Computational Science and Engineering using Python
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Lecture – 15
ODE Solvers

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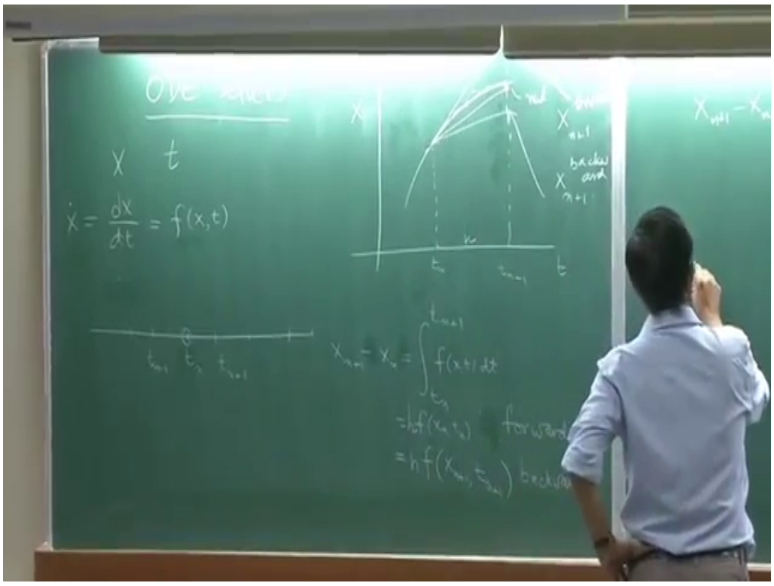

So I will start the ODE solvers. So, neatly I has to say that ODEs are the back bone of science, physical universe, the description is 2 differential equation assume time is continuous and it seems to be till good approximation we do not know whether time is really continuous or not. So, ODEs are very important and many equations are non-linear. So, you aware of non-linear know. So, most non-linear equations you cannot solve. So, then you have to resort to numerical schemes. So, it is becomes very important for you to understand how to solve numerically.

So, let us start. So, I am going to use the following notation my X is a dependent variable unlike the last class. So, let us just use that and the t is my independent variable. So, like mechanics. So, just think of X is a position and time is a time t is time. So, 1 equation I can write is for the velocity dx by dt is some function of X and t. So, we will try to solve this. So, we can also call it X dot is short hand useful notation. So, we will like to solve this equation numerically. So, some of them have exact value first order equation has exact solution, but we want to solve numerically.

So, the idea is that suppose I am at X n at time. So, let us divide time discretely. So, time it could may not be even. So, this need not be evenly spaced, but for I am here t n and I want to go to t n plus 1 I want to find X at t n plus 1 given my position or X at t n and what is given to me is this. So, is a velocity if you want to think of a mechanics, you given f which is function of X and t. So, idea would be, I will have to readout this again. So, let us draw t and x, this is my t n and t n plus 1. So, my real function is going like this suppose something like this, this is really has happening with us physical system. So, at this point I know the slope. So, I do not know what this is I have to numerically compute it.

So, what I could do is slope which is f. So, I compute the slope here or I compute f at that point and using a slope I extrapolate till here. So, at this point I extrapolate and I will reach here. So, this is not the exact value this is not the correct value correct value is here had the function will linear I would have reached there, but function is non-linear my X not by this is not f this is X is non-linear I reach here. So, this is called forward scheme, so this X n plus 1 forward. So, I go, I am sorry is it blocked some people can read this or no. So, this is X forward and we call it X n plus 1 now. So, this is forward scheme now I say well I mean look at this lot of error right.

So, I do not like that let me use this point and slope here of course, we do not know that point, but imagine for some reason or from equation which I am going to solve today the (Refer Time: 04:33) equation they are not real equations. Suppose I know the slope here then I can use this slope to extrapolate from here because I have to go from here this is my present position. So, I use this slope I use the slope. So, parallel to this I reach here which again is under estimate I am not able to reach my correct value, but this is called backward. So, X backward n plus 1 where somebody is these all none of them look good. So, let us use the midpoint.

So, what we will do is. So, somebody say that some reasons suppose somebody gives you the slope in between. So, I can use this slope which is this slope I use interpolation from here to that. So, this parallel line you draw I do some better, somewhat better know, if I choose a midpoint I am doing better. So, you can use this using the midpoint use with midpoint. So, we have to compute f now this is we can see chicken and egg problem I do not know my midpoint. So, I cannot compute f. So, I really cannot do neither this scheme nor that scheme, but there are ways to well the idea is that you go make an estimate of the midpoint. Because these are the tricks you know in the very cute tricks trapezoid device and you try to do as good as possible 1 concern do average of the 2, 2 slopes. So, this slope is doing over estimate this slope will be under estimate. So, do the average. So, that is like trapezoid rule. So, these are various rules. So, let us try to write a formal way to how to solve this.

So, formally I should write this as X n plus 1, so d. So, I just integrate this know. So, X n plus 1 equal to X n plus integral f x t dt or let us write like this equal to this now I have to estimate this. So, one way to estimate is that now I am going to write down all this stuff. So, say well f at X n t n multiply by h. So, that is the stepping know use this slope and multiply by h this is h. So, this is that estimate of integral using the value of the f at this point now it seems it depends on X n as well that is a problem if we dependent only on time no problem then I would have coolly done it, but it depends on X because X I do not know the future X that is a that is my issue.

So, this is forward scheme or you can say h value of the function at X n plus 1 and of course, you have to put time also at t n plus 1. So, this is future, so this called backward scheme or you could have X n plus 1 minus X n h midpoint. So, midpoint will be f of X we write as n plus half n is my time index. So, n is my time index n plus half t n plus half or, these a midpoint scheme or I could use trapezoid rule which is average of the 2 slopes, h by 2. So, this called midpoint method; f X n t n plus f X plus 1 is that clear. So, this how in fact, I am using my ideas from integration schemes.

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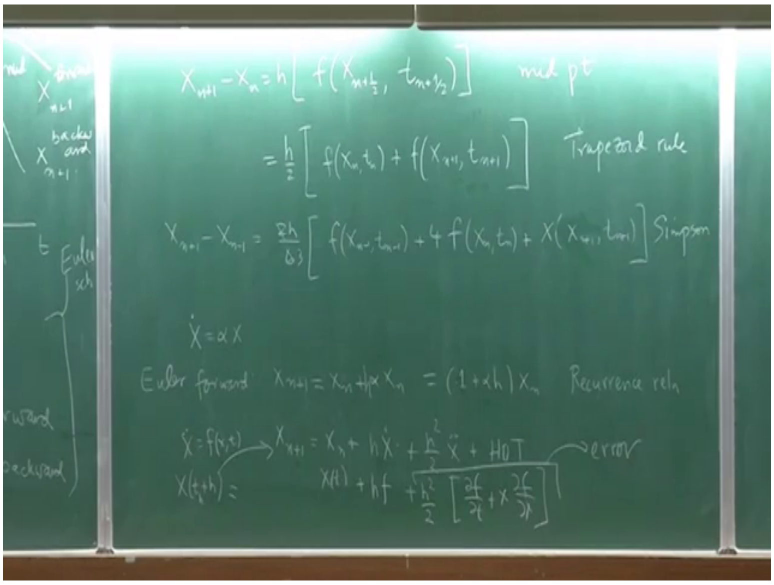

This is another nice way to says well if I here I am using only 2 points, now this as the integration of the function between using 2 points. Suppose I had 3 points, I have points point t n minus as well then I can use in fact, I have better estimate. So, my integral will be going from, I can write this as X n plus 1 minus X n minus 1 is equal to; now let us imagine that the h is equal h and h, so 2 h. So, what is the rule is called. So, 3 point is Simpson rule. So, this is f of X n minus 1 t n minus 1 plus 4. So, that is. So, this one issue here that I am jumping from n minus 1 to n plus 1 not from n 2 n plus 1, this method is has issues if we say more accurate, but problem is that I am making 2 jumps. So, 1 has to be careful with this scheme, but this is Simpson. So, these are all nice you can start coding it and try to solve it. This scheme is called this the whole thing this is this called Euler scheme, Euler famous oscillation Euler. We will discuss this bit later they have names, but, let us focus on Euler forward now somebody may ask.

So, let us say slight of keep it simple, very simple, so that I can get exact formulas and see how good is my Euler scheme doing. So, example I am going to use is X dot equal to alpha X whether alpha can be positive negative or complex I will allow all possible alpha x, according to this scheme forward scheme Euler forward Euler forward. So, I will get X n plus 1 equal to X n plus alpha X n. So, this is h times alpha X h times f computed at point X n. So, this is exactly solvable alpha h whether this is also called recursive relation. So, given X n I can find X n plus 1.

Now, I can put this in computer and crank it. So, typically we are given X 0 somewhere here t 0 and you time step equal to time march in or time stepping. So, this is technical name time step or time march now. So, this my approximate value. So, what is a error? So, you can estimate the error. In fact, you can estimate error for arbitrary f what is error in this scheme. So, let us do it for arbitrary f and we will say that this is will compute what should be the formula for here. So, I am going to do it by Taylor series X n plus 1 equal to X n plus h times. So, I am expanding from at this point at this point.

So, this is my formula please remember I am trying to solve X dot equal to f x t. So, I am writing this as X is my function. So, X t plus t n plus h that is X n plus 1 will be X t this is X this is X t this X t now Taylor series what does it tell you next term is h X dot right that is a Taylor series next will be X square by 2 X double dot its function of time. So, I just try to do it plus higher order term. Now this term is what X dot is f. So, I computed this is f, but my error is here X square by 2 and X double dot is what I do that the time stability of this f dot, but then it is function of X n t X both. So, I have to write this as delta f by delta t plus X dot delta f by delta and X dot is f again. So, given f I can compute any derivative. I have to just do it again and again. So, this is my error. You know (Refer Time: 15:50) scheme which is X 2 it is a bad scheme something which is just is accurate only up to linear order. So, any function which is quadratic is not good. So, this is single time step.

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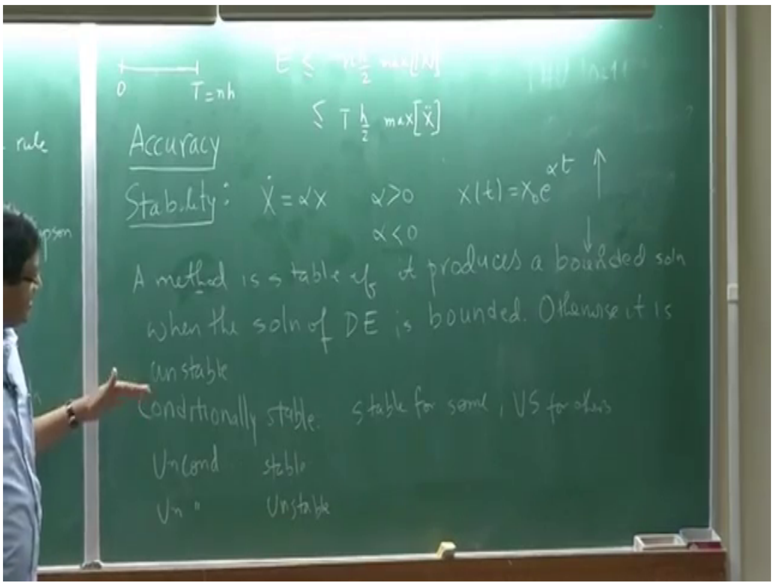

Suppose I go from 0 to capital T enhance steps. So, it is going to T times T equal to capital T n time h correct I divide into n steps of course, sometimes error can cancel. So, this thing can come with different signs plus minus sign. But suppose worst case is I knew that they all add up if they all the add up my error will be adding up. So, error will be s squared by 2 max of x triple dot multiplied by n error is less than equal to I should put mod of. So, I am putting a bound. So, this is n h is T its T times h by 2. So, something linear in h, so h I am taking ten minus 3 and my answer is order 1. So, I am getting accurate only up to point 1 percent which is not good. So, if t becomes large then it becomes worse suppose I am going to t equal to 100 non dimensional time again I am talking about non dimensional time T is 100, 100 times h is 0.10 minus 3. So, 0.1 is like 10 percent error.

So, accuracy is very bad for Euler scheme. So, this series issues called accuracy and you can make an estimate of accuracy by doing Taylor series. So, this scheme I will I will describe that this scheme is better is order h cube is accurate up to order h cube both this schemes are this scheme is h cube. So, we have to device higher order schemes. So, this is for accuracy. So, we will discuss it when we discuss better scheme. So, in for your project you should not use Euler even though we emphasize Euler for illustration Euler is not the scheme you should use we will describe Runge Kutta scheme which uses this scheme well uses this scheme I mean it is part of it Runge Kutta is not exactly this.

So, I will describe those schemes and you should use a at least Runge Kutta second order, Runge Kutta forth order is better. So, this is about accuracy now this is very important point called stability. So, how do I test stability? So, we are aware of stability in mechanical system know system stable. So, if I take this raw chalk like that is is unstable, but if I keep it like this is stable. So, stable systems are if I displace it from my equilibrium position it will try to go back to equilibrium position and unstable systems are one which is if you displace it then you will go away from the equilibrium position by terms are for differential equation that is not a definition, definition stability is very different and is very very critical.

You may not worry too much about in this course, but you should worry about it especially for your research projects. You need to worry about in this course if you are doing PDEs stability is a important criteria. So, how do I define stability? So, let us again look at this example X dot alpha X, if alpha is greater than 0 then the solution of course, grows with time. So, X t X 0 is grows with time. What if alpha is less than 0? Solution goes to 0. So, if my physical solution is growing in numerical solution it should also grow. But you may all this is unstable system right. In fact, this called unstable system in physics, but we do not call that unstable in numerical scheme both. So, you are talking about numerical stability. So, in numerical computer this is we do not talk about stability as, we do not call this unstable. So, what is unstable for computer scheme is if, let me just write down from here. So, method is stable if it produces a bounded is that clear a solution is stable if it produces a bounded solution when the solution of the differential equation is bounded. So, you have to test for this solution.

So, if my physical solution is bounded it. In fact, goes to 0, but if an numerical solution start oscillating then the solution will be call unstable and of course, if my numerical scheme also goes to 0 then is stable. Now there are some correlates to this some definitions which you should remember conditionally stable. So, when is conditionally stable when solution is stable for some unstable for some. So, I will show you some examples I mean this. In fact, will use the same equation and I show you. So, stable for some an unstable for others you can also call as conditionally unconditionally stable.

So that means, stable for all parameters it will stable for every all parameter is called unconditionally stable unconditionally support you know this is gives you unconditional support or unconditionally unstable. So, is unstable for any parameters so in fact, schemes are 1 of the 3, is either is conditionally stable conditionally. So, conditionally unstable is same as conditionally stable or unconditionally stable and unconditionally unstable now let us see whether what about this equation.

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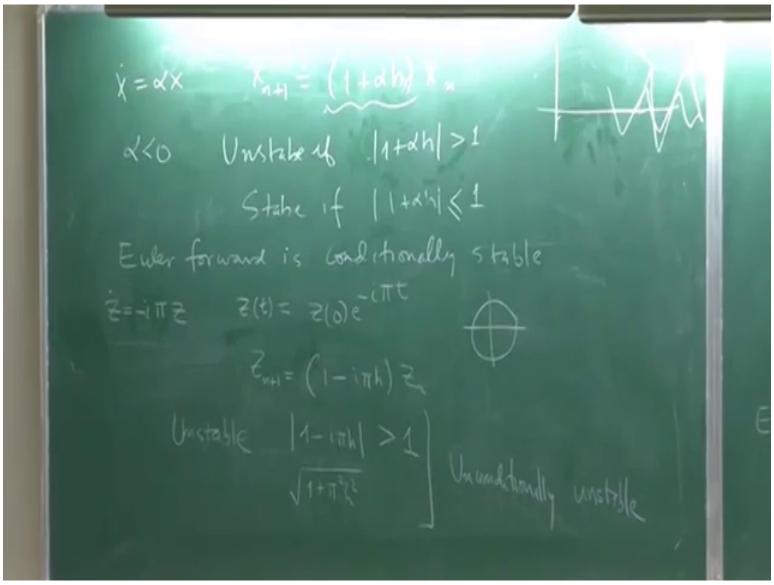

So, let us look at, Euler scheme X dot is alpha x, I showed that my is equation is X n plus 1 is, the stability for a scheme, so I am talking about Euler forward scheme. So, it is not I mean. So, every scheme will have this analysis. So, now, for alpha negative, remember, you have to test only for alpha negative alpha positive is both schemes are I mean numerous schemes we do not see anything my numerical solution will grow and my physical solution will grow, but for alpha less than 0 I have to check what about this term what happens to this for alpha less than 0. So, can your solution oscillate, no, solution can oscillate or no will it always go to 0. So, when will it not going to 0?

Student: (Refer Time: 25:18).

When alpha h is greater than 1 now we can chose of course, h so that it becomes greater than 1. So, this unstable if 1 plus alpha h is greater than 1, I mean alpha. So, imagine alpha is minus 1. So, just to give a trivial example minus 1, if I chose h h is your choice h I could chose as 3 h is 3 well you may laugh right now, but you will find situation you will make a mistake I will show you an example where whatever h you chose is unstable for this is trivial example of course,. So, here h nobody would chose as 3, but you use h equal to 3 here and then it is unstable. In fact, solution will is going to, you chose let us say alpha is minus 1 and h is 3 is going to do like this. In fact, it is going to grow it keeps switching sign. So, it is unstable if this condition is there ok.

So, this system Euler scheme Euler forward scheme is conditionally stable; that means, for this condition is unstable stable and of course, if this is 0 then is equal to 1 then is not correct the system remain constant which is again not true it should either go down or go up it should go down. In fact, I should say this equal to 1 is also unless you chose a solution starting point is X is equal to 0. So, Euler so that means, my conclusion is Euler forward is conditionally stable is that clear to everyone. So, let us do in slightly different example.

So, I am going to use instead of X Z dot alpha z, but Z is complex and alpha is also complex I use alpha as i pi. So, this example from (Refer Time: 27:53) book minus I pi. So, what is the solution look like solution is oscillatory. So, Z t is same solution know is Z is complex. So, Z 0 e to power minus i pi t it is oscillating is a imaginary is a complex number, but it going on a circle in the complex flame. So, is going on a circle in the complex flame. So, what happens? Yeah.

Student: (Refer Time: 28:31).

Solution will what.

Student: (Refer Time: 28:40) constant

That is true.

Student: Stable (Refer Time: 28:42).

Yeah. So, it is a good question. So, my answer is going to 0 well actually may be. So, I think I will give you grant me that I will just agree with that. So, if start from 0 I get that correct answer, but if I start from something else I stay there in the non correct answer. So, you are right is bounded. So, it should be it should be stable according to the definition. In fact, you should put equality here then right.

Now, what about this? So, is a Euler scheme stable or unstable conditionally stable which category my solution is changing with time. Now the formula this formula still the valid formula instead of X I have to write z. So, Z n plus 1 is 1 alpha is minus I pi 1 minus I pi h Z n. So, now what is a condition for stability? Now this is a complex number you know. So, I cannot simply say plus minus you know.

Student: Mod.

So, mod you have to put the complex mod. So, I have to put a mod 1 minus I pi h mod. So, if greater than 1 is unstable. So, is it is it true or not true is this quantity always greater than 1.

Student: Yes.

So, yes it is a complex number it is purely imaginary h is always positive h cannot be negative h is always positive. So, this is square root of 1 plus, so is always greater than 1. So, the system is unconditionally unstable. So, is a problem with Euler scheme, Euler scheme for whatever h I chose my system will grow.

So, I will illustrate always numerically in the next class, but this a bad news Euler scheme is that is Euler scheme is not a good scheme. We can write down. So, this is for particular alpha these particular alpha these alpha is positive. But this condition you can write down in terms of again sketch it in terms of arbitrary alpha.

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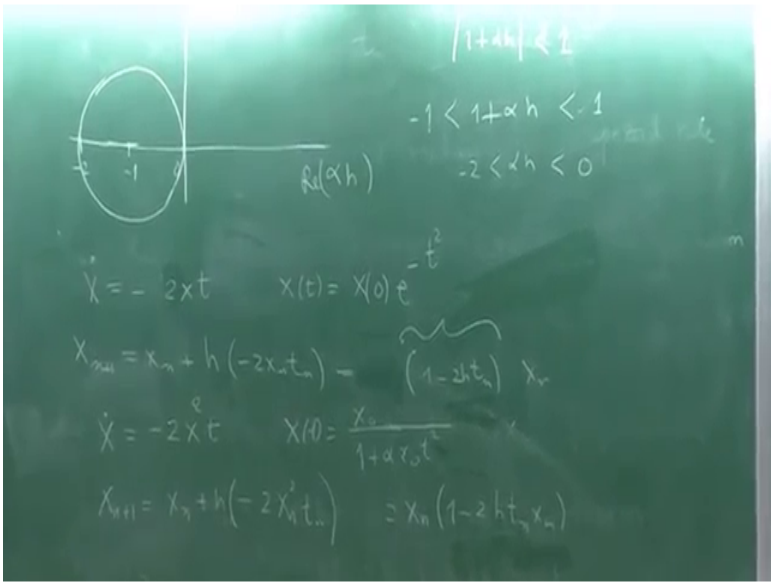

So, what the condition will be. So, I want to draw alpha h real alpha h imaginary. So, I am demanding that 1 plus alpha h is less than 1. So, what is does it [tr/transit] transit to alpha h. So, to see that let us think only on the real line. So, on the real line is going to 1 plus alpha h is less than 1 but greater than minus 1. So, alpha h is greater than minus 2 less than 0 on Euler line it lies between minus 2 in 0 and this is a circle with center minus 1. So, this region of stability, so this is a region of stability for Euler scheme.

Of course, if my equation is of this sort. Now this is a variation that we solve it in real space. So, you can write down equation for X and y. So, that part I may there in my notes, but I will not discuss it. So, this is state you that you can work in 2 t it takes X and y and again y t what eigen values and in which eigen direction it grow. So, all that can be done.

So, even though I am working right now with 1 equation, but is this 1 is relate 2 equation now let us think of slightly complicated example X dot X minus 2 X t still linear is linear or non-linear is linear is linear in X the t is the coefficient. So, this is linear equation. So, this is 2 t is a coefficient which can be function of time. Now this equation has exact solution. So, X t I will not derive it, but minus t square. So, if I just substitute just verify this. So, if I substitute is going to be X 0 minus 2 t exponential 2 t square which is same is that. So, this is exact solution.

Now, is this a same stable or unstable now how do I vary, I want all apply Euler forward. So, again the same formula, but I have to be bit careful. So, X n to equal to X n plus h times.

Student: Minus 2.

Minus 2, 2 X n t n. So, h times f, f is this. So, this is going to be X n 1 minus 2 h t n. Now this my, if I write this way, you demand this 1 be less than 1 mod of this now is that always true. So, I may chose very tiny h, but for large n of t this can become a problem know. So, you may think that h I mean look. So, if you are not careful your solution will behave properly in the beginning, but later on it will start oscillation.

So, one has to be careful I mean is stability is not trivial thing stability requires analysis and this is of course, equation is simple, but when your higher order schemes I will not do much of in the class, but you have to do it if you are working in this kind of issues you have to work out carefully.

So, another equation is which is there again from (Refer Time: 36:00) I just modified it a bit, this equation is again similar form. So, it also has exact solution in terms of first order equation you can always write exact solution. First order ODE there is a theorem it could be very complicated, but you can always write it you can integrate first order equation. So, this one it turns out its exact solution X t as X 0 e square.

Now, what about stability of this guy? X n plus 1 equal to X n plus h minus this 1 2 X n squared t n I just put f, but at that point. So, this is X n 1 minus 2 h t n X n. Now do well now I can see from the solution I sees I already know the solution I can reduce something. Now this of course, grows t n will grow, but X n drops faster than t n where this t square sitting here it turns out this guy always will be bounded we chose appropriate h. So, this system is for of course, if we use h very bad h in the beginning itself it becomes unstable.

But if we chose proper h then this system is stable even though t n is growing. So, this system is conditionally stable of course, is not for all h, but you can be rely on Euler scheme it give at least stable solution. What about the accuracy? So, I will show you in the next class when I do all that numerically all this systems are not very accurate because error is of the order of h for h squared first step h order h per in the full time scale. So, you will find that the numbers very off so, but one thing you definitely want a stability and of course, you like accuracy. So, you need to work on both the angles. Now Euler scheme is unstable, but Euler forward scheme. But can we make some amends so that I can recover stability. So, the idea is in spite it is only small trick and your system becomes very stable. So, let us think of Euler backward scheme.

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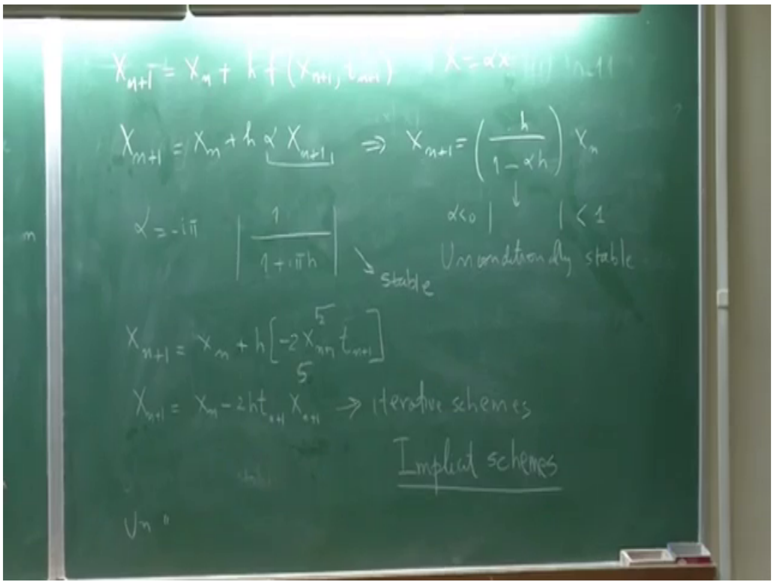

So, what is a Euler backward scheme? X n plus 1 equal to X n plus h function calculated at n plus 1 t n plus 1 now of course, a problem is I do not know what is X n plus 1 in general, but for this example which is a very simple example X dot equal to alpha X this is. So, this is a very simple example, but it is good for illustrate.

So, let us plug it here and see whether this system Euler backward scheme is stable or unstable. So, X n plus 1 is X n plus h is going to be alpha what expect 1 not X n X n plus 1. So, this is computed at n plus 1 is that clear to everyone. Now I can easily solve X n plus 1. So, what is X n plus 1? This implies X n plus 1 is X n divided by 1 minus alpha h now is this equation is stable now remember problem is when alpha is negative is this equation is stable or unstable for alpha negative what is it, alpha is negative. So, whatever h I chose this point is less than 1 right is guaranteed to be less than 1 as long as alpha is negative.

So, for alpha negative this object mod is always less than 1. So, this conditionally stable sorry unconditionally stable is stable for all h. So, this unconditionally stable. So, Euler backward scheme at least has 1 advantage that unconditionally stable accuracy again a problem, but is very stable. So, the first one, this one will be stable. What about this one when alpha is a complex number, suppose my alpha is minus I pi what happens. So, this factor is 1 divided by 1 minus, minus is equal to plus I pi h what about this guy is also less than 1. So, is also stable.

So, it turns or it will it will my oscillation when I do the numerical solution we will find that this will go in what is stable is not is not growing. So, this also stable it does even this guys are stable. So, we can work out this one or both how will you solve this problem with Euler backward scheme. So, Euler backward scheme will correspond to plus let us solve this one, this one. So, Euler backward scheme will be X n plus 1 equal to X n minus h plug in my f which is minus 2 X n plus 1 square t n plus 1 .

Now, this becomes X n plus 1 equal to X n minus 2 h t n plus 1 X n plus 1 square. Now you said possible to solve like this now this is Euler backward how do I solve it?

Student: (Refer Time: 43:25).

Sorry.

Student: (Refer Time: 43:27).

So this one you can use quadratic formula I can be bit nasty and I will say what about change this 2 case power 5 then what do I do. So, then I am really do not know how to do it analytically, but then I can apply iterative scheme which is one of the exam questions which in exam question was not that difficult exam was just iteration, but you can iterate it by trial solution. So, this is called Newton option I am not sure you done in your earlier classes 1 of the iteration scheme you start with some guess and you iterate and you read the solution. So, one of those schemes are useful of course, you chose right guess and right scheme if you do not do the right scheme you may run away to wrong region.

So, these are solved by iterative schemes. Actually so in fact, let me just mention one more scheme and then I will stop. So, you see a advantage of, in fact, these of call implicit scheme. So, let me just write this word. So, my solution is in terms of solution itself is like integral equation in code of mechanics. So, these are called implicit schemes and these schemes are got explicit scheme. So, my solution is in terms of X n plus 1 in terms of X n. So, is explicit, but my X n plus 1 here is in function of X n plus 1 itself. So, it is called implicit scheme. So, implicit schemes are typically more stable and, so we will come and you do PDE will I tell you that you need to use implicit scheme for stability.

So, I think I will stop at this point and then we will, I will illustrate first by simple codes and then we will do higher order schemes Runge Kutta trapezoid rule. So, we will do all that. So, I will stop.