Computational Science and Engineering using Python
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Lecture - 07
Errors & Nondimensionalization

So, we start numerical analysis now. So, first thing we need to understand is error ok.

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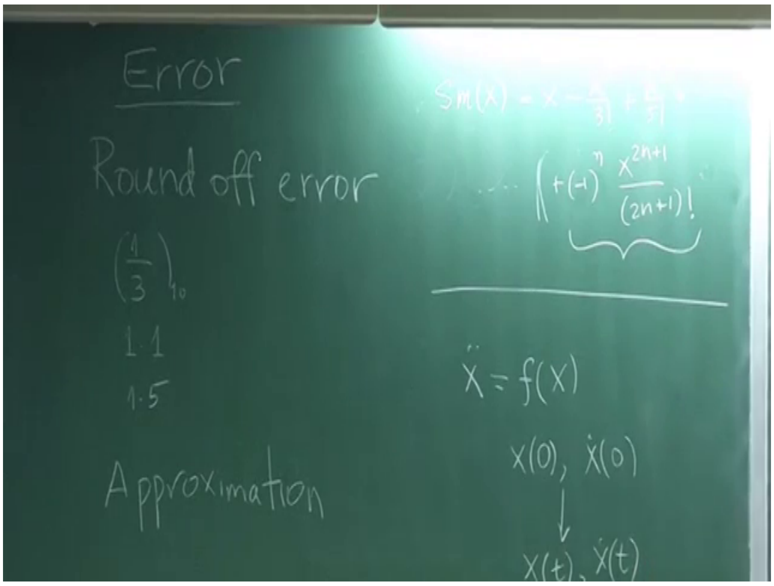

So, the result you get is coming from computer, unless you do symbolic processing like that I am not covering right now may be I will do it depending on the time. So, (Refer Time: 00:44). So, without symbolic processing there will be almost always some error of course, we want the error to be small, but you must know how much the error and sometimes if you do not careful error could be very large, and it could be bogus your answer would be bogus. So, what kinds of error we get in numerical computation?

So, one error is round off error right, we discuss that round off error. I discussed this before. So, no number were very few numbers floating point numbers are represented exactly. First thing is any irrational number cannot be any represented by finite number of digits, but even if it is a rational number, that to cannot be represented quite accurately inside the computer ok.

Like 1 by 3 is a rational number, but it cannot be represent inside computer both in decimal as well as in binary, but the number example I gave you like 1.1 is quite in decimal I mean only 2 digits, but in binary it cannot be exactly represented we did some example. So, this is the curious examples, it tells you that no number well very few numbers can be exactly represented in a computer very few of course; that means, the large number, but there are even larger number which cannot be put in the computer . 1.5 can you put inside accurately decimal 1.5 see all decimal this can be put accurately is 1.1ok.

So, round of error is critical, you must understand how much is the accuracy what how are we storing in the computer, but second error is also approximation. So, we make approximation, example I am going to give you. So, we would not compute sin of X, x is some number floating point number then how does computer compute this series. So, one does the series like this, but again I cannot compute all terms of the series, right.

I need to truncate. So, this will be some loop. So, this is implemented there is some clever track spot most of the time it is just simple implementation of series. Now this series I will truncate somewhere, but as soon as I truncate this error right. Suppose I truncated x 2 n plus 1 by n 2 n plus 1 factorial depends the sin towards sin will be n is one is odd n. So, I just truncate here. So, I do not keep this trunk.

So, this plus other terms will be error, but we say well error is of this order where of course, error will be all of these which I ignored, but I am going to say the error is of this order we expect the series to be convergency these. So, each term is subsequent term is smaller all right. So, this is the error which we get because of approximation. We will do later that when I solve deferential equation derivative calculation, will be not exact again we will be make approximation. So, all our numerical computation will be approximation and there will be error because of it. So, error comes of these two types broadly, now it may happen. So, is that clear? So, is this part I mean, this quite obvious.

But you will have to see for every algorithm how much is the what approximation I will choose. Now this error as well as this error could add up in each step. So, just imagine that I am computing. So, we I am doing in a loop. So, weather protection of temperature of Kanpur. So, to reach tomorrows temperature I am going to do many time steps, take initial condition and time step. We solve Newton’s equation x double dot equal f of x we going to solve this kinds of equations and this is that differential equation, but I will given the initial condition x 0 and x dot 0, I am going to loop time stepping reach x t n x dot t this is a Newton's law.

Now this is all we done in one shot in computer compute loop small-small time steps and is going to reach just to make it more explicit. So, I start from here position as a function of time, I will be going to delta t delta t delta t like this, ok.

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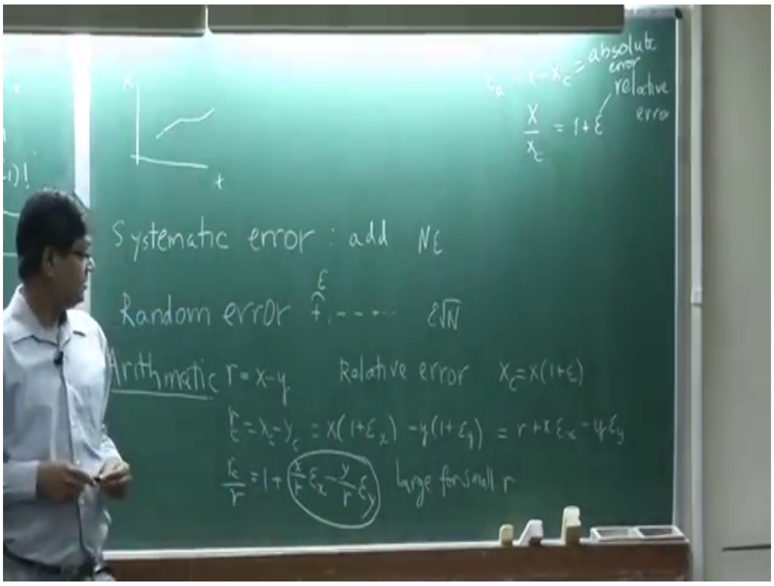

Each time still I will be committing an error now the errors could add up. So, that will be systematic error if it is systematic error this you know from your (Refer Time: 06:56) physics course your systematic error; that means, well each time my error is of same sin and they just keep patting up.

So, systematic error you just you have to add them, but there could be error which a random. So, in a round of errors typically will be coming with the both the signs plus minus. So, if you are round of. So, if random errors; the random errors come with both the signs. So, it will come plus minus minus.

So, in n times suppose each let us now theory of errors someone there huge number of books and I am not expert of this, but we should know how much I mean to elementary analysis. So, if let us imagine each and each step I make an error epsilon; assume it to be equal epsilon. Then if systematic error then n times step what could be the error size n epsilon. Now if it is random then a random walker a drunk walker you know he is walking from origin, and each time this person in 1D takes one step forward randomly or one step backward randomly.

So, its deviation from the starting point is of this order square root epsilon x root n x epsilon. So, this is these are two types of error we get and. So, we should keep this in mind how much is going to be the error. So, let us also look at these are broad categorization. Now there is one more thing I did I should have mentioned it there one I should I think I should add here one time error is arithmetic error actually it should basically belong to this round off error approximation error arithmetic error. So, even if a number can be accurately represented there could be error because of my numerical operation addition subtraction. So, let us look at example, I want to subtract x minus y now there will be well in my.

So, there could be some error in x it could come from round off or my experimental I mean when I input data I make error. So, there could be some error in x. So, exact value is r which is r equal x minus y, but my computed error c for computation. So, my value of x is x c and Y is Y c. So, this computer value and this computer value for y. So, the difference will be rc, now this what I will get in computer not this.

Now, let us estimate what is the rc. So, we will also use a word for relative error. So, relative error is not the actual error is what is error in x minus x is absolute error, but relative error is written as x equal to actually x c equal to x 1 plus epsilon. So, this epsilon is called relative error. So, x 1 and x c sometimes if in floating point numbers and it represent numbers as exponential right 10 to the power something remember. So, large number will have if the number is large x minus x is large, if number is small then x minus x is small does not mean that I am doing it right number byte.

So, nature is formed; however, if I say what is the error in this. So, if this small and this small then we write this one plus epsilon. So, this is a good measure of your operation. So, this for relative error and this is absolute error. So, now, let us estimate what is rc minus rc. So, this going to be x 1 plus epsilon, I am going to call it x epsilon x error in x whether two quantities, the errors could be different and then other one is y 1 plus epsilon y, epsilon could be positive or negative it could be either epsilon either sign. So, this is equal to x minus y which is my exact value r plus x epsilon x.

Now, let us look at relative error in r there is. So, rc. So, my space is getting heater now. So, I am going to write it here rc by , what a rc by r. So, this becomes 1, 1 plus x by r epsilon x. So, these are my relative error now when does it become large relative error.

So, this one danger you know something it tells you that when my numbers are of certain type I have danger you know this number could be very large when r is small. In fact, when r equal to 0 this should be 0, but these were the error can be very large relative error. So, I am going to show you an example where I subtract two numbers which are somewhat of same order and the error is relative error is large, and your number your answer would be very wrong. So, this quantity is large for small r. So, how do I estimate this? So, when x is equal to y approximately.

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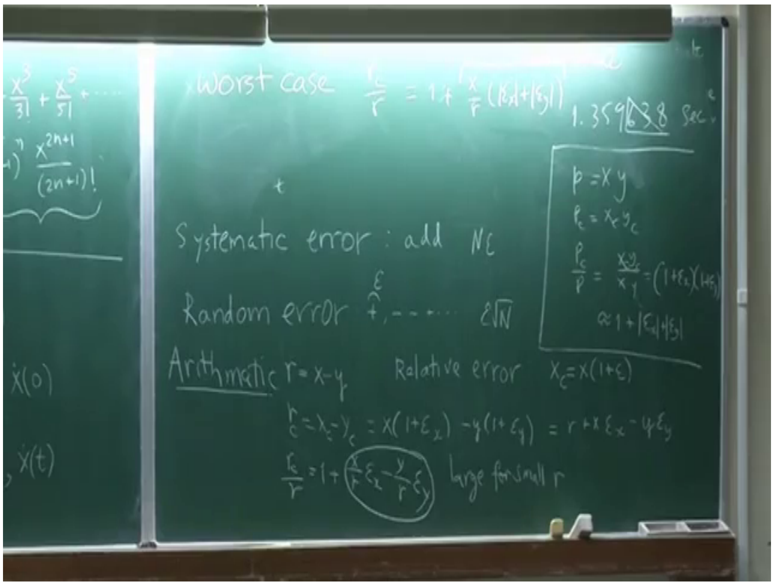

So, I am looking at max worst scenario. So, worst scenario is when r is worst case.

So, rc by r is it I am probably blocking because I am also cautious of the camera. So, is it clear I mean visible to everyone. So, rc by r. So, these one thing you should remember. So, I am going to make only estimate I am not going error is always estimate you should not say error is 0.1, 2, 3, 4, 5, 6, 7, 8 like that, few elementary stuff which every student most student make mistake is you should not write your numbers for large number of digits how many digit should you use? So, somebody says that time period of pendulum is 1.3596 seconds. So, should I write like this? So, where should I cut off?

Student: (Refer Time: 16:00).

So, your watch has accuracy. So, accuracy of watch let us say millisecond. So, I should not have any of these digits, micro second then I should can keep this. So, we should keep only digits which are reliable. Similarly I want to make only estimate I am not going to say error is this number error is bounded by this number. So, I say well worst case is when of course, r is closed to 0. So, x and y are roughly equal. So, I say x by r and epsilon. So, this even though I am subtracting it epsilon y could be negative and epsilon means positive. So, the error will add up. So, you can say well epsilon x mod like epsilon y. So, these are approximate. So, the error is error estimate these why error estimate error estimate always positive, you should not say error is negative.

We can do the same analysis for product so in fact, this analysis straight forward. So, let us say take product of 2 number x y. So, let us call it p. So, we can do the same stuff so. In fact, let us look at quickly pc in computer is going to be xc yc. So, Pc by Pe is xy by xc yc equal to now I apply the same logic. So, other way (Refer Time: 17:52) xc about.

So, I just do the same logic the next file will cancel and I get 1 plus epsilon x, 1 plus epsilon y. So, these approximately 1 plus epsilon x will product can be ignored leading order, epsilon are supposed to be small is the relative error. So, epsilon x plus epsilon y and you can put a mod that is to be safe. So, my error is sum of the errors. So, product is not that dangerous subtraction is dangerous or adding numbers which have different sign that also is a problem.

So, any number with two different signs something while doing this some operation if I get 0, then there is a possibility of large error. So, I am going to illustrate by two computer course. In fact, let me do some more ground work before I go to the programme. So, just to summarize we going to have round of error or error due to approximation. Now these two errors can add up in systematic error or it could be random error. So, they will cancel somewhat. So, error will be not an excellent, but it should be epsilon square root n. Now one example of error which comes in is arithmetic.

So, in arithmetic operation in subtraction we estimate the error, and find there is most dangerous when the numbers are of the same order ok.

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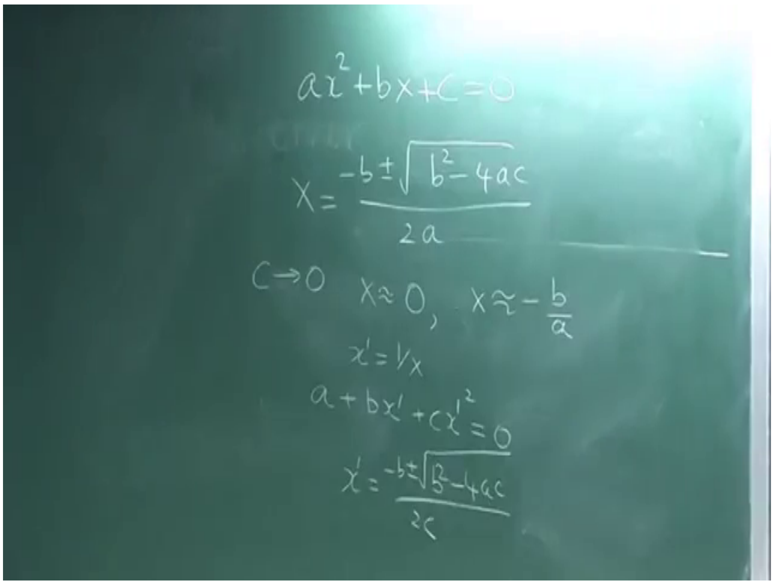

So, I am going to do an example solving quadratic equation rules of a quadratic equation. So, this equation is a x square plus bx plus c is 0. So, my answer is minus b ok.

Now, let us workout when c goes to 0 c small. So, what is the answer when c is small approximate answer? So, one is sets this to 0. So, I get x equal to 0 is the answer approximately. So, c with key finite, but small and or minus b y somebody say that I do not want to solve this equation I want to rewrite it in some different way. So, let us call it x prime equal to 1 by x. So, what is the equation for x prime? Is going to be a plus b x prime I just 1 by x prime square 1 by x, prime plus c x prime square 0. Now let us solve this equation. So, x prime is minus b, b square minus four ac by 2 c. So, what is the value of x; so, again the value of x from here. So, let us write it here x equal to 2 c x, x equal to 1 by x prime.

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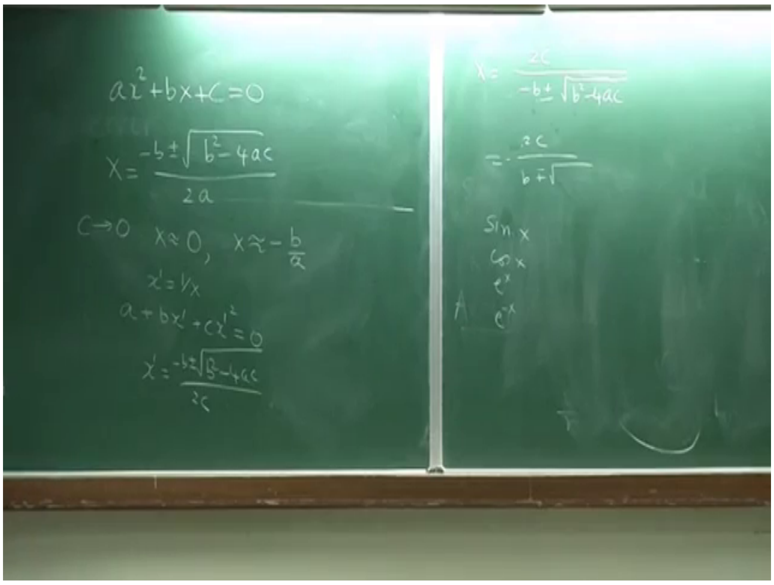

So, two c divide by minus b. So, problem is expected when this number and this number are of the same order and you subtract and that is where error will be large and you get a wrong answer. So, in a subtract division and subtraction it is a problem. So, I will just show you what the results are for these two and. So, the numbers I chosen is a equal to 1 b equal to 1 both are equal, but c is ten for minus 10 small number and I just coded the formula.

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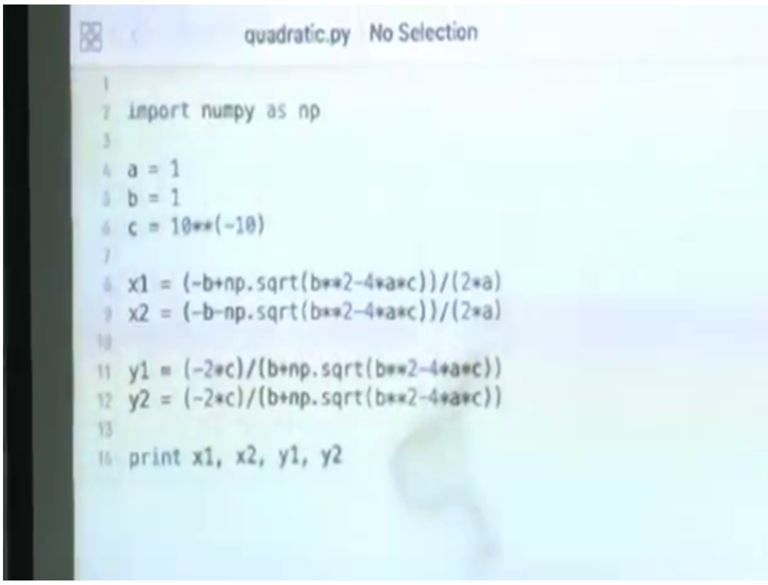

So, use num 5 then np and. So, first two answers are these values and next one is y 1 y 2 are these two values. They should minus sign right. So, there should be minus sign here. So, minus 2 c is taken minus sign outside; so minus 2 c divided by ok.

So, minus outside; so there will be minus sign. So, let us run it the error of course, is larger here. So, numbers are not so bad but.

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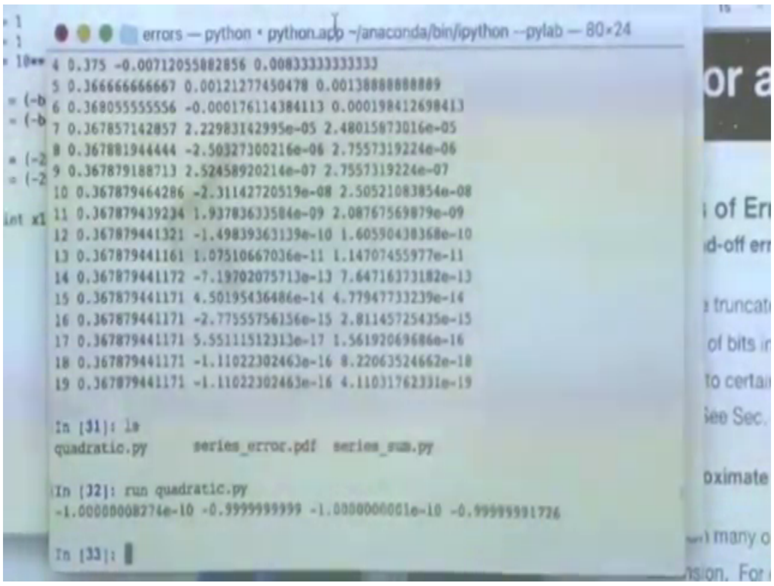

So, these are the first two numbers, the first two numbers these two numbers are coming from first two formula. So, the next two numbers are. So, this number is correct this error this is significant error 1 7 2 6, it is not I mean is not off way off, but there error is more on the second formula. So, I use the same exactly same arithmetic I use the same formula right I just made the change of variable, but it has come below and just by doing it you are lost precision. So, these purely because my error is more in this operation in the numbers are closed by if I make my b c even smaller, then I should expect more errors. So, let us see whether it happens.

So, I will make it minus 20, c is even smaller divided by 0. So, it is already creating problem infinity divided by 0. So, minus 20 it does not like it. So, let us make it minus 15 or something. Now you can see that error is quite large. So, this is illustration of error occurring due to subtraction now you may say that why I am doing all these, but it turns out that this kind of stuff will happen. So, in the homework for floating you will get 1 by r for electric field. So, you have to handle 1 by rm, you do not go close to the origin you avoid that origin.

Now, this one example the second example is how to estimate sin x cos x exponential by series method. So, any computer does this computation using series. So, I wrote a code to do this calculation. So, they are four plots. So, they will compute cos x. So, let us turn it on cos x. So, this loop is going to cos x by series some number of iteration, I am going to do is 20 which is large ok.

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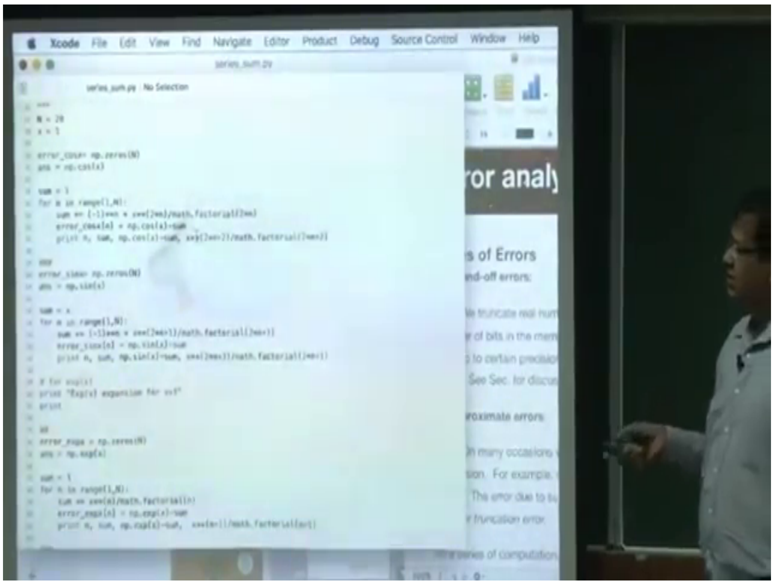

Now, I am going to compute a x equal to 1. So, I am looking for value of cos 1, I can do the same thing for sin x now these for exponential one and these for exponential minus 1, I made a error here. So, this loop is for exponential minus 1 ok.

Four functions now a make a guess which has largest error. So, I am computing for x equal to 1 the four functions, sin x, cos x, cos x, exponential x, exponential minus x, exponential minus x is largest error a smallest error. So, I will compute the error right now just is not the relative error well these values are approximately close to 1. So, it is basically same as relative error, but which has largest error make a guess ha.

Student: E to the power x.

E to the power x second.

Student: 0 minus x.

Great. And so it has the expo.

Student: Then explain them also.

I see. So, let us see. So, this code when you run it. So, this is a plot another four plots are sin is sitting here is red, green is co sorry green is cos, this is error, cos green is cos third is exponential which is here loop.

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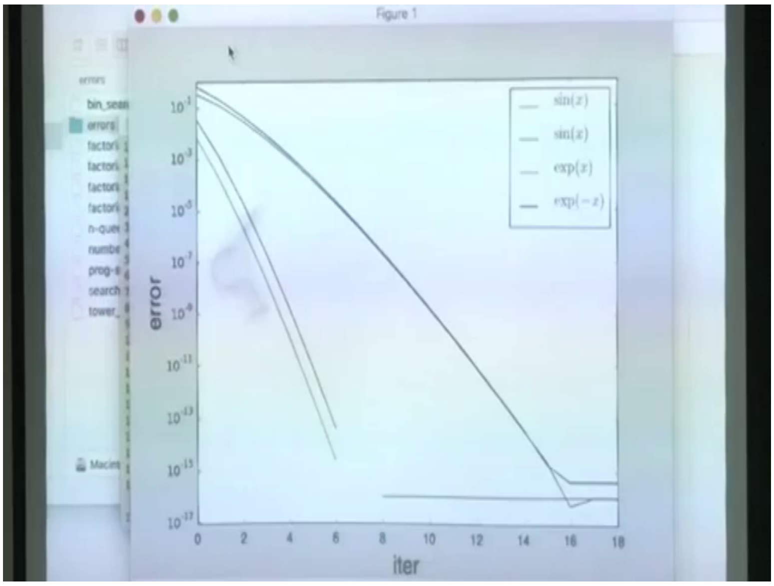

So, error the y axis is error and x axis is iteration. So, of course, first iteration as largest error and when you keep more and more terms error decreases, and what plot is called? This is linear here and this is exponential, this called semi log blog. So, you can say semi log y, I plotted using semi log y. Now exponential blue here and black is exponential minus x. So, sin and cos converts quite quickly by 8 terms, my error has gone up to 10 power minus 15, which is quite big I mean 10 minus 15 really accurate, I reliable computation to 8 decimal place maximum. So, this is quite accurate, but here exponential error is I mean need 18 terms to get error of the order of 10 to the power minus 15.

Why they look this is jump here and error is basically 0 for sin and cos not 0, but 10 power minus 16, but exponential error is significantly large and it becomes very small only for 18 terms 16 terms here. So, exponential is a very dangerous function not dangerous exponential is slowly converging function and you one needs to keep large number of terms in the series. So, that is why exponential is the most expensive operation. Among the computation of functions exponential happens to be very expensive operation, and your exponential minus x you might expect that because of the sign change plus minus plus minus this should be converging quickly (Refer Time: 29:27) slow. So, this is how we compute this error because of approximation, when I had this long infinite series why I truncated it and I get error. So, this is about error I mean nothing more I want to say about error; any question?

All clear is it good now is anyways simple you know from your experiment for this course. So, next thing I want to cover is this is my favourite is dimensional analysis. So, you will not want to non-dimensionalize equation, your variables for example, if I am doing extra physics calculation then my size of the galaxy could be large I feel loo is centimetre it is from 10 to the power 30, 10 per like that it is a large number and errors will be large if you put large numbers or quantum mechanics plung constant, you know size for me. So, that is too small.

So, computer does not like either too small number or too large number I mean you can see round off error, will be more for small numbers. We do not know deal with division by small number you know that is going to be a problem. So, your number should be order one, and that can happen if I non-dimensionalize it. So, my size of electron is of one unit not one Armstrong. So, in that you have to use appropriate unit and that is what non dimensional is means. So, I think I am just going to do the quantum oscillator not the classical oscillator, classical oscillator also useful, but let us use do quantum oscillator. I will leave it I did in the last semester.

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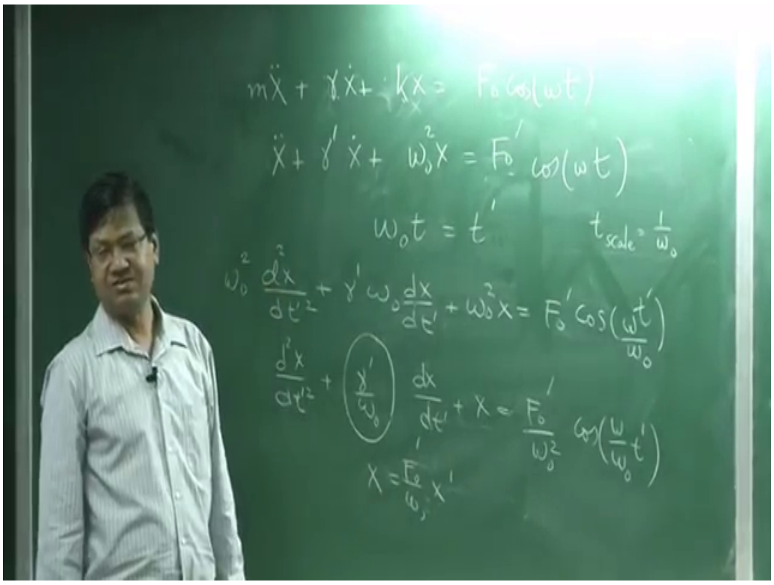

So, if you have some difficulty with classical oscillator. So, let me just write down the classical oscillator and write the answer m X triple dot gamma X dot K X cosine cos omega t. I mean I have 15minutes. So, I should be able to finish. So, I am backtracking I am going to do classical oscillator quickly. So, there how many parameters: 1, 2, 3, 4, 5. So, we do not want too many parameters. So, first thing get it off divide by m ok. So, divide by m. So, I am going call it gamma prime gamma by m x dot plus k y m s v omega naught square x f naught by m.

So, I got to 4. So, this is one parameter, now what should I do what is is the length scale here for classical oscillator. Well that is why you got in the get in the wrong territory, you should length scale will come from force, but let us wait for that let us first divide by time let us get it off the time scale. So, what is the time scale? I am going to choose omega naught is 1 by omega naught is my times scale. So, omega naught t is t prime.

So, t prime is dimensionless and my time scale t scale will 1 by omega. So, I should replace my t by t prime by omega naught. So, do the algebra straight forward, d square x by d t time square, omega naught square will come here. So, this is unit of 1 by time square x by time square. So, omega naught square will come here gamma prime omega naught t.

So, divide by gamma naught to omega naught square, but this should also be replaced t should not be there now only t prime should be there. So, this should be t prime. So, I just divided. So, I get d square x by dt time square plus gamma prime by omega naught these one variable, dx by dt prime plus x this prime. So, how many variables I got now? So, this one two please remember as the f naught prime is f naught by m and 3. So, I got I reduced from 5 to 3.

So, by just choosing my time scale I got rid off it, my time is now in one unit. So, it is not the time period is not 2 pi by omega naught is 2 pi for this problem. Now I need to get the length scale, this will tell you what is the length scale. So, what is the length scale for this problem? Gamma does (Refer Time: 35:13) no that is not these are what is what is the dimension of this object?

Student: (Refer Time: 35:21).

No, this as dimension of length, this as dimension of length this is dimension of length, this is dimension less it has no dimension. So, dimension of length is here. So, I should take this is the dimension of length. So, I should say x equal to F by omega naught F prime x prime, now x prime is dimension less, ok.

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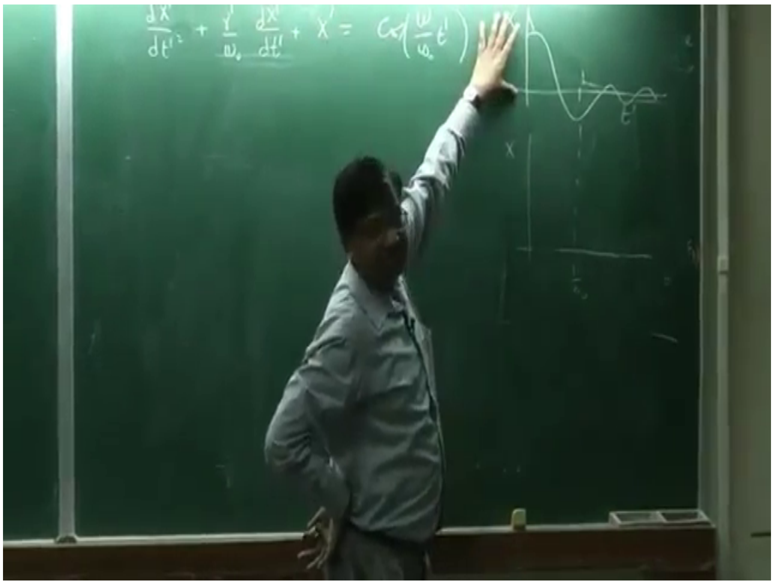

And then d square x prime by dt prime square, plus now I have to divide all that gamma prime now actually the division does not exists here. So, no problem dx prime, dt prime plus x prime. So, this will go away right I just I am replacing x by this quantity multiply x prime. So, this will cancel from both sides. So, that goes away and I get cos. So, I have already two parameter friction coefficient, non-dimensionalized friction coefficients and non-dimensionalized forcing frequency and I should work with these two parameters only. So, I can solve for x prime a function of t prime. So, it could be well oscillation depends.

Now somehow I want to go by to original variable then what should I do? So, the person will ask no this is what is the position of the particle, how should I get the position? Now I have I get it got the answer 5 x prime. So, I just use that transmission. So, there will be x here, and t prime called it should be replaced by t. So, when I say one here, let us say this one this 1 corresponds to what 1 by omega naught. So, time axis. So, everywhere there is one should be replaced by 1 by omega naught that is it. So, solve this problem; that means, you also solved the original problem. You should be able to convert from one to other, and if you know this plot then you can go back by this transformation this one and this one, ok.

So, this classical oscillator, what about quantum oscillator? So, let us quickly do quantum oscillator and 7 minutes is that clear. So, in computer, there will be projects or homework or exam question. So, you need to work out non-dimensionalization.

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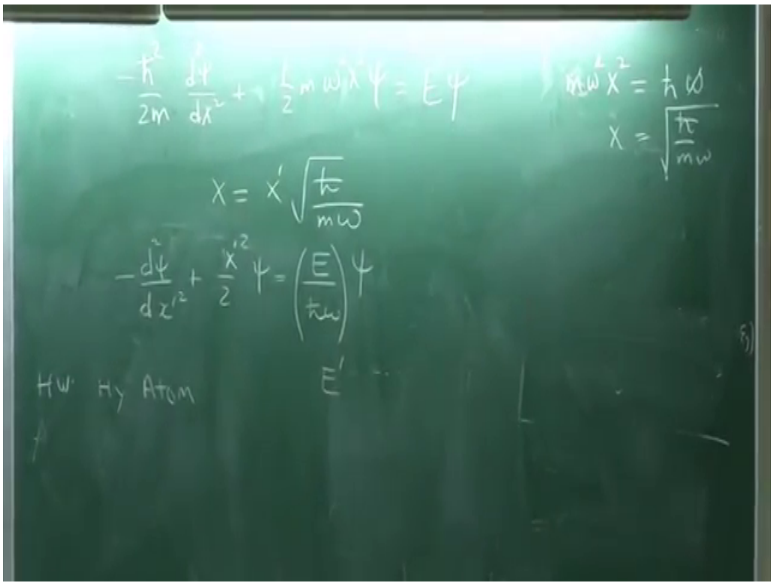

So, let us workout quantum oscillator. So, the equation I will do time independent oscillator v. So, v is half k square. So, this is a starting equation for oscillator. So, I need know non-dimensionalize this. So, what should I do? Length scale; so length scale of this problem is come on what is it, how do I get length scale.

So, now by this would this is if you are not doing it then you are not doing it properly. So, half a omega square x square these potential energy or total energy if you like h bar omega. So, energy is a obvious order. So, x will be h bar by m omega. So, dimensional analysis gives you very quickly the answers, you do not need to do some fancy mathematics Lizandra polynomial and Hermite polynomial, it is here case or this from dimension analysis energy equated it to h bar omega. So, let us for short hand keep like this ok.

Now, please remember you need to do this kind of operation, I mean this not fancy mathematics, but simple things must be done first. So, x equal to x prime square root h bar by m omega. So, x prime is dimensionless I will not non dimensionless side, I will let it be. If we put it here I will skip the algebra you can do it I did it, sometime last semester. So, everything cancels dx time square plus half. So, what comes here?

Student: (Refer Time: 41:06).

E divide by. So, this is dimension of psi, this is dimension of psi, this should be dimension of psi. So, this should be dimension less. So, what should divide here? H cross omega. So, this is E prime. So, we have only one parameter E prime no h bar m omega all are gone, and we solve this differential equation nice looking right you do not need to worry about h bar m so on. So, in computer we feed this. So, it simplifies your mind can think simple and you get your answer, I mean this will be exponential times hermits polynomial.

So, in our project in our homework we solve these equation, here my x will be order one not Armstrong or very small number. So, homework related to this is hydrogen atom non dimensional hydrogen atom. So, I will look at any question I also first let us non dimensional that is what you should do it.

So what we need to start next is numerical method, now non numerical these are general things we need to keep in mind, error analysis and non-dimensionalization, but now we need to start each algorithm and some of them very clever, some of them are intuitive easy I just to tell you that great men like oiler mostly men and very few women. So, oiler

Gause Zender Hermit all these guys u seen in mechanics mathematics. So, Newton; Newton has very clever algorithms for solving equations and they were they did not have computer that time. So, they were doing by hand, and they wanted quick conversions I mean computer I am lazy. So, 20 terms fine let it do, but they had very few I mean wisely they had do by hand.

So, they want to get the result as quickly as possible Ramanujam; the some of the series of Ramanujam conversion very quickly. So, pay attention well I am not very good at it, but I know some algorithms which are very clever like integration there are very clever scheme called Gaussian Quadrature. You heard of Gaussian Quadrature it is very quick it converges very quickly. So, there is some interesting maths in it. So, your knowledge of mathematical method will help do not think that is uninteresting that is number one, people think that it is very uninteresting.

So, I just wanted to say that if Gause is doing it that cannot be uninteresting you know it has something in it. So, we will start in the next class.