Computational Science and Engineering using Python
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Lecture - 14
Numerical Differentiation

Today we will start differentiation numerical differentiation or derivative. So, how do I get derivatives numerically?

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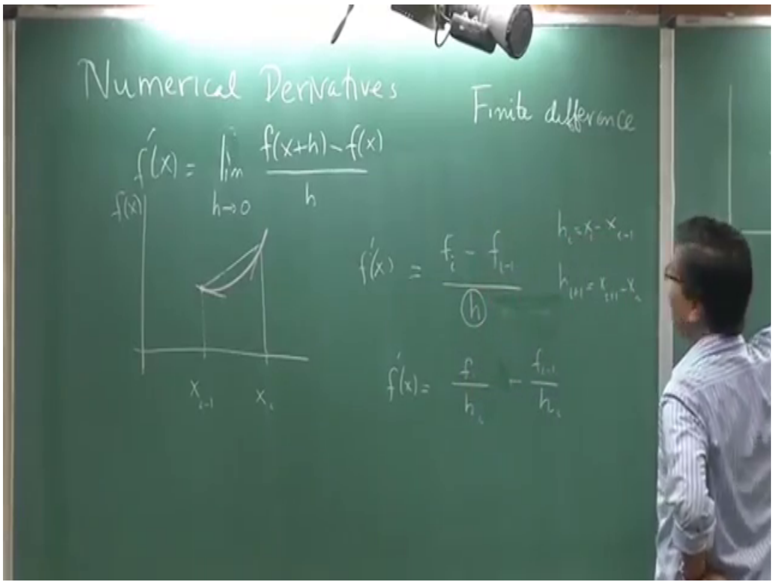

So, we will use what Newton said. Now what is a derivative I said difference of the function between 2 points and divided by delta x right. The definition is f prime of x is f x plus h minus f x by h, but in reality we can in computer we cannot make h 0 h standing h will be small, but you have to choose a finite h and that is where all this confusion and well not confusion approximations come how good is your algorithm. So, I will are there quite a few ways to do it.

So, right now I will describe something called finite difference. In fact, there is a way to derive derivatives using 4ier transforms as well, so that I will do it later. So, when you do 4ier transform. So, we will worry about derivative using finite number of points that is called finite difference. So, simple idea is I have 2 points discretized. So, let us call it x i minus 1 and x i and the y axis is a function here and here suppose a function is linear then it is straightforward know linear is my this idea will work even if h is finite for linear function you can just say slope is constant. So, f prime at any point in fact, but I am interested in the derivative at the given points. So, all my calculation will be derivative here or here, but derivative same everywhere and that is f of. So, I am going to put a short hand now.

So, f i it means function value at x i this shorthand. In fact, is the formulas are bit long. So, we need to make it as shorthand as many shorthand is possible f i minus 1 divide by h which is h is this is same as x i plus x i minus 1 this is good this is. In fact, exact for linear functions this formula is accurate, but if the function is not linear. So, just imagine that I have a function which is going through this 2 points, but like this now this formula is not good right my derivative number is this slope, but the value of the derivative at this point is in fact, slightly negative here it is positive, but is. So, here is at this point is overestimating at this point is under estimating.

So, as soon as you put non-linearity higher order terms then this does not work. Maybe what I will try is I will put a midpoint. So, let us say that I have 3 points there are 2 points let us put 3 points.

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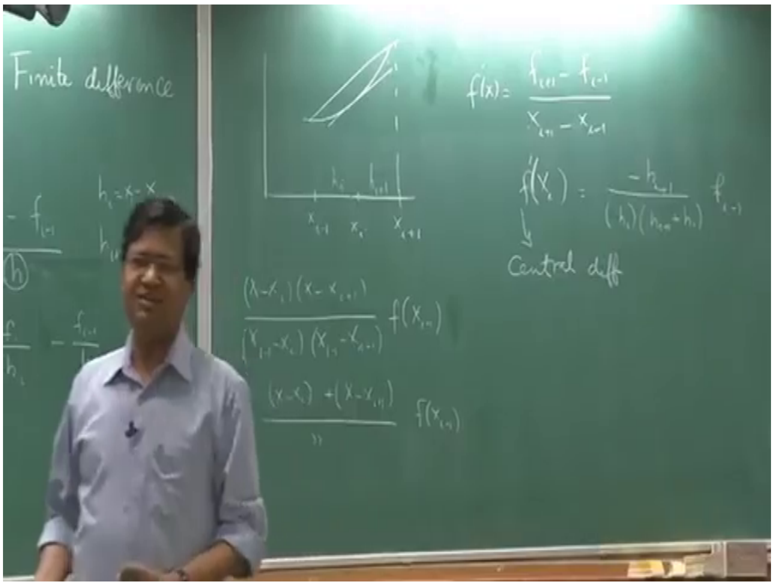

So, I will do it right here or I can make a new one. So, take 3 points x i minus 1 x i x I plus 1 and we have 3 points. So, the function goes like that right. So, what I could say as well is better if I want the value of the derivative in the midpoint. So, slope is real slope is this, so I can take this 2 points and. In fact, if I want the slope at the midpoint I should take the difference of the function that the 2 adjacent points and this is better. In fact, is exact if it is quadratic if the function is quadratic then I will get a exact formula f prime of x is f i plus 1 with.

So, this is better formula and, so I will prove it actually why is it better what is the error so, but suppose the function I mean I want to use more points like let us say I want to use 4 points now this is 3 points 1 2 3, I use want to use 4 points. Now with the intuition you cannot really derive these formulas. So, you do got get to some mathematical formalism and we can again go back to Legendre polynomial interpolation and you can derive what should be the formulas any order. So, I will just illustrate how do get derivative using 2 point and 3 points you can also use higher order schemes. So, let us just look through this slide, because I do not want to really write differences are quite long. So, so the idea is to derive any order of derivative with any number of points with Legendre's interpolation.

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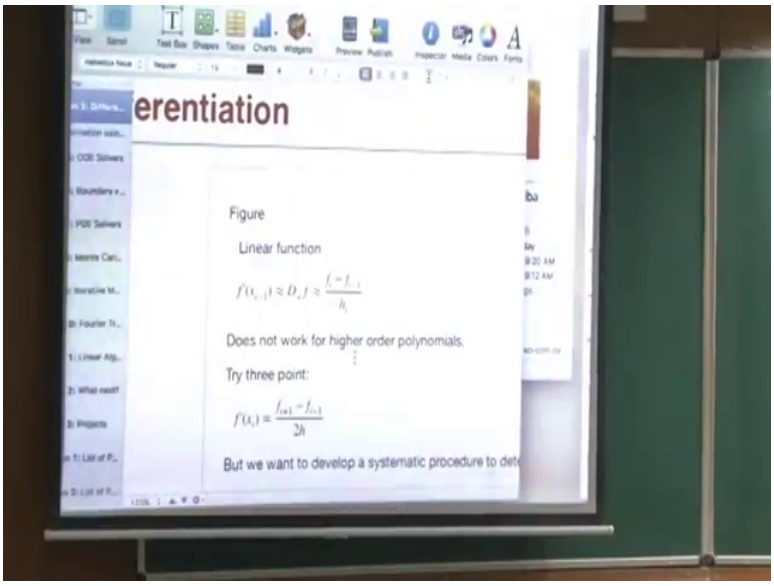

That is why I hope you realize that this is a really good framework to derive a lot of numerical schemes Legendre's interpolation and that is why interpolation is mother of many numerical schemes. So, you have to look at the slide I did not make a slide, but because typing there and keep I mean keep it also it just takes too much time. So, what we will, so I have 2 points x i minus 1 and x i. So, make a interpolating function or Legendre polynomial which goes through these 2 points.

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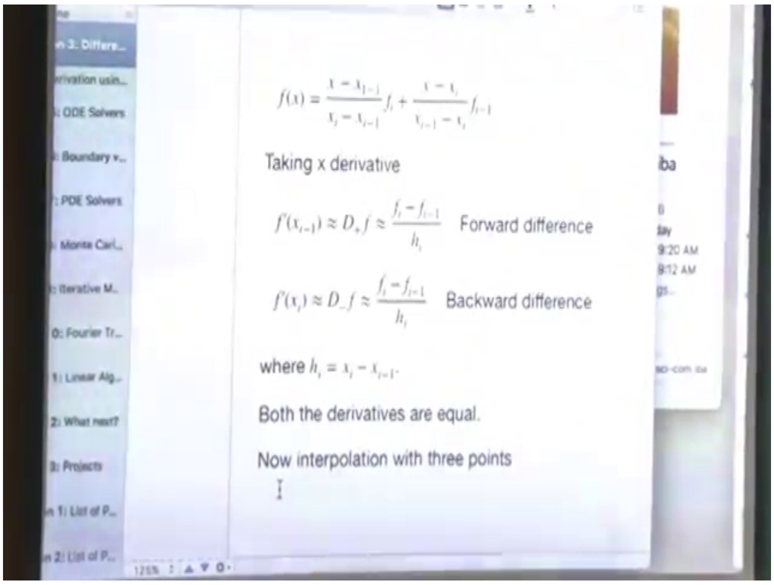

So, these are interpolation you recall. So, it is linear because I am using only 2 points. And using these 2 points I can take the derivative of this function now these are function of x. So, I can take the derivative of it. So, f prime just take the derivative of the function. So, I will get a term here which will be f i divided by this one and here also f i minus 1 by this, but both of them are opposite sign this has opposite sign is that they are equal, but opposite sign. Please keep in mind that this difference need not be equal. So, sometimes you keep this large small especially near the walls you need to make fine grid and away from the wall you make a coarse grid.

So, if I take the derivative I mean you can just see that now it turns out that this derivative is formula will be same. So, let us just do it for 1 expression. So, f prime of x is f i I am going to write is h and next one is f i minus 1 and this will be minus h so, in fact, I can put a minus h, this is derivative at any point but. So, now, there are some notation we need to understand the notation I am computing derivative. So, this is exactly same formula is what I wrote here now it is exactly same. So, I derive it using Legendre's polynomial. Now if you want to take the derivative here using the point which is to the right there is called forward difference. So, I am sitting here I am looking towards ahead, so forward. So, it is called forward difference and is d plus.

So, this is an operator d plus is an operator is called forward difference operator acting on f which is this formula I turns out since derivative same at any point. So, it is the same formula for if I take derivative here and look back. So, I go on ahead, but I want to use a point behind me to compute the derivative. So, it is called d minus it is called backward difference, but it turns out both this formulas are equal for this linear in linear polynomial. In fact, it is h i this is for. So, h i is defined as x i minus h i. So, higher of the 2, so that is again you have to keep in. So, x i minus x i minus 1 what about x i plus 1 will be x i plus minus x i ok.

So, now I want to do better now this formula as I said is good for linear function, but I want to work out function like this or even higher order polynomials then I can look at higher order Legendre’s polynomial.

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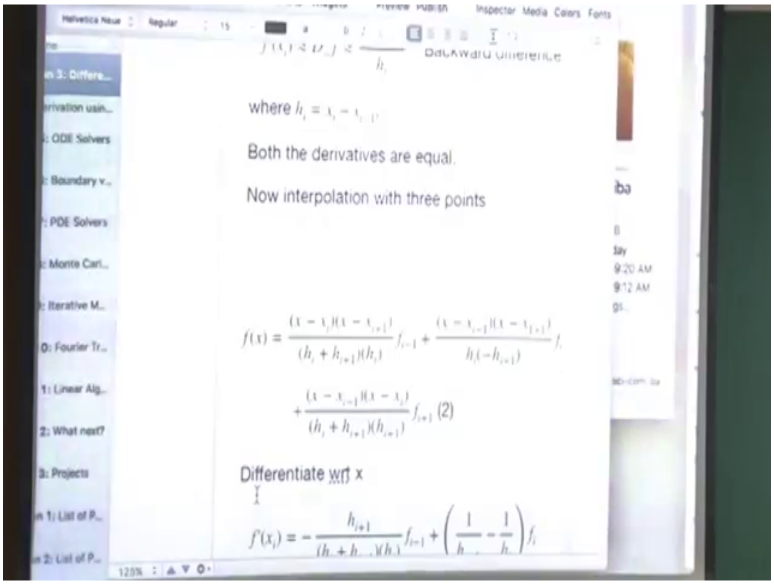

So, I have 3 points. So, x i minus x i x I minus x i plus 1 divided by what is the denominator which is missing here. So, the first is x minus x i x minus x i plus 1 divided by what please do not (Refer Time: 10:20) Legendre’s again, Legendre’s polynomial is the basis of everything x i minus 1 x i minus 1 minus x i plus 1 now what should did this function be.

So, if I put x i x equal x i minus 1 I get 1 and this would be f i x i minus 1 it is simple, whatever is here should be here these 2 plus 2 more terms that has 2 more terms now. So, these are Legendre formula now you can take the derivative of this function. So, derivative will be now I have to take the derivative and then compute at given points, so the 3 points x i minus 1 x i and x i plus 1. So, let us take the derivative of this.

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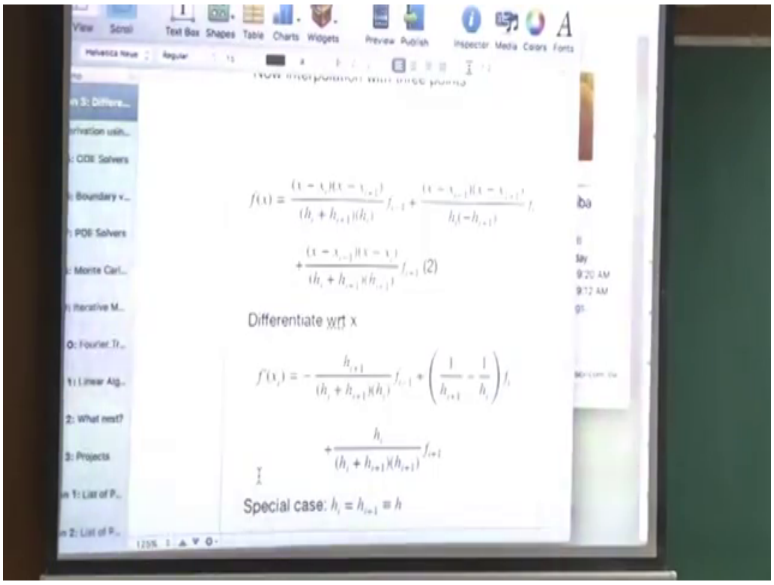

So, you take the derivative it is a chain product rule. So, bottom remains as it is. So, if it I have to apply the product rule this is remains unchanged and this is one know this is x is sitting in front and if I keep this function and take the derivative I get x i i plus 1. So, I keep this function and take the derivative with respect to now. So, this is what I will get as the first term.

So, I will not write more terms, but now I had to substitute one of the 3 points. So, I want to compute the derivative this prime is derivative this one at x i. So, put x equal x i you put x equal x i this goes to 0 only survive is this. So, it is x i minus x i plus 1 which is minus of h i plus 1 this is minus sign here say h plus 1. Now divide by what is these guys this is minus h i. So, let us write this one you agree that if I take the derivative at x i. So, above is minus h i plus 1 bigger bit 2 divide by now these guys. So, x i x m minus 1 minus x i is minus h i minus h i and what about this. So, this is h i and this is h i plus 1. So, you have to add them together it is this difference, so minus minus becomes plus I am going to remove this h i plus 1. So, this is the first term and f i minus 1 of this.

So, we can do the same thing for next 2 terms this term in that term. So, you get this. So, this is a formula for the derivative where at the midpoint this cause central difference you doing at the midpoint that is called; so this is central and the expression is given here is Ferziger is a nice book which has these details derivation, but I have put it here. So, you can just look at it.

Now if I put the case when h i. So, if this difference are equal then the formula becomes simpler there are cancellations in fact, this term will cancel right I mean this term will definitely cancel.

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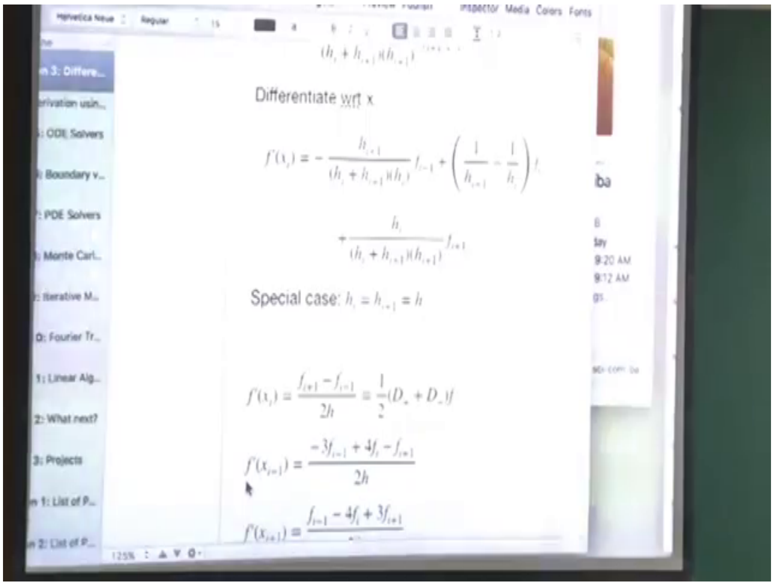

And you get a pretty simple formula which is this f i plus minus f i minus 1 by 2 h. Do you see it on the board it is where is it I erased it for this, this is the one this exactly same as what is there. So, we have derived it mathematically now we can also compute derivative. So, this is the derivative computed here what about derivative here how will I do it. So, I have derived this derivative know this function. Now substitute x equal to x i minus 1 and you get a formula and the formula is this. Now please do not expect me to do it you also probably not do it sin pi is good thing actually sin pi could do it I mean you will just give the answer you know all the algebra will be done by sin pi.

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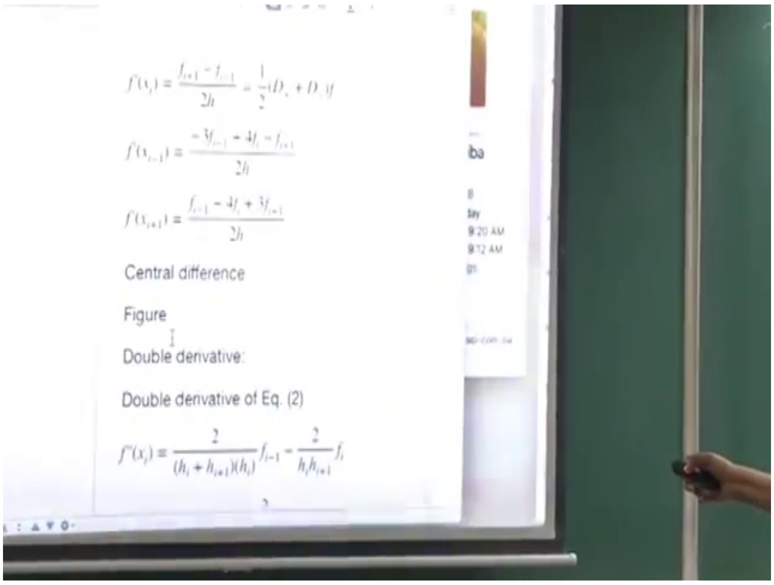

If you interested you can write it and should get the answer. So, these are the formula for f prime x i minus 1 this is x i plus 1. So, this will be forward difference the 3 point and this will be called backward difference. So, your 3 names forward difference backward difference and central difference now suppose somebody says what is the second derivative you will need second derivatives on many physics problems do not laugh second derivative equation there are second derivatives. So, how will I compute a second derivative with 3 points with 2 points for this second derivative it is just 2 points 0 there is no second derivative.

So, you need at least 3 points. So, how will I do it if want to do second derivative double this do it twice. So, use this function Legendre this effects this one and take derivatives twice. So, you have to take the derivative second time and if I take derivative second time this is becomes 2 right there one here and one here. So, just do it twice and you get the second derivative and I just. So, is it clear I mean this quadratic straight forward. In fact, coefficient of x squared is just put 2 and you will get the answer you do not need to worry about the linear term they will not vanish. So, that second derivative is easy.

And it turns out this is the formula they do not look very nice know they do look ugly. So, I will give a table where you can read off from the table. So, this is a formula for the second derivative now when for equal interval when h i plus 1 and h i are equal then it simplifies a bit and this is a formula in fact, this formula you should memorize.

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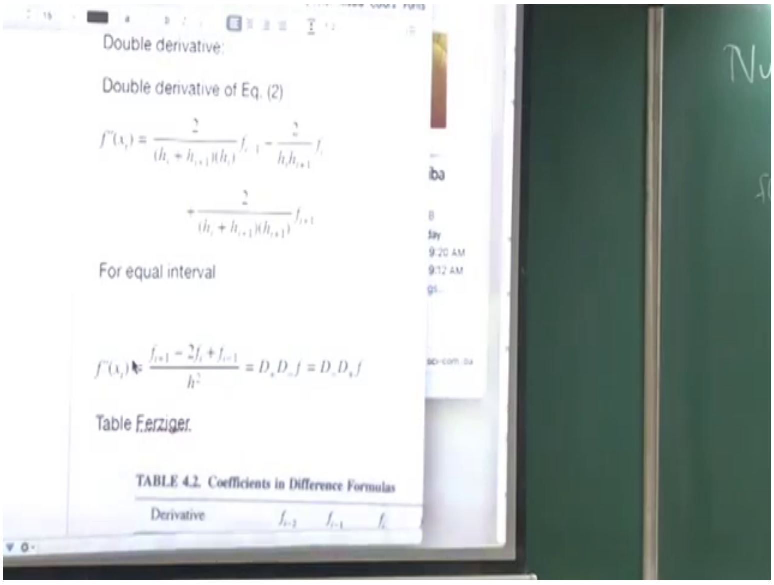

You will need for your homework and projects definitely you will need this if you are doing, but most of the projects are based on differential equations. So, these are formula. So, what do I take? So, add the values of the function at these 2 points these 2 points and subtract twice in between you can also do this by compute the derivative here.

And derivative here first derivative and subtract off you will get the same formula what are this is I have derived it here for Legendre polynomial. So, now, all this derivation is you know if you want derivatives with 3 points, you cannot derive it every time.

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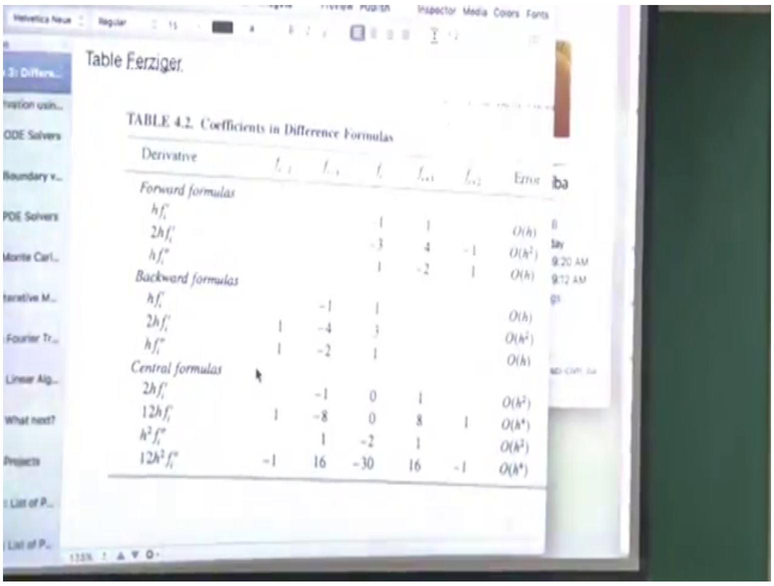

So, there is a table and let us see how to understand this table and also gives the error. So, I will basically tell you a little bit how to compute error, but let us first understand what this table means. So, we have 5 points. So, let us write it here. So, I have there is a i minus 2 as well right ok.

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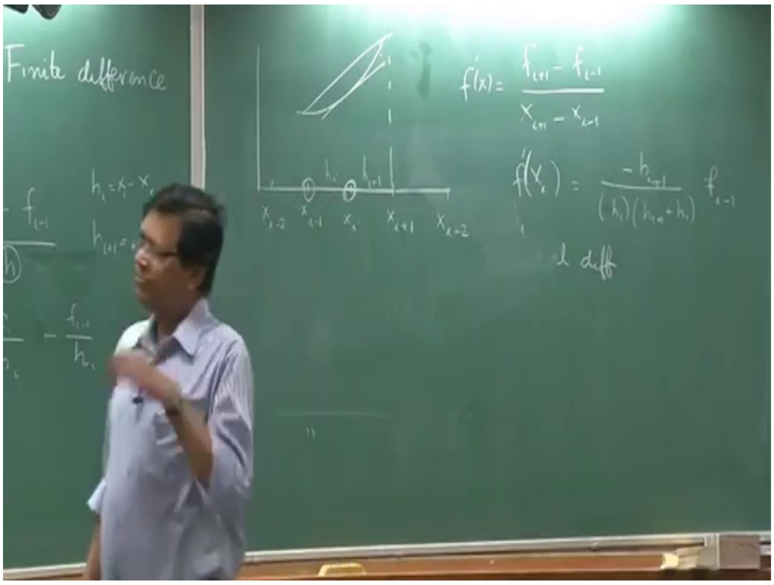

So, I want to compute function it. So, it is the formulas I will not block them I want to do it here at i so; that means, I want to compute my derivative at point i.

So, what is the power difference using 2 points which is f i plus minus f i. So, that is this should come in with the minus 1 sign this should come with 1 and divide by h. So, h times f prime i is f i plus 1 minus f i is easy to read now this table you should really use it now somebody said well I want with use 3 points, but I want to compute derivative here now this we already derived before. So, let us look at which formula I should use. So, I had the points of course, my points for I minus these 3 points, but. So, you should just see that I am using a derivative here, so 2 in the right. So, there is a forward difference and the formula which I mentioned it I am sure this one. So, using the points ahead of you.

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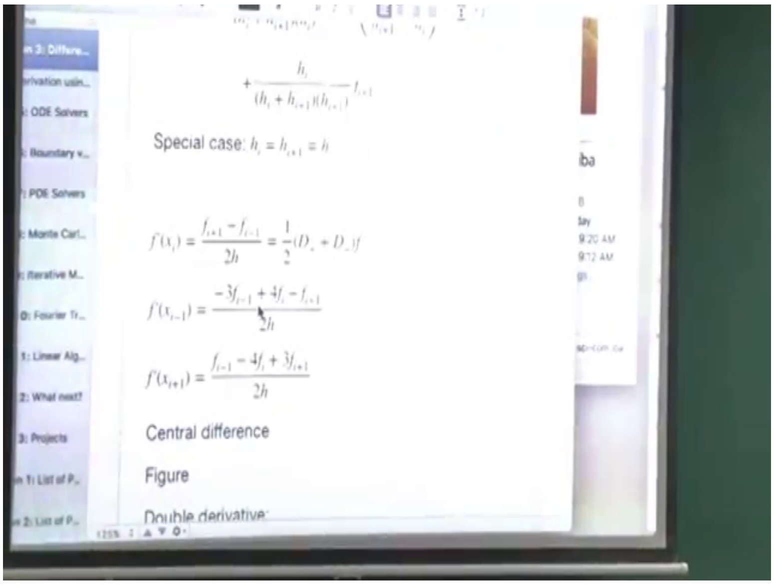

So, the point at where you are is minus 3 then 4 and minus 1 and divided by 2 h. So, I say I take this 2 h to here and give you the coefficients. So, coefficients are minus 3 4 1 4 minus. Similarly double derivative I just derived it at the at the point I using I plus 1 and I i plus 2 well it turns out the double derivative same double derivative again for you are using only 3 points. So, double derivative here, here and here are equal it is quadratic the way linear. So, when I did the first derivative my Ferziger here in here are equal. So, second derivative at 3 points will be equal and that is why is 1 minus 2 1. Now this is called backward formula. So, I want to compute derivative at i.

But using the point left of me or behind. So, is minus 1 and 1 this is again you can see in that. So, this formula corresponds to this guy, so behind me. So, the where you are is 3 and minus 4 and 1 is this symmetric actually symmetric of this with the opposite time and that is what you got 3 minus 4 1. So, I hope you understand how to read this table.

Now this is not well now this is there some new stuff this is using 5 points this I did not derive it right now if you want to use 5 points and this is what you should use 1 minus 8 0 8 1 using 3 points are derived it this 1. In fact, this formula, but with 4 point 5 point this is what you get and double derivative is this it is more work.

And, but you can get this formula, what is the error? So, this column tells you the error. So, you can derive some errors from here. So, how do you get error for this formula? So, let us try to estimate how do you get error. So, somebody says well the formula I am using. So, the way to well that one simple way to do it is f x minus f x i minus f x minus h this what is right this way equal to I use Taylor series. So, f x will remain as it is minus f x minus h f 1 of h.

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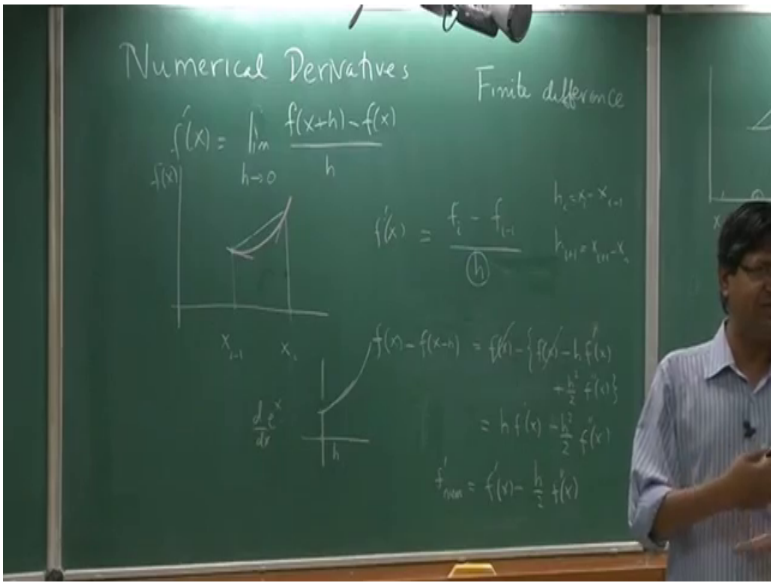

Now the next outer term is x square by 2 double derivative. I will stop I mean there are higher order terms, but my error is here this will cancel and I get h f prime of x plus s square by 2. Thank you.

So, I divide by h that is what we got here if we divide by h. So, f prime numerical f prime numerical is f prime which is real value minus h by 2 this is easy this is just simple analysis now if I function with linear this is 0. So, that why that is why it was exact the function is quadratic then I get error right away and h is a big error order linear this called linear error order h is huge and you should avoid it h will be typically small. So, like what Newton described h should be small. So, this is a order h. Now I will not derive this it is order h square, so you can do similar ways, but I will give you another scheme another method derivation in a minute.

So, this table you can we just read from here now with, so which is best here in this table h 4. So, first derivative h 4 you should use for 5 points. Now it is more work in while coding, but it is not much much more work if you use points you get accurate results you can use seven points you can get more it. So, you can derive this formula in other way.

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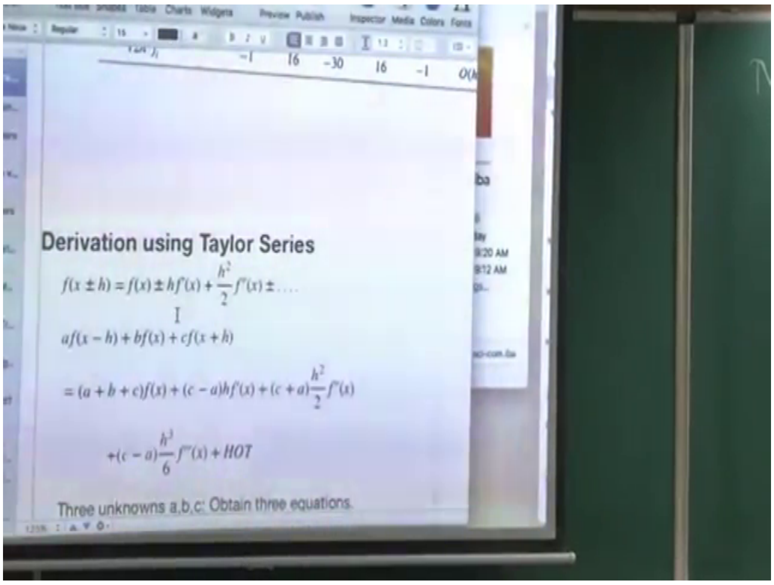

Now, this is a cube derivation some of this ideas well whether there are more sophisticated way to compute derivatives of higher orders. In fact, a lot of computations PDEs partial differential equation like all the fluid flows, Schrodinger equation in (Refer Time: 23:42) dynamic solvers right DEM solver is derivatives and people need accurate derivative. So, this is another scheme which is called compact scheme I will not have time in this class.

So, there are very sophisticated schemes to get very good derivatives, but this will give an idea how you can get formulas derive formulas. So, let us imagine that I want to compute derivative first order derivative and also estimate the formula error. So, I have choose 3 points. I choose these 3 points again with equal interval.

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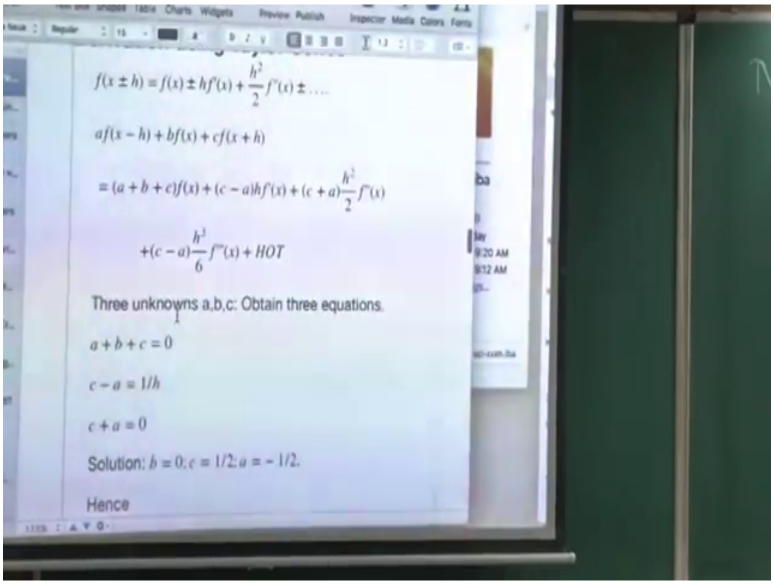

So, my points are x minus h x and x plus h. So, I will do a Taylor series of this and see if I do Taylor series I will get this expression right. Should I go one by one I mean these are first derivative term is coming from both of these, second derivative will come from again and third derivative will into symmetric. So, this is exact formula for Taylor series 2 cubic order and HOT means higher order terms.

Now I want the first derivative, so what should I do? I should set this to 0. So, I want this expression c minus a should be 1 by h 3 minus a is 1 by h and c plus a must be 0 I want accurate up to second order h square. So, set these then what will I get? I will get f prime x ignore this ignore this term. So, I keep if I delete this I equate this to this. So, I set this to 0 this equal to 1 by h. So, this becomes 1 and this is 0. So, I get a formula for a prime x. So, these 3 expressions will give you what are the values of the coefficients a b c. So, b 0 c is half is a is minus half. So, that is central difference scheme. So, the formula is and what is the error? Error is here this is a error which I am not including in the formula.

So, c minus a h cube by six. So, c minus a is 1 by h. So, h to basically you get h squared by 6 f triple prime; that means, cubic as third order derivative. So, am I too fast? The slides do tend to become to get too fast. So, using 3 points I want to derive a formula for prime h and that is what I have done here. I just equate with the Taylor series and set appropriate terms to 0. So, this is the formula I get and also I get error right away the term which I ignored which is c minus h cube by 6 is that. So, that. So, error is of what order in central difference scheme s squared and forward difference scheme with it was h this was h and this was, in fact, this is h squared.

Now, how many numerical operations you are doing here? Numerical operation is addition subtraction and division. So, there is 1 division involved here is 1 division involved here and well I mean there are 2 subtraction if you like or if h is given to you there is only 1 subtraction. So, the operation is exactly same in these 2, but this gives you x squared and this gives you h. So, which we should do I mean never apply this, this is what Newton said, but no you should not obey Newton for this we should do that. So, this is how we (Refer Time: 27:12) get this. So, I mean this of course, I just derived it here. So, let us do 1 exercise computer code is easy. So, I think I will skip computer code I just wrote a simple code.

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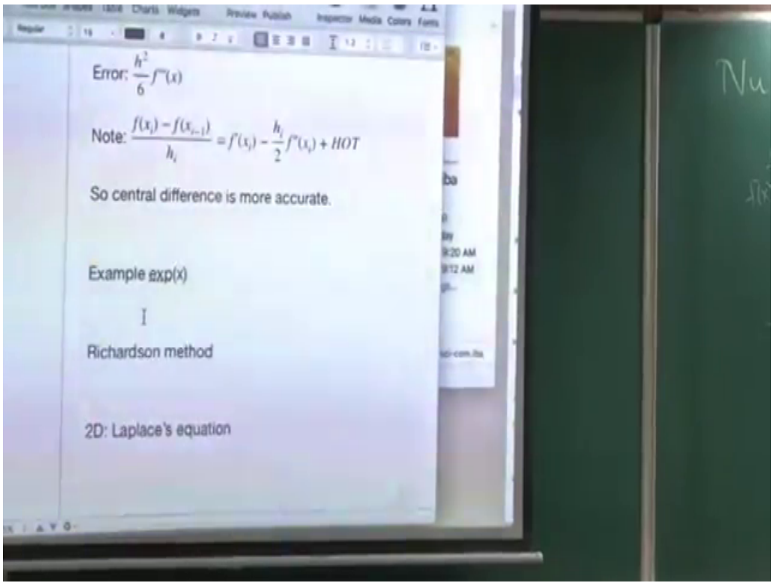

But you can write a code now I mean this given a function can compute derivatives. So, the exercise I will give you is exponential x, compute derivative at x equal to 0 using forward difference scheme, central difference scheme and backward difference scheme both first order and second order derivative. So, this I will not show you how to do the computer code I mean this python is straightforward you just implement this you will get it. You can vary h and see how the error changes. One thing I will request is that you vary decreasing keep decreasing h. So, I want to compute it for x derivative of this at x equal to 0.

So, take 2 points this is x equal to 0 and then vary h. So, a function goes like that know. So, derivative here is 1 if I should be it should be going like that 1. Now if I vary h, I will get better and better accuracy. So, you verify this by doing different schemes and get the error central difference scheme should give h squared. So, use h different h and sit.