was the derivative of the hat function on the interval xi - 1 or xi +1, so that was fi - fi – 1/ h, the same thing, okay. So, we are essentially representing in a sense, we are representing the function when we do this; when we go through this process we are representing the function using hat functions; linear interpolants, okay.

So and of course we will ask ourselves the question, it can be do better than this and we can obviously do better than this because we know that we can represent the function using quadratics, cubics and so on because this function; because this approximation involves x + h and x and the derivative is at x, right, we are using a point that is ahead; we are using a point that is ahead.

So, I will again; so this is xi, this is xi + 1, right, so if I call this point, the function value here is fi, so I am saying that f prime, I have already dropped the h to indicate, so I know it is f prime at the point i is fi + 1 – fi/ h, since I am using a point that is ahead, this is called a forward difference, this difference is called a forward difference; a forward difference, right. So, it is a forward difference approximation, is that fine.

So, if you can have a forward difference, the natural question that you have is; can we have a backward difference? So, in order to do that just like we did earlier, you say f(x) = h is f(x), we just follow that process, same process + h times f prime of x + h squared/ 2 factorial, second derivative of x + cube 3 factorial; I am sorry, I am making a mistake here, I have to pay attention, thank you very much; h cube f triple prime of x and so on.

The sign change is important, okay, so in therefore solving f prime, I just write it in the same notation; f prime at i is f at i - f at i -1/ h and what is the truncation error? h/2 times f double prime at i, this is –h/2, this is +h/ 2, is that fine, -h/2 and +h/2, the signs are opposite, this is called a backward difference; backward difference, so that is a backward difference approximation, is that okay.

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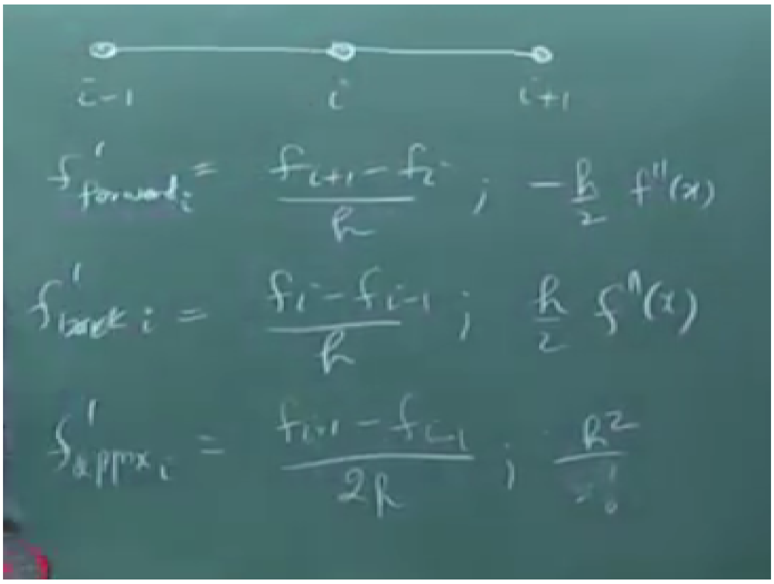

Okay, so we have a forward difference approximation, we have a backward difference approximation, look at this so at the same; across the same interval; across the same interval, I have these 2 across; I am not go there just a second; so, I have i, i – 1, i + 1, so I have 1 representation for f prime i, which is a forward difference, 1 approximation for the f prime, which is forward difference, right at the point i; at the point i which equals fi + 1 – fi/ h.

I am just rewriting that –h/2 f double prime of x, then I have another approximation backward, I will just write back at i which is fi - fi – 1/ h and the error here; truncation error here is; okay, is it possible for me to get a better or better approximation if I give you these 2 to get a better approximation? It looks like if I add this estimate and that estimate, this error will just cancel, you understand.

It looks like if I add this, so if I take the average of these 2, so this is just by way of suggestion just way of from observation; just from observation, f prime some approx. i is; what is the average of these 2? fi + 1, the - fi and + fi will cancel, - fi - 1 / 2h, this goes away, so I will have to go back and calculate; recalculate my truncation error, so what would be my truncation error?

What does my truncation error going to be like, I have - h cubed/ 3 factorial which is + h cube by; truncation error is 2h squared/ 3 factorial, it was has a; you can just do it, there is a -h squared by; there is a -h squared/ 6 here, okay and what we going to get here? You have a +h squared/ 6, anyway what we will do is; we will do; we will do this in the legal way, let me not so you can try going through this process.

You will see that will actually go through this legal straightforward fashion instead of this intuitive, so here all I am saying is if I look at this; this gives me a clue, I have a forward difference approximation, I have a backward difference approximation in this fashion and it turns out that these terms cancel, okay. So, when I say let us go about this legal way, what I am saying is if you want to find the truncation error, there is only one way to do it.

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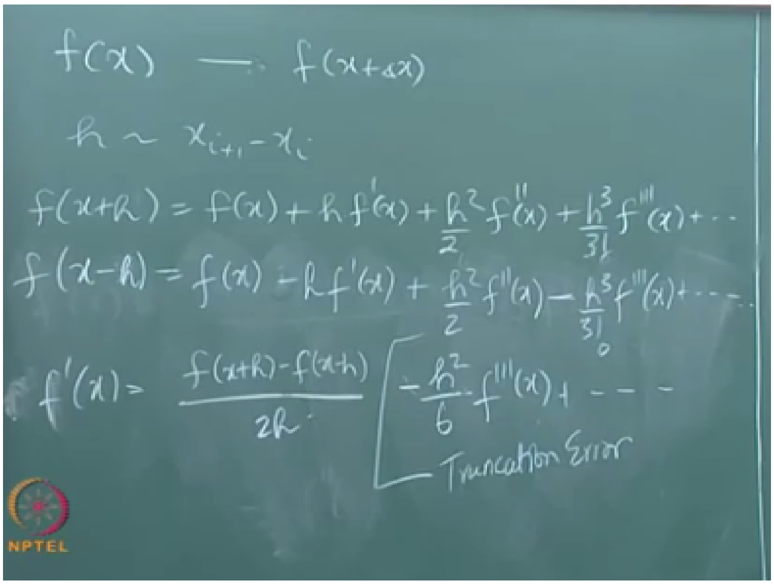

You have to get the series and actually do the truncation error, so we have to get it from Taylor series okay. So, let us get back to the first one, we get it from Taylor series, so it involves the points $x + h$ and $x – h$, so I will rewrite my Taylor series for $x – h$, $f(x) - h$ is $f(x) - h$ times f prime of x + h squared/ 2 factorial f double prime of x - h cube/ 3 factorial f triple prime of x and so on, is that okay.

So, what I am going to do now, I want to solve, so this is how you would do it, right so please do not go around taking averages and all that was just for; that was just a question to lead us intuitively to this part, so this is how you do it. What do I want from these 2 equations? I want to get f prime of x that is my objective. I want to solve for f prime of x, so which means that from the first equation, if I subtract the second equation, I will get 2 f prime of x is $f(x) + h - f(x) – h$/; well, so I will remove the 2h.

So, I am dividing through by 2h, what happens to this term? It cancels, there are 2 of these but I divide it by 2 okay and therefore, I get and we have to make sure that the sign is right, we have a - h squared/ 6 f third derivative of x and so on and other terms that would be the truncation error, okay. So, in this particular case as h goes to 0, we converge quadratically okay, the error goes to 0 quadratically, h squared.

And what about the polynomial that we are using, that is also quadratic; that is also quadratic okay, that is also by chance it happens, then that it is also quadratic, it is also a second degree polynomial, we can represent a second degree polynomial; we use a second degree polynomial for f, this term will be 0 and f prime we will get the right answer, is that fine, okay. So, essentially we are using parabolics to represent the f in this case, right.

Though we are not actually constructed the quadratic, all we have is those points, if you go back and try to find the coefficients, right for the quadratics and cubics, if you go back right, we did; you have done as repeat we have done hat functions, quadratics cubics I have not used quadratics and cubics to represent functions, right I would suggest that you try it. If you go back and try to do it, when you look at you will get a system of equations for the coefficients.

And when you look at the system of equations for the coefficients and solve for the coefficient, we will be surprised that you should not be surprised that you will get terms like this, just try it out, right. There is the reason why I asked you to do it, if you done it this should look familiar, right, you should; there is suppose, to be an aha moment for you saying that ah, I have seen this right, when I did the quadratic, I got exactly the same expression, okay.

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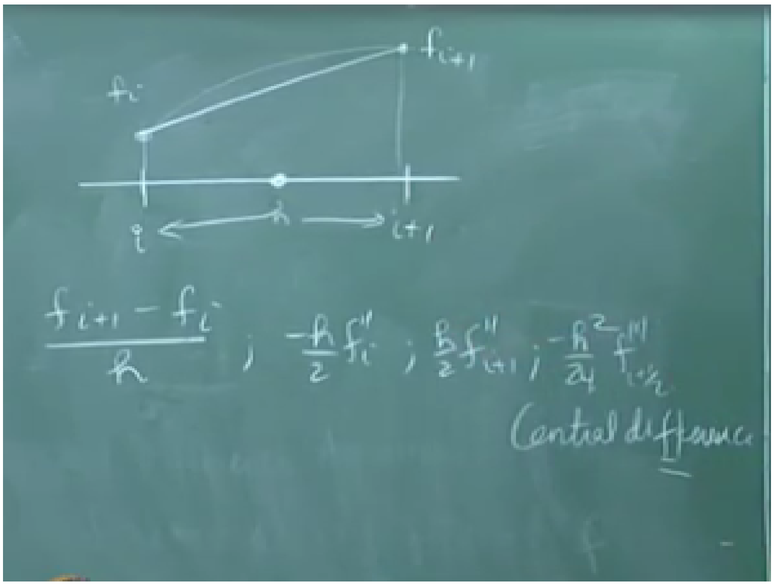

So, there is a connection between this and that the quadratic; coefficients of the quadratic, okay, well so this is what we have, let me make an observation here and then we will see what is it that I am going to choose an interval to see what it is that we have. This is i, this is i + 1, so I can have some function in between, right there is some function that I am sampling, this happens to be a fi that happens to be fi + 1.

What I am doing is; if I look at fi + 1 – fi/ h, so that you get a clear idea so what it is that we are doing here, right, fi + 1 – fi/ h, this length is h, right just for clarity, I am actually calculating the slope of that line; I am calculating the slope of that line. If I were to take the slope of that line and assign it and assume let it is the derivative at the point i, I will be doing forward difference, right.

And the error that we have; the truncation error that we have is –h/2 f double prime at i, if I take the same slope, the same number; the actual number that you calculated, if I would take the same slope and assign it as a derivative at this point at i + 1, right then I would have backward difference, the same number, right; the same actual number that you calculate, it is a backward difference.

And the truncation error would be h/ 2 f double prime, be careful with this; i + 1 okay and interestingly, if I take that and assume that it is the derivative at some midpoint, right derivative at the midpoint, now my h is not the same h there, this is right but it still, I mean it; so 2h actually becomes h in that formula, so it is the same expression; the same expression you have to be careful with the truncation error, okay.

Then the truncation error if I take it as a central difference for this would turn out to be h squared/ 24 third derivative, you can think about that 24, right and this is at some intermediate point, we do not know what is that value but it is some intermediate point i + 1/2 I will just call it i + 1/2, it is a midpoint. The same number, right is first order approximation there, first order approximation there, forward difference, backward difference this is called central difference, okay.

So, central difference; the same number central difference is a better approximation, so that basically, actually if you think about it, this should remind you of mean value theorem, right mean value theorem simply says that if you are going on a continuous path; if you are walking on a continuous path right from one point to another point, if you are walking on a continuous path from one point to another point, then somewhere in between in that trajectory; somewhere in between in that trajectory, what does mean value theorem say?

You are walking parallel to the line joining those 2 points, if you start at a point and go to another point you understand; if you start at a point and go to another point, it does not matter you have all go following a continuous path somewhere along the line, you must have been walking along the line joining those 2 points that is all mean value theorem says. It does not say where that is our problem, okay, it does not say, where.

So, this line joining them, this line join; the function is tangent to it at some point, the function is tangent, the problem is we do not know where, we do not know where. If you give me the point at which it is tangent then I have the exact derivative at that point, somewhere in between it is the exact derivative, here it is an approximation which is first order; here it is an approximation which is first order, in between it is an approximation which is second order.

And at some unknown point, it is an exact representation somewhere in between for a continuous function fi + 1 – fi/ h is the derivative, is that clear okay and it is the fact that we do not know it that gives us this truncation error, the fact that we do not know at what point it is the tangent that gives us the truncation error, so it is possible for us to calculate the derivative to approximate the derivative, to estimate the derivative at any given point it is possible for us to estimate the derivative in a given point using forward differences, central differences, backward differences.

And the forward difference, backward difference and central difference have the appropriate truncation errors, okay; associated truncation errors, right, so and each one of them, you will see as we go along there is a reason why you would use one or the other, okay. Are there any questions? So, then there comes the natural next question, if I could use x + h and x - h to get a second order, right we are little greedy.

Why do not I take it; is it possible for me to use the third equation and get one more; right, a higher order approximation, is it possible for me to add one more term one more equation to that and get a higher order approximation and it is possible, okay. So, I will go back here, so what happens is something; no, I want to solve for; I want to solve for f prime, I want to solve for f prime, okay.

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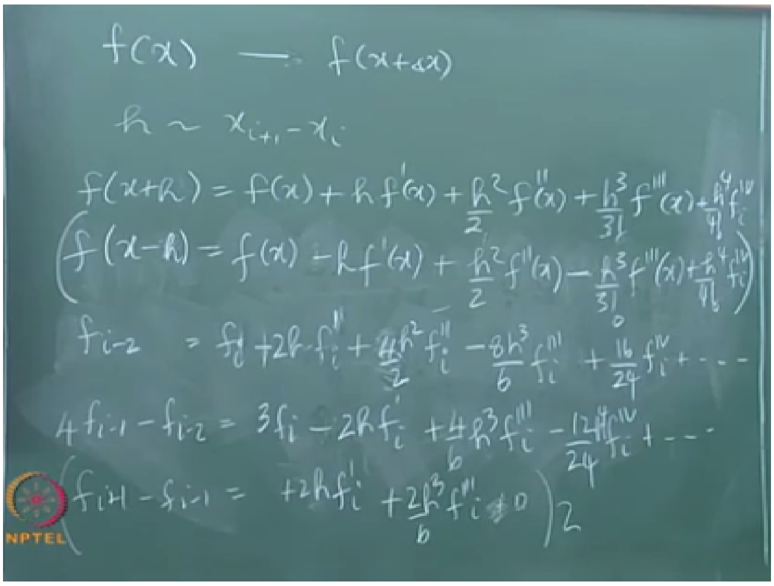

So, just to be careful, I will add one more term and you allow me to change the notations slightly, h to the 4th, 4 factorial, f fourth derivative at i and + h to the 4th/ 4 factorial f fourth derivative at i, is that okay, fine, so I am going to go with this subscript i, though I have left the other terms as x, I am not going to rewrite the rest of those equations but you allow me to change to this notation.

So that f of; you want to take one behind one ahead we have to decide where to take it, if I take i - 2 that corresponds to f(x) – 2h, okay, f of i - 2 is f of i – 2h second derivative; first derivative at i; got a mistakes, +4 h squared/ 2 second derivative at i - 8h cube/ 6 third derivative at i + 19/ 24, it is 4 factorial; 4 derivative at i and so on, it should be possible now for us to what should we do; how can we go about this?

What do we want our objective is to make sure that we retain the first derivative term; the f prime term, we retain the f prime term, okay. So, when we had; when we had 2 equations, we essentially eliminated the f(x) and retain this term, okay and eliminated the f double prime, the f double prime term, right, we do not mind having the f(x) actually, the f(x) got eliminated as a; right that was just one of those side things that happen.

What we really want to do is get rid of this, now in this case I want to get rid of the third derivative term also. Am I making sense? It is clear, so you have basically 3 equations and I want to get f prime of i at i out of it, how can we do this, what is the deal, how should we do this? I have a double prime here; I have a double prime here, okay, so I want to knock this out, what do I get here?

So, if I take this equation and this equation, so this is basically 2h squared; 2h squared or 4/2 is fine, so I need to multiply the first equation with the; if I multiply this equation by 4; if I multiply this equation by 4 and subtract to save the second equation from the first equation, right that should get me something. So, if I take this and multiply it by 4 and subtract this equation from there, what am I going to get?

4 fi - 1 - fi - 2 equals; 4 fi - 1 - fi - 2 equals 3 or 5 and they have a - and +; -2, no not -; - 2 h f prime at i, then - i same minus but I write plus, okay, -2 h f prime at i + this term and that term are going to cancel that is the whole objective then I have 4 of these, I have 8 of those, right; I have 4 of these, I have 8 of those + 4/6 2 thirds h cube f triple prime at i, then what else? I want to retain the fourth derivative; I have added the fourth derivative because it is likely that I suspect that my truncation error is going to be like the fourth derivative, right.

So, there are 4 of these and 16 of these, right; there are 4 of these and of 16 of these – 12/ 24 fourth derivative of i, fine, h power 4, most important; h power 4, okay, so let us taking these 2 and of course earlier we had knocked out the h squared term by subtracting these from each other, which gave me fi + 1 - fi - 1 equals, I just repeat that no fi's + 2h f prime at i, this quadratic term cancels out + 2h cubed/ 6f triple prime at i.

And what happens to the fourth derivative? Fourth derivative cancels; fourth derivative cancel + 0, fourth derivative cancels, okay with move on, what does this give me, what do I want to do now? I have a 2h f prime here, which I want to retain but I have a third derivative term here that I want to eliminate, I have a third derivative term here that I want to eliminate, so if I multiply the second equation by 2; if I were to multiply this equation by 2, and then do what?

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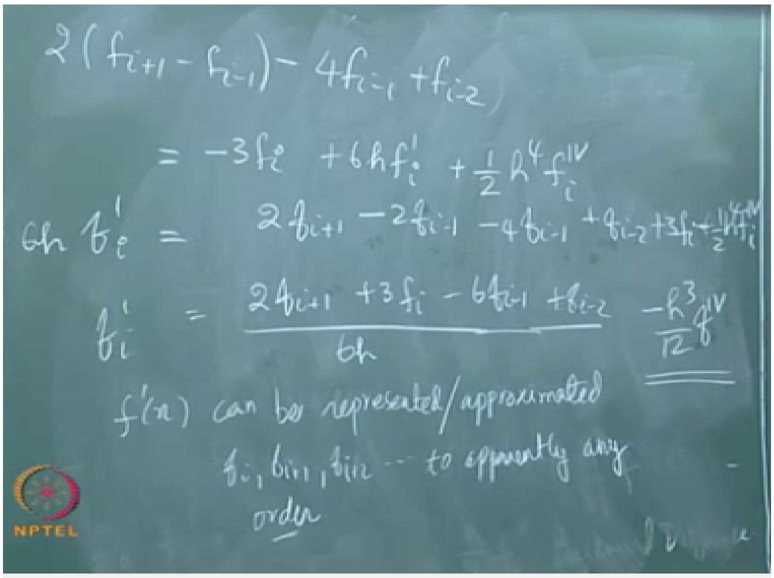

Subtract one from the other okay, so from maybe the second equation; from this equation, I subtract that equation, so I get 2 times fi + 1 - fi - 1 - 4 times fi - 1 - fi - 2 times; 4 times, so I made a mistake, I have to be bit careful; 4 times fi - 2 - fi – 1, this gives me - 3 fi +; there is a 2h f prime and the 4h f prime; 6h f prime at i what else, the triple prime goes away and we have multiplied this, so it will be +1/2h to the fourth or that is + fi – 2, h to the fourth derivative, right.

Is that okay, fine, so what does this workout to? I want to solve for the f prime, so I will take everything else over to the other side and swap the equations around because I want the f prime. So f prime at i equals I have 2fi + 1 - 2fi – 1, then we leave the 6h here, I do not skip any steps; - 4fi - 1 + fi - 2 – 3fi; + 3fi + one half h fourth derivative at i; minus, so clearly I am going to make a lot of sign errors today okay.

This gives me, somewhere it is added up okay; 2fi + 1+ 3fi – 6fi -1/ 6h – 1/12 h cubed f to the fourth derivative i, yeah fi, I am sorry, I should not say fi + 1, where did I get fi + 1; fi + 1, fi, fi – 1; fi - 2; fi – 2 - h cube/ 12 f to the fourth derivative, let me add them up and check that I am performing, the check; I am performing a test here, you may not see obvious that the tests that I am performing is I am adding up the coefficients in the numerator.

I am adding up the coefficient in the numerator and in fact they do add up to 0, okay in fact, they do add up to 0, so here you have some mechanism by which; you have some mechanism by which we have got something that has third order; converges this third order okay and the representation is third order cubic, is that fine, has any questions, okay, right. So, it is possible;

so one thing is for the representation of f prime at x, right can be represented; can be represented or approximated.

And slowly switch from representing on the computer to approximating on the computer represented slash approximated, right using various points, the sample values at various point, so you can use fi, i + 1, i + 2, i - 2 and so on can be represented to apparently any order that we seek, any order is just a matter of adding points, as you add points as you add more and more points right, as you add more and more points.

So, if you have i +1, i, i -1, i - 2 then apparently you can get right, very higher order as higher order as you want, so there are; it is possible that you can actually get higher and higher order representations or approximations okay. So, right now I just make that as a broad statement, what we need to do is; we need to find out and we have this truncation error, everything seems fine right, everything seems fine.

But you have to little bit careful okay, so what I do is; I will give you an assignment, I ask you to you try this out and see what you get, so we can use this representation that we have. To check whether we are get; actually getting it, so pick a function since we are talking about trig functions in the last class, I will use sin x.

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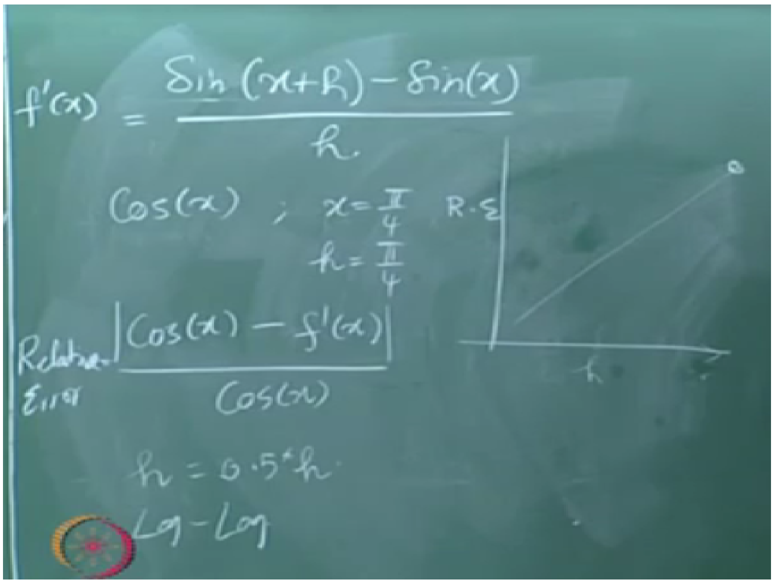

So, you try out sin of x + h or x + delta x or whatever, - sin of x/ h, calculate this, okay, so this is a candidate derivative; this is a candidate derivative for sin, let us use; let us assume it is forward differences so at x right, so this is a candidate derivative f prime at x, you also know that the derivative is actually cosine x, pick a value of x, right pick a value of x, say x equals pi/ 4 and pick a value of h; pick a value of h, say h is pi/ 4, okay.

And evaluate this for different values of h, evaluate this for different values of h and what I want you to do is; look at cosine of x - f prime of x/ cosine of x, you can take either, right take the modulus, if you want to keep it positive and what is this? This is some kind of a relative error, fine okay, so far so good, now this is what I want you to try to do, you try to make h smaller and smaller, so in your program you keep having the value of h.

So, you say h is 0.5 times h in your program, you keep having the value of h and keep calculating this relative error and I want you to plot on a log log plot; on a log log plot, I want you to plot the relative error, this is h, is it okay, is that fine, okay. So, now that is clear, you tell me what you expect, now that the assignment is clear, what do you expect? I want you to try it for different schemes, that is I want you to do it for forward difference, backward difference, central difference.

What is it that you expect? Remember h grows larger in this direction, h grows larger in this direction that means you are starting somewhere here that is pi/ 4 and you are going to work your way towards 0, okay. How many times are you going to divide by 2; how many times are you going to; how many values of h are you going to try this, h; weather h should be below machine epsilon or whatever it is you figure out whether it should be does it have to be below machine epsilon.

Let it you do it just see what happens, right so what is it that you expect? Say for a first order; for a first order scheme for a forward difference, this is forward difference, what is it that you expect, what do you expect the graph to look like? You expect a linear curve, linear curve like that something like that, try it out and see what you get, right and if it is second order; if it is second order, now you would be careful, it is second order it is still going to be linear.

This was a 45 degree line, second order will be; you expect the steeper line, is it go through the origin I do not get it, some problem or maybe it starts somewhere else, I do not know if I am making sense, you are taking log on both sides, you have log error, relative error equals whatever look at the truncation error work this out, you try to work it out, we will get back, we will take a look at it, try to work it out okay, try to work it out.

And as I warned you before always some little trap in something that I asked you to do, so keep your eyes open, okay. So, having this maybe you know try 64 times possibly, it is a lot, rate of 50 times, try having it 50 times, okay that should not get you into trouble, try having it 50 times, try it for float and double; float double, you try long double, okay try a combination and see what happens, is that fine, okay right.

So, let us get back to this as it turns out we are able to get derivatives of; we are able to get; we are able to get derivatives of various orders approximations to a derivative; first derivative of various orders, so can we get second derivatives, right. So, we look at these 2 equations and in fact, it turns out we can get a second derivative, if you just add the 2 equations, it is clear now that these terms will cancel.

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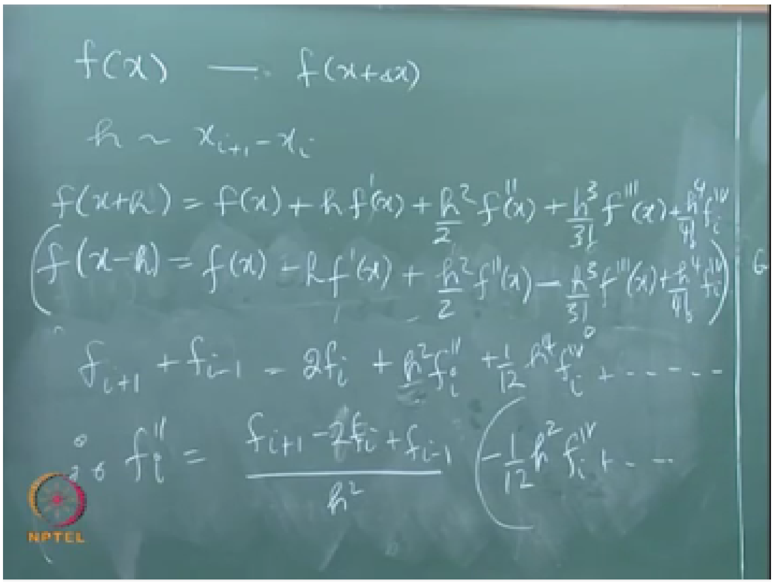

So, we have f(x) + h, which is f of i + 1 + f(x) – h, which is f of i – 1, as 2 times f(x), which is f of i; fi, this term cancels + h squared/ 2 goes away f double prime at i which is what we want, this term cancels, leaving us 2 of these + 1/12 h to the fourth derivative at i and there are higher order terms, we can solve for the second derivative and therefore the second derivative at i equals fi + 1 - 2fi + fi – 1/ h squared.

And the truncation error is – 1/12 h squared fourth derivative at i okay that is the truncation error, is that fine. I wanted to; so it pretty actually, one I wanted to do it today because it is straightforward, the expression is here we can just subtract, get the second derivative, it is possible to get the second derivative in terms of i, i + 1, i – 1 and so on. I also wanted to do it because I wanted to make one thing here.

What is the rate at which the truncation error goes to 0? H squared, it is quadratic, it is second order, right, second order. What is the polynomial that we can for which we can get the answer, let us cubic, right, so I do not want you to get in your mind that the function representation is quadratic, convergence is quadratic you write that was only for first derivatives. When you go to second derivatives, the error term converges as h squared.

But the order of the representation of the function, you understand the order of the representation, right is the fourth derivative; the fourth derivative and therefore you can represent a cubic exactly, is that make sense, right. So, only if you plug in a fourth degree polynomial will this be nonzero, okay. So, even for the third degree polynomial let us going to work but this convergence is second order, okay.

Right, just because for the first derivative approximations they seem to match, i do not want you to get in your mind they matched because we were dividing by h but here we are dividing by h squared and I suspect looking at this that maybe for third derivatives we end up dividing by h cube, okay, so that is one thing to remember, so you have a h squared order of convergence, representation is cubic for the function, is that fine, okay.

So, it is clear using the values of the function at various locations that we can actually approximate derivatives, right. So, we are now in a position to actually approximate differential equations, is that fine, right. So, we now; once we are able to approximate functions, once we are able to approximate derivatives, we are in a position to approximate differential equation, we can approximate the differential equations and actually represent our functions on the computer and systematically hunt for the solution, okay.

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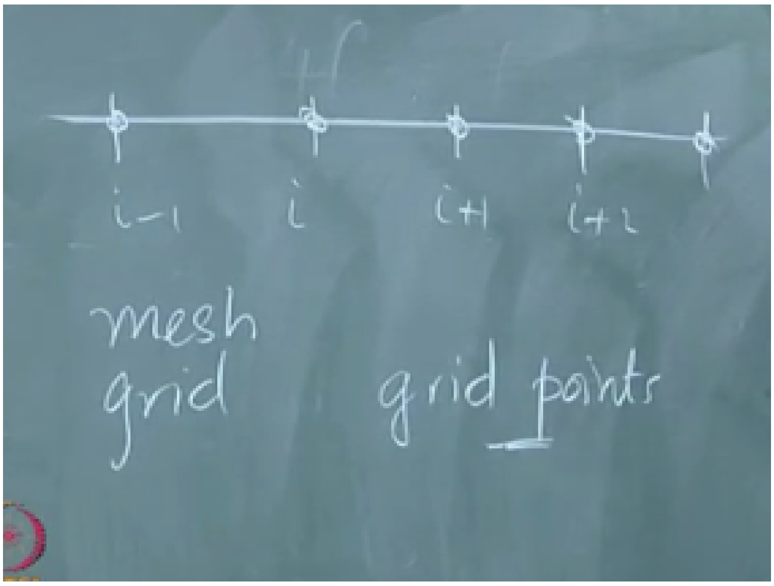

So, this we will do in the next class, what we are going to do is; you look at an equation in 2 dimensions, so all my derivations are in 1D, I am going to look at the equations in 2D but before I finish, I just want to emphasize some terms that I am using. So, these are; if i – 1, i, i + 1, i + 2 and so on, you will see me refer to these, this whole interval being broken up into a mesh or a grid.

I will explain these terms more detail later and these points I will typically refer to them as grid points but you may hear people referring to them as nodes okay, right. So, I will typically referred to them as grid points. So, given function values at grid points were able to represent functions, were able to represent derivatives and therefore we will be able to represent on those on that mesh a differential equation, right.

Because they are able to represent derivatives and also extract out a solution, which you are able to represent on that mesh, is that fine? okay that is our objective, fine, next class thank you.