Numerical Methods and Simulation Techniques For Scientists And Engineers

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Lecture 01
Introduction
Error analysis and estimates, significant dig

So, good morning everyone welcome to this course on numerical methods and simulation techniques for scientists and engineers, the courses likely to give an overview of different numerical methods that we use for solving different physical problems. And there are simulation techniques which are needed in order to either time evolve or evolve in another parameter space of systems and then see that how things behave in the time evolved say for example, case such as you know, markets or the financial groups.

They need such simulation techniques to know that how the market is going to behave in a few months down the line or maybe even a few years down the line. But of course, that is a very complicated problem, numerical problem, which had a lot of you know, external factors that influence we are mostly going to talk about the very established numerical methods and the simulation techniques that are also quite established and are needed in a big way for solving physical and physically relevant problems and engineering problems.

So, in order to see an introduction to the is let us understand that since the middle of the last century or other the latter half of the last century, the personal computers have been available in a big way and they are rather inexpensive these days, which have made these numerical computations of various physical things quite easy and feasible.

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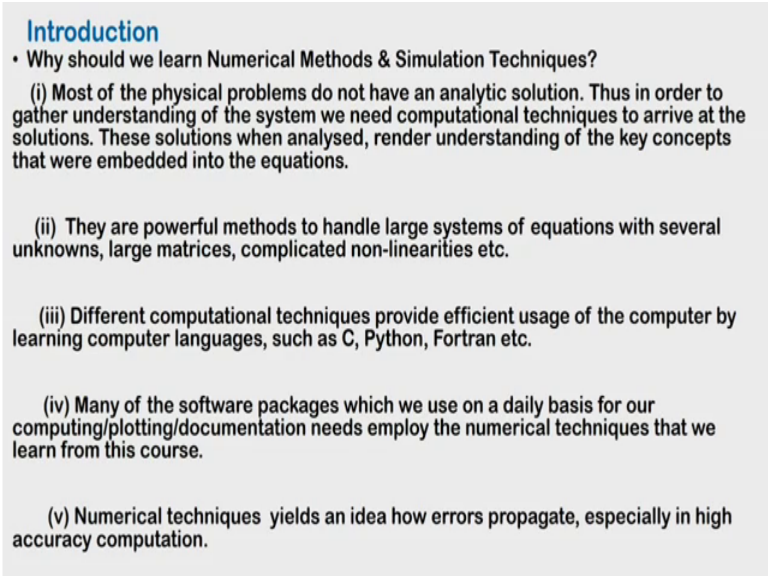

So, is needless to say that these inexpensive personal computers with a reasonably large RAM, they have given access to powerful computational methods and techniques, and which have evolved in the last maybe 20 years or so, in a fairly massive way. So, let us you know, cite few reasons that we should do this course or rather learn this method of numerical techniques. So, the first question of course, that why should we learn numerical methods and simulation techniques.

So, are most of these physical problems that we come across do not have an analytic solution, even the best of the mathematicians could not solve a large number of problems or a differential equations that may not have a clue solution or an exact solution, even if it is there, it has not been discovered as yet. And there are approximation techniques such as perturbation techniques and so, on which we have seen in course of say quantum mechanics or sometimes even in classical mechanics, they only give approximate solutions.

But that also subject to certain conditions such as the perturbation term or the interaction term being small as compared to the non interacting term such that you can use the basis or the V functions or the Eigen functions for the non interacting problem in order to find directions due to the interact interaction term. So, in order to gather understanding of those systems were exact numerical methods or rather exact analytic solutions are not available computational techniques are the only solutions to those problems.

And we need to arrive at the solution. So, we need to resort to new metrics. And these solutions when we analyze them, they give you understanding of the key concepts that are embedded in the equations, equations do not make any sense to us, unless they are solved and they are put in perspective, and they are physically they are made physically meaningful. In order for us to gather information about the system, its properties, its characters is dynamics, behaviour with respect to different parameters, etcetera.

The second is that, they are powerful methods to handle large systems of equations. Of course, we cannot physically solve maybe more than one particle or two particle or maybe a few particles, but, these computers are these computational techniques can solve a large number of simultaneous equations and with several complications such as they can have several unknowns and large number of unknowns, large matrices, they can handle large matrices diagonalization of large matrices are made possible and they can also handle complicated nonlinear entities, usually non linear equations cannot be solved by hand you need to have computational methods or numerical methods in order to solve the non linear equations.

So, these are some of the very basic things where numerical methods come to have us and they are heavily used in most of these situations. And of course, very correctly that different computational techniques provide efficient usage of the computers and which of course necessitates learning of computer languages such as C, C++, Python, Fortran, etc, etc. And many of these software packages that we actually use on a daily basis for reasons related to computation related to plotting of graphs, so, as to make meaning of those results that are you know, visual meaning of those results that we actually find.

All documentation purpose, we often use a large number of documenting software's where we simply write letters or write document or write you know, notes, which are, which could be class material and all that, they apply number of numerical techniques, which have few of which we would learn in this course. And importantly, last and not the least, the numerical techniques each and idea how the errors propagate, and especially in high accuracy computation.

So, when you need results, which are, you know, you need accuracy of 10 to the power -6, then, of course, you have difficulty of getting anything up to the 5 decimal places, or 4 decimal places, and so on, you need accuracy up to the 6 decimal place. So, they are the small errors, which are, you know, even of the order of 10 to the power -5, etc, they could make a lot of difference in our results, such as, you know, these rocket propulsion or there are other things where accuracy is very important.

If a satellite or a rocket deviates by a very small amount from its path, there could be, you know, serious and fatal consequences, which is what we do not want. Now, it is important for us to have an idea that how are these techniques propagating from one step to another step as we carry out this computation. And as I said that these are essentially relevant in high precision or high accuracy computation.

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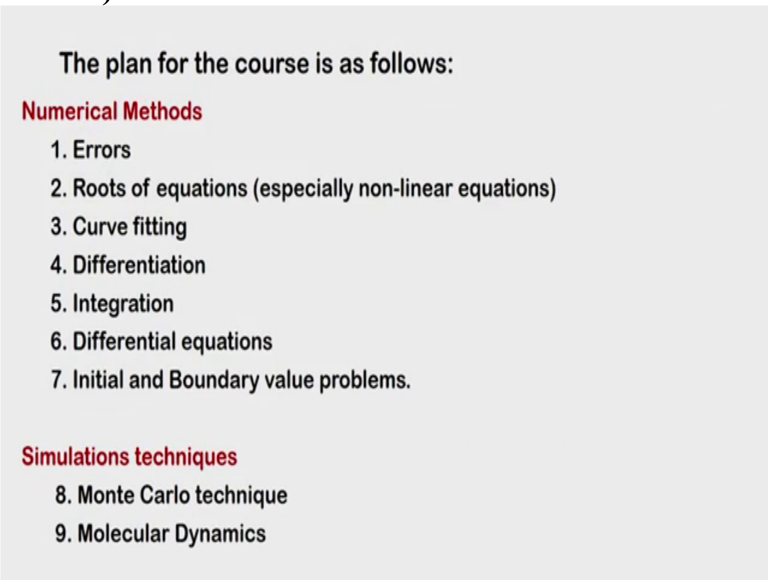

We will talk about the errors in a while, but let us look at the plan for the course. So, the plan for the course is roughly or other will follow this by and large, which will be all backed up by examples, which are from the science and engineering fields as the name suggests, that this should be for both science and engineering fields, some of these things are better to understand and visualize in various science problems, that one is actually exposed to right from school level onwards.

So there could be a more you know, component or more focus on the scientific problems rather than the engineering problem, but nevertheless, we try to address both. So, we have exactly like two distinct sub headings of this course, one is called as a numerical methods, this involves errors, it involves the roots of equations, especially the non linear equations, and will learn methods how to handle the non linear equations.

And before we actually say, all these things, it is important for us to understand that each of these methods will be backed up by their corresponding error calculations. So it is important that we have these, methods very clear, and each method will come with its own error calculation, then, we will talk about curve fitting, and how to actually make sense of a result and aid it visually that how a particular function behaves as it is dependent parameters.

And there, because they are numerical data, they could be scattered about certain, you know, a variation. And it is important for us to know that what the variation is, because in some cases in physics, or even otherwise, you would like to know that what is the variation of a function for its dependent parameter say X, X going to 0 or x going to infinity or x going to 1 and so on. So, there are these golf fitting will tell you what is the nature of the function, what is the you know, polynomial fit best polynomial fit, or, any kind of fit that is available for this function.

Then we will talk about differentiation, numerical differentiation, it is an important part, the thing is that that differentiation or derivative is liable to have a lot of errors, while knowing that there are situations in which we cannot just do without learning derivatives or differentiation, because differentiation actually, if you recall the definition that you have learned in school, that is divided by age and the limit is tending to 0.

So, you are actually dividing quantity by a very small quantity and hence the there could be serious errors which are associated with this. So, we have to understand and learn what are the different methods of you know derivatives that are used, then of course, we do integration and this is one of the most common things that is done in numerical methods, if you want to find out the area under the curve or if you want to know the you know the distance travelled in case of a non uniform motion or even a uniform motion by particle or by a body by system and so on.

So, we need integration techniques, differentiation, differential equations, will look at differential equations and how to solve differential equations in an iterative manner. And then we will talk about the initial and boundary value problems, this is again a very important part of this numerical methods, because a large number of problems are actually subject to certain initial and boundary values and these are needed for us in large number of situations such as say wave propagation in a media or say heat transport in a certain metal or in a certain material or across a junction of materials.

So, you need to solve for the heat conduction equation and subject to the you know, the boundary conditions or the even sometimes the initial conditions are needed for finding out x as a function of d that is distance as a function of time among the simulation techniques will only touch upon two of them Monte Carlo technique, it is a very important technique, which is used it is initially used for doing integration.

But will use that and actually learn that how one can simulate a system and on based on this technique, and will also learn molecular dynamics, which is solution of Newton's equations subject to you know, the initial conditions and so.

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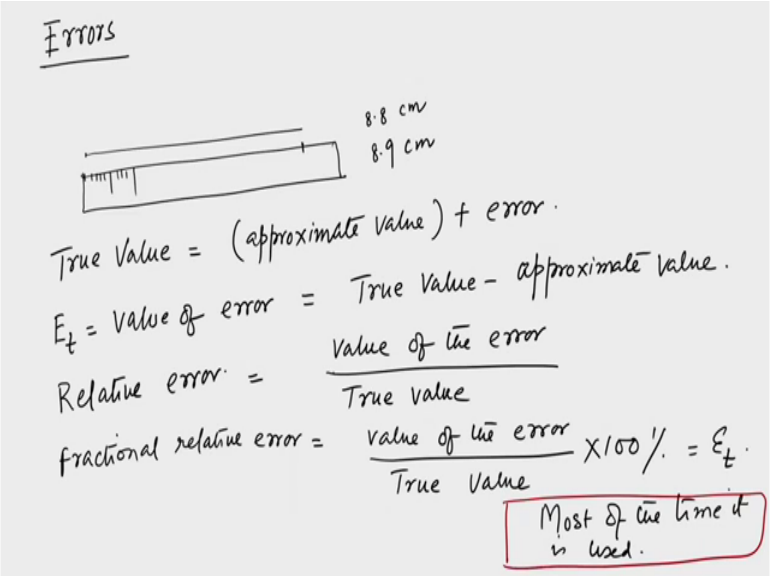

So, having said that, let us try to you knowing, sort of giving you an idea of errors. So, how errors actually arise, okay, if you are trying to measure a line, okay, with a scale growing very approximately what you can understand that this is a scale with you know, with all these markings that you have, and so on. Then, this one comes the end of the scale, say, suppose you actually, you know, align it with the 0 of this scale.

And it comes to around a between say 8.8 centimetre and 8.9 centimetres, and then you have no way to say that it is closer to 8.8 or it is closer to 8.9. So, there are what I am trying to get at is that every system comes with or every measuring device comes with a least count and you cannot do anything better than the least count this has a least count of .1 centimetre. So, for example, you could have better scales with you know, larger accuracy and so on.

Of course, meter scale is not the way you if you want to actually find out the thickness of a air strand. And so, there are screw games is and there are other things which are there, but the thing is that that it is always impeded by the least count of the apparatus, you cannot do anything better than that you can some student can say it is 8.8 some students can say it is 8.9, but that is what it is one has to accept that what is the mean what is it the this line is closes to whether it is 8.8 or 8.9, subject to some parallax error and so on.

So, there are these errors that are always there. And mostly we are interested or rather we talk about the errors that come out because of rounding off of decimal places. So, what we mean by rounding off is that every measuring devices I said including a computer has limitations of how many signal difficult digits you can calculate with the aid of it anything more than that is not possible anything with larger accuracy or higher accuracy with that kind of measuring device is not possible.

So, we if you leave the if you take only up to the significant digits and leave out the non significant ones, these non significant ones actually can come out in sort of you know, they can get snowballed or other they can get added up as we go across the various stages of these iterative stages of these computation, and they can become very significant. So that is one kind of error. And we will mostly talk about a round of error in various situations.

So, just general definition is that true value is equal to an approximate value + error okay. So, let us call this value of error Et equal to the value of error which is equal to the true value - the approximate value okay. So, this is quite simple that we have the error is simply the true value, which we may know which we may not know, but we of course, know the approximate when value the true value is only known when we have an analytic solution, and we can actually solve it exactly so, a true value means and exact value of this and an approximate value.

So, mostly when we talk about these round of error and things like that, we it is assumed that we know the exact value by some other means, okay, by probably a much better method, which leaves out some of these are rather overcome some of these approximations that have been used in this particular method. So, another quantity that is often use this call as a relative error, which is equal to the value of the error and divided by the true divided by the true value.

And a more frequently, what is used is that it is called as a fractional relative error. Let us call it SPT. Okay, so this is, you know, most of the time this is used. Okay, so we will see some example for calculating error and how that actually affects our results will start with a problem, which is essentially problem of civil engineering. And then we will of course, as we go along the way we show for each method or for all those numerical techniques that we have described how each method is subject to error due to round off or otherwise, and we will discuss all that.

So, through this example, let us show generic you know problem of errors or how you know the significant digits make a difference.

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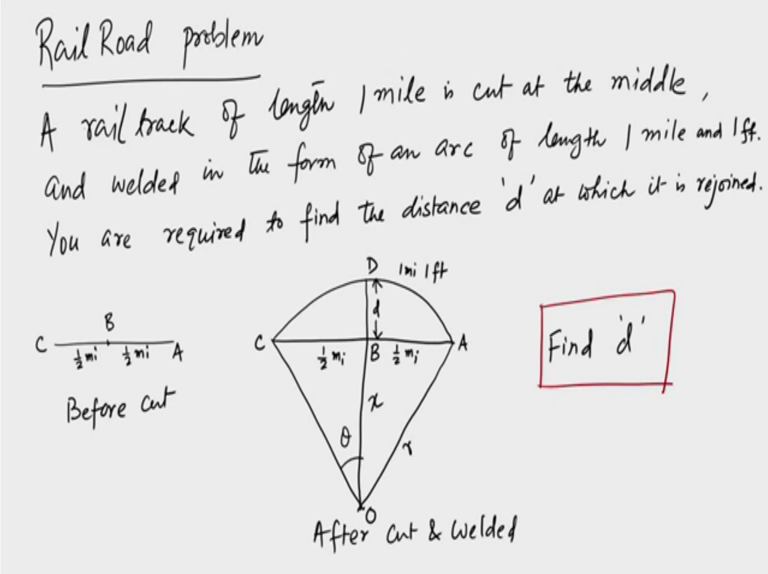

Let us name this as the railroad problem really road or a crack whatever problem. So, let us give a statement of this problem rail track of length 1 mile, so, this is in older units, but does not matter the unit is not important here is cut at the middle and welded in the form of an arc of length 1 mile and 1 foot one you are required to find the distance d at which it is rejoined. Okay, so, what it means is the following, so, there was this track which was initially you know, like this, and then it was picked like this and it is bent, and we put all these things w have been drawn need figure.

So, all right. So, this is, so, this becomes, this is the rail track to before so, this is the midpoint of the rail track. So, before it is been cut so, this is after cut and welded. Alright, so this is one mile. So this is like half mile, let us write it with small MI for a mile. So, it is a half mile, so this is like half mile. And this is like half mile. And so this is let us call this as O, that is the point and this point, let us call it as d. So, this distance is d, which is one has to find that how far away from the track that it has been joined.

And this is of course, these are arc as length of 1 mile and 1 foot okay and let this be r, let this angle be Theta and so on. So, this is a situation and let this length be x and this let us call this as C and this is A and so, this is that and there is a B here. So let us just write it as A B and C. So ABC is the rail track, which has now become ABC and we like to find the okay. So, so, the question is find d okay.

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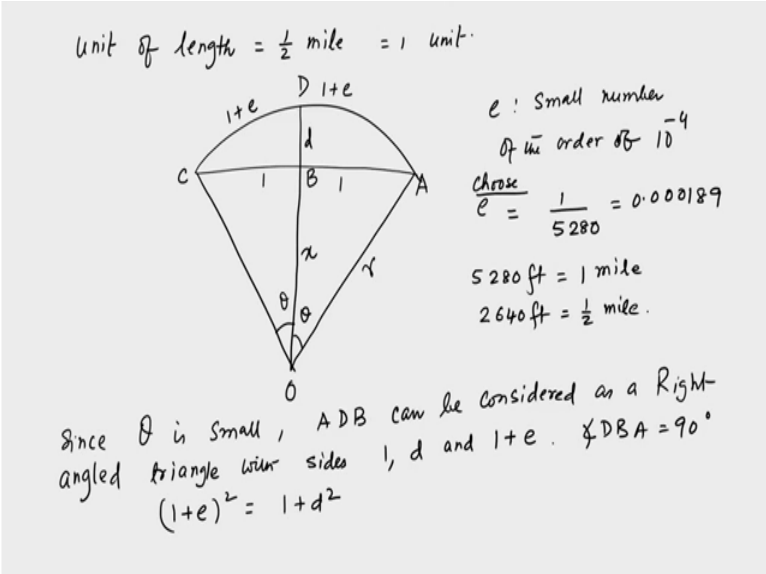

So, if that is the case, let us take the unit of length as unit of length for our case equal to half mile and the figure can be redrawn as the same figure is as we have drawn earlier, it is redrawn like this just ignore these protrusion that are at the end and so, there is a theta there is 1 and 1 and there is a d there is a C there is A and then there is a so because this half mile is taken as equal to 1 unit okay.

So, this is a 1+e that is the one side the other side is also 1+e where he is a small number and this is of course x this is of course d. So, x is as we have said, x is this distance and so on. And so x and d and this is 1+e and this is also 1+e where he is a small number maybe of the order of 10 to the power -4 so we do not have an idea of the magnitude, but one can choose e to be so we will just say that we choose e to be like 1 divided by 5280 which is equal to a .000189 where 5280 feet is equal to 1 mile.

Okay, so that is the conversion so it is so if you need half a mile then this is equal to 2640 feet which is equal to half mile. So, either ease of this or it is twice of this because is the unit is taken as half miles anyway does not matter for us as much. So this is my r and this is where the problem starts. So we have just reduce the problem a little bit where the miles have been taken into a half and so on there is a B and there is O there so of course since Theta since Theta is small, because it is only 1 mile + 1 foot.

So Theta must be small, so ADB can be considered as a right angle triangle with sides as 1 d and 1+e okay. So, of course, the right angle is at DBA is equal to 90 degree, so that we have the hypotenuse being formed by 1+e. So, if that is true, then 1+e squared that is equal to 1+d squared

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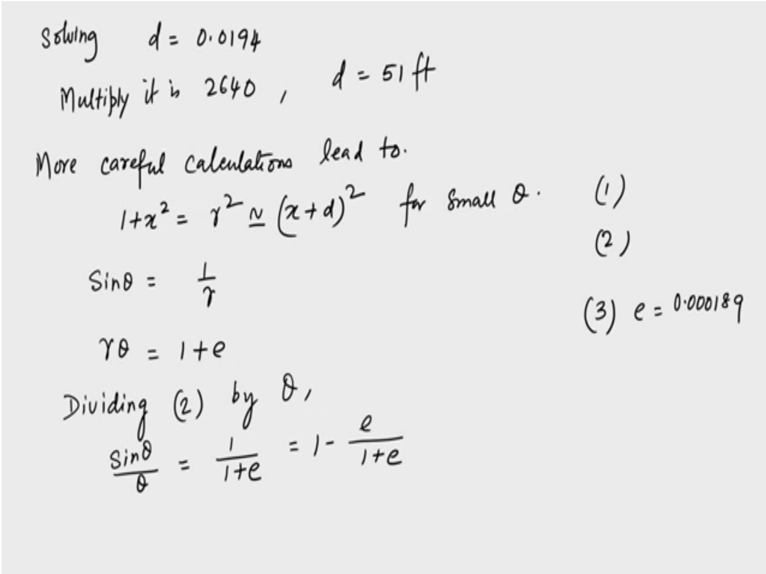

If you solve with the value of e that we have chosen, solving d comes out to be .0194. And multiplying it by half mile, which is 2640 feet, we get be equal to so d equal to 51 feet. So from this it is clear that if you have to make this part this at the middle and weld it and join it like an ark, it has to be done at a distance of 51 feet. But if you look at it a little more carefully, so more careful calculations lead to if you refer to the finger, then it is 1 + x square equal to r square.

Remember that this is one and this is x so the right angle is that ABO so it is 1 + x squared equals r squared. And which is nothing but equal to so r squared is nothing but equal to x + d the whole squared because the angle Theta is small so r and x + d are nearly same. So we can put this is of course for small theta. Now if you look at it, sin theta becomes equal to 1 over r so let us call this as this as equation one sig theta as 1 over r because this is 1 that is the right I mean the perpendicular by the hypotenuse that 1 over r and then it is r theta equal to 1+e now we are taking into account that r theta an arc which is 1 over e.

And as we have said that e equal to .000189 and so on. See if you divide 2 by theta so sig Theta over Theta. It is equal to 1 by 1 + e, which is equal to 1 - e divided by 1 + e. So that is my equation. Say, so that is that is comes from equation 2 when we divide by Theta so we have divided by Theta and Theta equal to 1 by 1+e divided by r so that our cancels and you have this for now.

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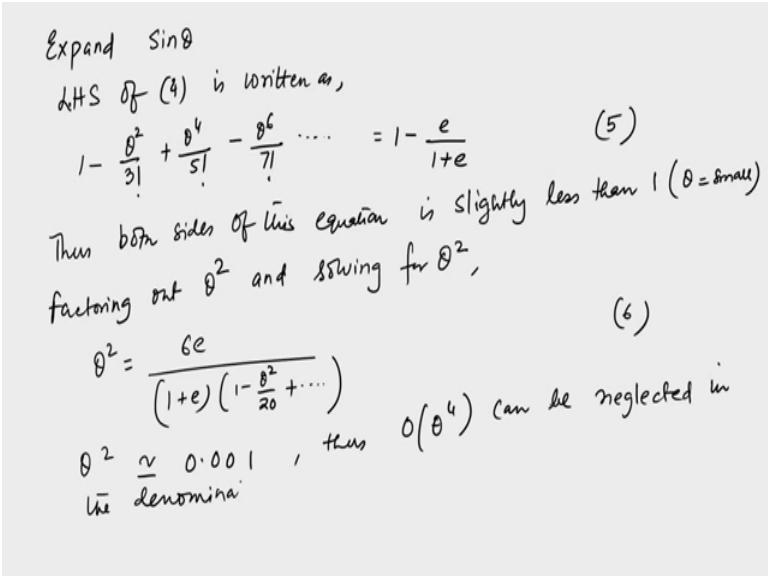

One needs to now expand sin theta. So that is equal to, so LHS of 4 we have not named it but let us name it as 4, so LHS of 4 is written as 1 - theta square by 3 because it is Theta – Theta Q by 3 factorial plus Theta 5 by that is the expansion of time sin theta 5 by 5 factorial. Now one Theta goes away from everything, so theta 4 by 5 factorial - Theta 6 by 7 factorial, etc, this is equal to 1 – 6 divided by 1 + e, let us call this as equation 5.

So basically, does both sides of this equation is slightly less than 1 again, because theta is small ok. So, the leading term is of course 1 and these are of the order of the leading order is of the theta square and all that and now what we can do is that we can factor out theta from these things, the 1 anyway cancels out and we can factor out Theta and can solve for, so let us just write factoring out theta square and solving for Theta square.

So Theta squared is equal to 6e divided by 1+e, 1 - Theta square by 20, plus and all that. So that is the value of Theta squared, which is coming out from here. So of course, this is equation 6 and Theta square is of the order of maybe .001 this one can actually theta 4 can be neglected in the denominator. That is why we have written it only one term.

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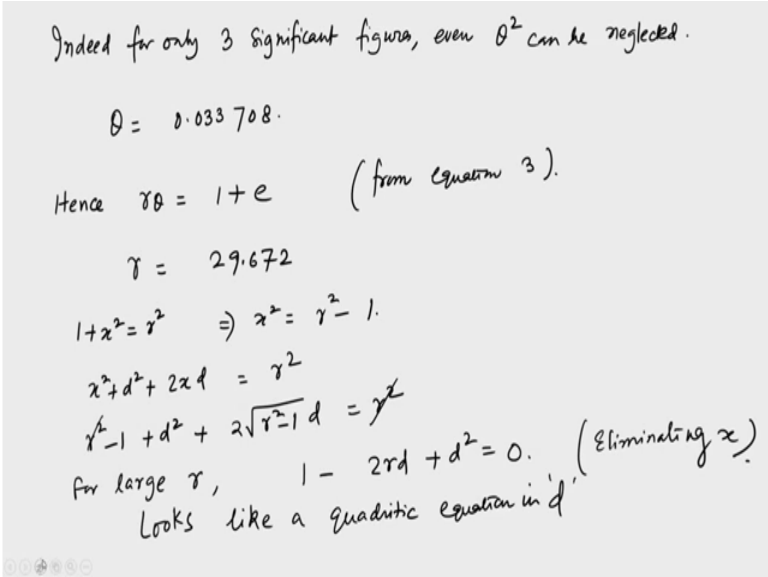

So, indeed, for only 3 significant figures, as we have been saying before that the significant figures are important. I mean, even theta square can be neglected in front of theta. So solving for theta it comes out as .033708 Okay. So, hence r theta equal to 1+e which we have already written here as equation 3, this is from equation 3. Now r with this value of theta r comes out to be 29.672, e we have already quoted. So this is r equal to this. And now we can actually get a quadratic equation for be using this e.

So how we can get this is that we have 1 + x squared equals to r square. So that gives that x square is less than r square -1. And we have actually x squared + d squared + 2xd, which is x + d whole square, that is equal to r squared that is there in this equation, equation 1. So if you use this, and you can put now here to put x squared equals to r squared -1, so we have r squared -1 + d squared + 2 into r squared -1 into d equal to r square. So, this will have you know the r square will cancel and for large r one gets 1 – 2rd + d squared equal to 0.

And other way of looking at it is that we are eliminating x. So it looks like a quadratic equation in d which is of course, solution will give us the answer. But if you look at it carefully, it is actually a linear equation with the quadratic perturbation. So it is, this is the last term is the perturbation.

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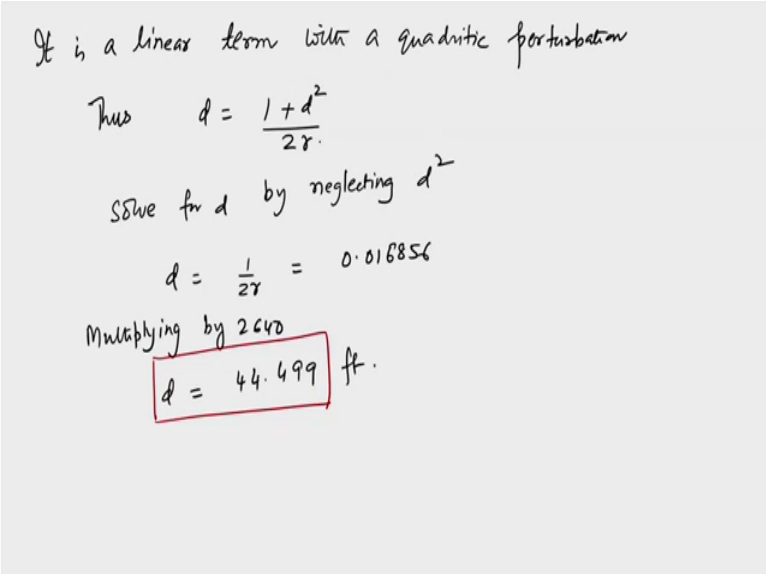

And so, we can write this as quadratic perturbation. So, that is if we take this then d equal to 1 + d square by 2r and if you all for d by neglecting d square So, d becomes equal to 1 over 2r and putting the value of r, d becomes .016856 these are the numbers that you should check and it because to get it into the units that we want in mile or feet multiplying by 2640, d becomes equal to 44.499 feet. Now, this is 44.499, almost 44.5 feet and the earlier answer that we got was 51 feet as we as we saw it here.

So, one method gives you 51 feet, the other method of course, gives you a much lower value which is 44.5 feet. So, this is certainly not an ignorable discrepancy, that you actually want to think if you think of that if a civil engineer is actually doing this 44.5 feet versus a 51 feet would make a lot of difference. So, he has to take a call that that whether he should do a sort of more you know measurement that is based on the first method which is just taking that arc to be a straight line and using Pythagoras theorem in a right angle triangle.

Or a more involved analysis, which also nevertheless has some approximations made such as we have made approximations I just theta is more and d is also small compared to the unit of length, which is half mile and various things. So, basically, your r came out to be around this value, one can multiply it and get a value in a feet that is much larger than d. So, we have actually neglected the square and treated this equation and have gotten a value which is 44.5 nearly 44.5 feet.

So, this is the difference in numeric computation. So an algorithm is very important the correct algorithm would give you get you values which are much closer and if you choose a much simpler algorithm, which is more inaccurate, then the chances that one gets values which are far away from the actual value that is that is going to be there. So it just an example how in such a simple problem. Looking at the problems in two different fashions would give you such wildly different results.