Computational Science in Engineering
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Lecture - 25

Okay, so let us continue our discussion. Now we have so far, I mean, we have done discussion on starting with linear algebra and then we have looked at ODE and differential equation and meanwhile, we have quickly touched upon some of the fundamentals of Fourier analysis and Fourier transform and Laplace transform.

So that these are I mean, we did not do quite a bit of details discussion, the reason being the Fourier or Laplace are quiet, I mean these are, I mean standard methodology that transformation and all these and which are I mean essentially available in any of the textbook or any mathematical textbook or higher level mathematical textbook.

Now then we have discussed on PDEs where we have also kind of looked at lot of theorems and their inequalities, their existence, uniqueness, and finally we closed down the discussion with some sort of an example how to actually handle them with the different kind of approach, that we have discussed.

Now with that actually, now we will move to the discussion on the numerical analysis part, where now we will look at different aspect of the numerical methods and especially how to solve these ordinary differential equations and linear systems. But, before doing that, we would discuss some of the things like polynomial equations and root findings, because that may help. And then, we will move to the other discussion.

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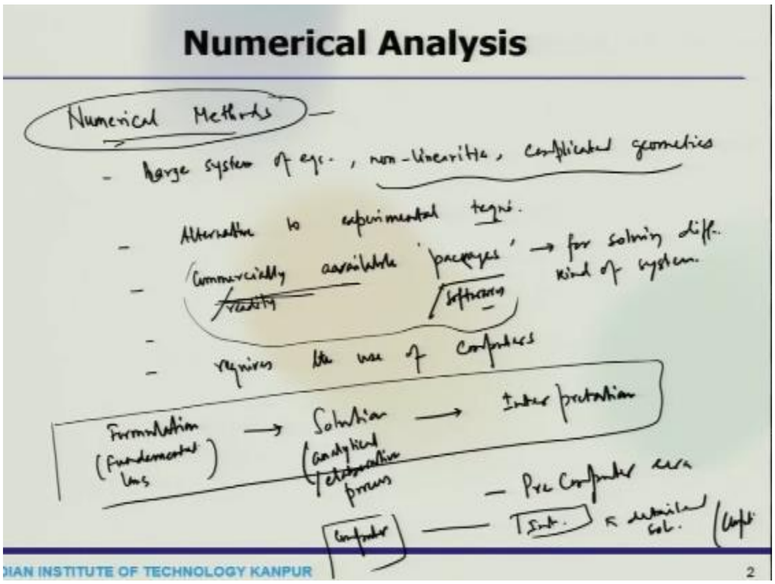

So let us start with the discussion on what you call the numerical analysis, which is sort of an what, so this or rather you can say the numerical methods. So, these numerical methods, which are sort of an they are very powerful problem-solving tool. I mean obviously, so they are capable of handling large system of equation. So also, nonlinearities, complicated geometries.

So, which are quiet, these are the things which are quite common in any of the engineering applications or engineering practice. And these systems are not very easy or often one can solve analytically. So, you need to have some sort of numerical methods. So, this also sort of an alternative to the experimental technique.

Because, what happens when you have this complicated system and such kind of situation, it is not that easy that sometimes you can carry out the experimental measurements or look at the detailed system. So, this way this can complement that thing. Then obviously, in your career actually, if you are pursuing these things, you might have seen there are commercially available packages for solution for solving different kind of system.

Like whether it is a problem related to fluid mechanics or problem related to solid mechanics or problem related to microscale phenomena, there are different things and there are different packages which are available. Some of them are commercially available, some of them are sort of an open source, so one can use it.

But often what happens is that, I mean while using these kinds of available, readily available packages, it may lead to some sort of a problem. The reason is that, these readily available packages also use some sort of a fundamental baseline methods which are associated with that. So, knowing that would always help to use these readily commercially or one can say readily available packages or codes or software whatever you call it.

So, this would always help so that one, so the point here is that one should essentially know the backbone of these different package software so that one has to know the fundamentals of the numerical methods. So also, this numerical any numerical method to lead to a certain solution, it requires the use of computers, so that we can actually do the programming and finally, get out the solution.

So, and other way one can say that numerical methods provide sort of a vehicle for you to reinforce your understanding of mathematics. So, one function of numerical method is to reduce higher mathematics to basic arithmetic operation. So, they get a nuts and bolts of some this. Now when you talk about this, like you have kind of an to lead to a system.

So, you can have a formulation, which is essentially the fundamental laws. Then this would give you a solution, which is elaborate and often complicated method too. And then finally, one has to interpretation or interpret the results. So, this was what one has to get these things, I mean this process. This is where the solution is pretty much, this used to be analytical or kind of an elaborate process.

And this used to happen when you have the pre-computer era. Now due to this computer era, the thing is that you still have the same basic fundamentals building blocks are same, like formulation remains there. But what happens to the solution process? So here in the computer era one uses the computer to solve the problem.

And then finally, obviously in the interpretation, now you have access to the detailed solution so that one can look more carefully or in depth analysis of the system. So that this is what you do in the computer era. So, you can see how things actually evolve in the.

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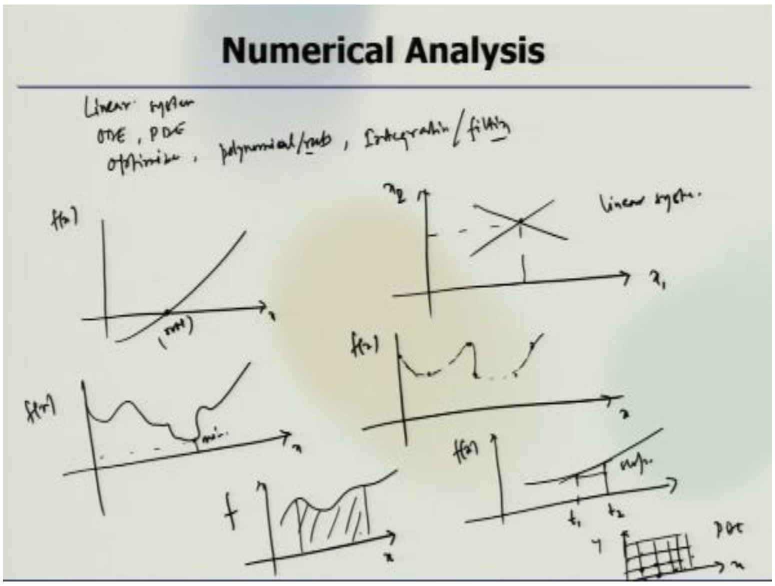

And when we say the numerical methods required the mathematical background, so that one has to understand solving of the linear system, then ODE, PDE, sometimes you need to optimize your system, then polynomials or roots. So, these are things and sometimes also one can look at integration or fitting, curve fitting something like that. So, these are the things one can look at like that.

So, for example, let us say you have a function x, which is going in x, and it is going like that. So that is one of the roots. So, this is where finding root becomes important. Let us say you have two variables going in two different directions and they will go like this. So, this is the solution. So, this is linear system. Or sometimes you have a function which is going in this direction, and the function goes like this.

So, you can find out the minimum bond. So, this is sort of an optimization. Or you can have a function and you have some sequential point like this, then the best curve fitting would be the one of the things that one can look at that. Or sometimes you have let us say function which is like this, so you can find the area under that curve. So that would get to the integration.

Then you have, so all these are basically kind of now you have an ordinary differential equation where you could get the slope. So that is the slope. So, you can find out the solution, let us say t_1, t_2 and you solve this. Or I mean the final situation where you can have a system like x and y, where you can solve these queries at different points. So, this is also possible. So, all these things that what we look at it here, so that is going to be the part of the numerical methods.

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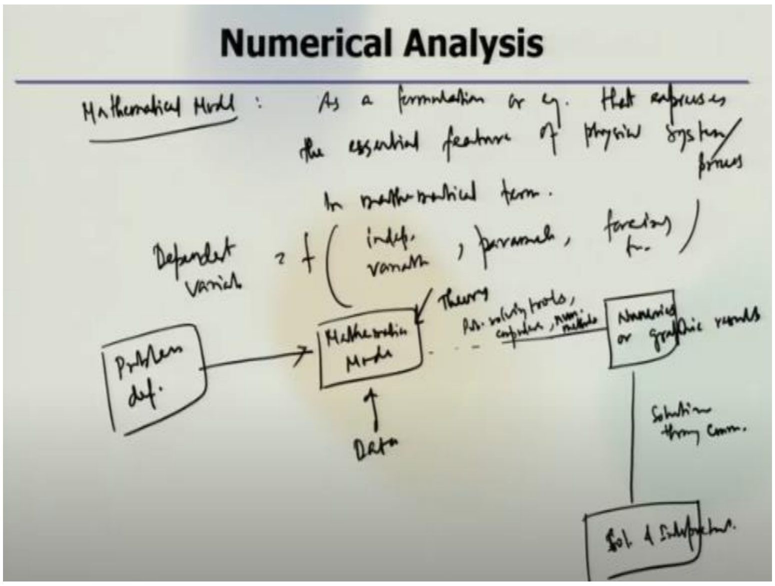

So, what we can say that any mathematical model, so this can be defined as a formulation or equation. So, this is an explicit essential feature of the physical system. So, where it is like a mathematical model can be broadly defined as a formulation or equation that expresses the essential features of physical system or process in mathematical term.

So, one can say that there could be some dependent variable, which are function of some independent variable, parameter space forcing function. So, what one has to do like if you have a let us say, problem definition, then your next building block is the mathematical model. So, where your data goes as input. Also, this is from physical definition to comes to mathematical model. Also, your theory comes into the picture.

And then with this, you go to the Numeric. Numeric or graphical results or graphic results. Now so here you will have problem solving tools. You need computers, you need numerical methods, etc. So, all these will fit to that. And finally, what you get is the, so here you do the solution through interface communication through communication. And then finally, you get the solution and interpretation. So, these are the building block where you can actually solve like that.

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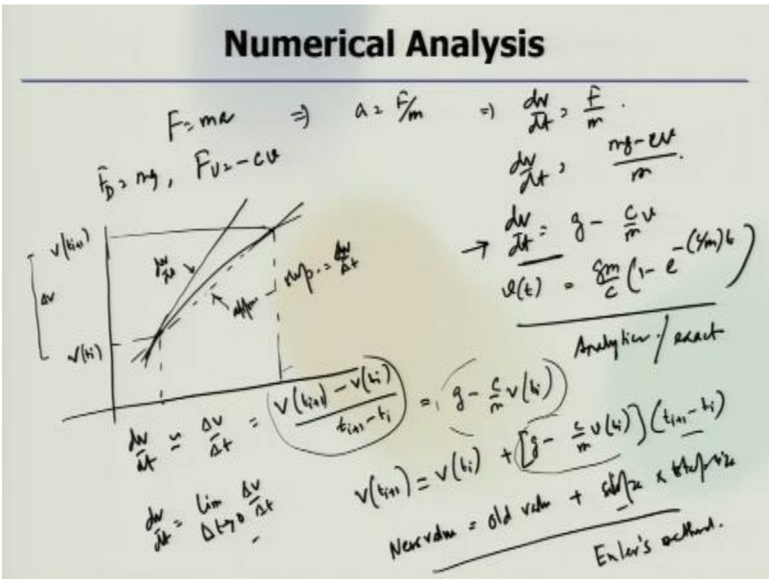

So, for example, I mean the simple way to look at like, you have Newton's law of motion which is F = ma. Now where a is defined as $\frac{F}{m}$ which is acceleration. Now we can write

$$\frac{dv}{dt} = \frac{F}{m}$$

Now the forces could be, let us say weight or upward forces. So let us say we take the drag is mg. There is another upward force which could be constant into v, proportional to v.

So, this

$$\frac{dv}{dt} = \frac{mg - cv}{m}$$

So, once you simplify this, what we can write

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

Now one can solve this and get an expression that

$$v(t) = \frac{gm}{c}\left(1 - e^{-\left(\frac{c}{m}\right)t}\right)$$

So that is a purely analytical approach what one can solve. So, this is what one can look at it.

Now at the same time, so this is either analytical solution, or one can say it is an exact solution, which you can get. Now when you use the same expression or the equations here like this, we can solve it numerically. And once you do that numerically, you need to basically do some sort of an, so let us say, if you look at that plot, so this is how it is probably going to go.

So, this is the starting point where $v(t_i)$ and it reaches a point where like this, let us say $v(t_{i+1})$. And this is the difference between that Δv. So, one way to look at this straight situation and this is what and there would be kind of a tangent. So, this is the slope of the curve which is dv/dt. And this guy could be the, this is the approximate slope.

And what do you can write that

$$\frac{dv}{dt} = \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} = g - \frac{c}{m} v(t_i)$$

So, there is a time difference. So, Δv and Δt is the differential velocity. So, what one can say this is when the limit

$$\frac{dv}{dt} = \lim_{\Delta t \to 0} \frac{\Delta v}{\Delta t}$$

Now we use some sort of a finite divided difference, so this is nothing but

$$\frac{dv}{dt} = g - \frac{c}{m} v(t_i)$$

Now this can be rearranged and one can write

$$v(t_{i+1}) = v(t_i) + \left[g - \frac{c}{m} v(t_i)\right] (t_{i+1} - t_i)$$

So, t_{i+1} is the new time level where from here when you move to there, so this is an approximate. So essentially one can see that new value is the old value plus slope into step size. So that is the step size into slope. So that is what it is.

Because, when you look at that, this is the approximate slope which is nothing but dv by rather delta v by delta t which is this guy or rather this expression. So, this one is the slope, approximated slope into this. So, this is how you can find. So, this is typically or formally known as the Euler's method, okay. So, this is how one can approximate and get the solution to the system.

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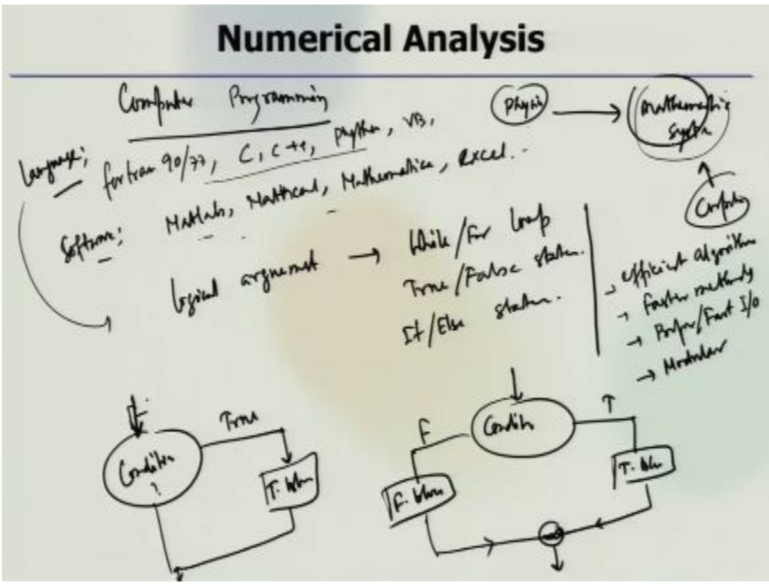

Now when you do that another important thing, which will come into the system is the programming or computer programming. So now for doing that, so you have a physical problem. Now you have approximated that thing like this. Now this expression is nothing but a mathematical expression. So, your physical problem, where is your physical system now goes to a mathematical system or equation.

Now this mathematical system one has to solve. So now here you are actually using the computer to solve it. Now computer means you need to do programming. So, one can use different kind of programming language. Also, some packages like one can use Fortran. So, which could be 90 or 77 whatever it is. C, C++, Python or Visual Basic, Visual C++ whatever.

Or one can use some of the software packages which will also allow some like MATLAB, MATHCAD, Mathematica, sometimes Excel. So, these are different packages what one can use to so, but essentially what you need to do that you need to actually transform this system of equation or the mathematical expression and so when you do the programming that time you can have a lot of logical argument that you need to put in like a while or for loop.

Sometime true, false statement. Sometime if, else statement. So, these are the building blocks. Like for example, let us say I have an input. And then there is a condition. So, this condition could be anything. Now if this is true, then it goes to some true block or if it is not then it comes to like this, okay. Or sometimes one can look at this okay they are my condition; this is the input.

So, if it is true it comes to true block, it comes here or it is false it comes to false block. That means do some operation, come here. And then finally it gives the output. So, this is, this kind of logical statement that one has to put in place and there could be multiple of like this. I mean one block, multiple blocks and depending on that what you are trying to do. So, you can actually put in.

And now these things if someone tries to do through his own programming like using some programming language then that is okay or one can also fit this kind of. But anyway, even then, if you use a software like MATLAB or MATHCAD or something like that, so you need to feed the information to the software.

So now this programming also could be multiple layered like not only the logical argument also one can have very efficient algorithm like reducing number of these kind of technique. Then there could be faster methods. Then proper or fast input, output. That means data read data writing system. Then it could be also modular.

So, this could be also modular in the sense that one writes in a like different blocks and then the blocks are kind of finally put together to get a single main programming code. So that is there. Now while do all this, so that means, one thing is understandable that when you have a physical problem.

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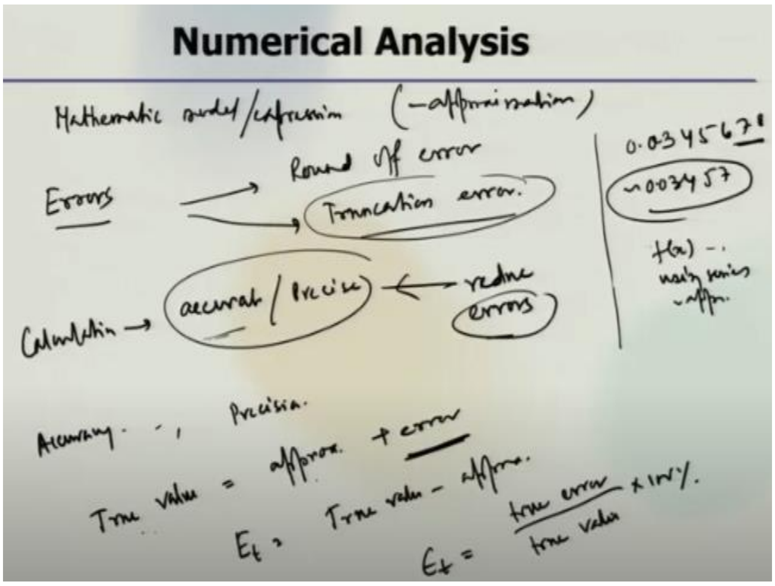

Now the physical problem you go to some sort of a mathematical system and where you do the approximation. Now when you do the approximation, then that time obviously, you have this getting that mathematical model or expression you are already doing some sort of an approximation like we have seen that simple example. Now when you do that, now there are things which are going to be important like in this error.

So, in the numerical analysis, there are two kind of errors what one can actually encounter. One could be round off error, that is one error or other way it could be truncation error. Now these are two different kinds of errors. Round off errors one can understand that whenever we have for example, you have a number like 0.0345678 like that and you can always round it up 0.03457 like that.

So, but now you are eliminating the last few digits. So, these kinds of things and when you do series of arithmetic operations or and then at the end this may lead to some sort of a huge error. And some precise calculations, because again the calculation what you do, this has to be accurate and precise. Now once you try to do that, achieve that, so you have to reduce all sort of errors.

So, rounding error can lead to a huge problem when you try to get very accurate and precise solution. Now then another thing which could be truncation error. Truncation error, like whenever we have some sort of a polynomial function, then we use some sort of an, using some series we try to approximate. So, in that approximation, we are leaving out some of the term, which could lead to some sort of a truncation error.

So, we will see how when we do this kind of system, we will deal with the systems and what kind of error it will lead to. Now when you say accuracy or accuracy of the solution, accuracy refers to how closely the computed, closely a computed or measured value exists with the true value. Or the other one is the precision. Now precision refers to how closely individual computed or measured values agree with each other.

So that is a precision. So, you have accuracy, you have error. Now when you talk about any true value, so there could be approximation plus error. So now you can see if this term goes to 0 so the true approximation would be close to the true value. So now if I write like the error, so this could be true value minus approximation. So, one can have the relative error which is ϵ_t, which is

$$\epsilon_t = \frac{true\ error}{true\ value} \times 100\%$$

Now true error could be what is the error you are getting.

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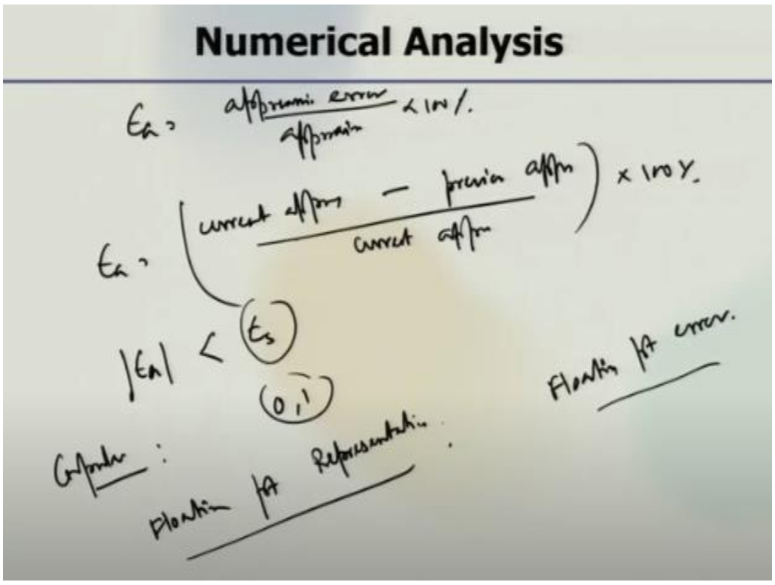

Now there is another one which could be there, approximation error, which is like

$$\epsilon_t = \frac{approximate\ error}{approximation} \times 100\%$$

So that could be another percentage of the error which can be lead to that. So, one of the challenges of numerical method is to determine error which estimates in the absence of knowledge regarding the true value. For example, certain methods are iterative methods.

So, you keep on doing iterative so you do not have the exact value to see what is the true error. So that time we use percentage relative error, which is like this current approximation minus previous approximation divided by current approximation. So, we look at that in the relative sense, what is the rate of the error and what that is and we can always define that, that is always less than certain small number.

So, this is a small number which could be user defined. Now then another thing which will come is that in computer things are in binary digit like in computer things are in zero and 1. So that is where the round of error comes into the place because computer actually feeds the things in that everything in that digit bit mode, where every number is stored there, and when you try to do.

Now these are coming then there could be other things when you are doing floating point representation. So that time some errors may occur. So that could be the floating-point error. And now these days whenever do really floating point calculation, so actually people call it how many floating point operations the computers can do.

So, the kind of the advancement or the architecture of the computer is so high and that it can do huge level of floating point calculations so that your computer architecture is powerful to give you the number of floating point calculations. So, these are the things which will also I mean these are the just the some of the kind of issue which will come.

And just to see what the error comes in and like and those errors which are going to propagate and like that. So, the other thing which we will quickly look at that the truncation error when we do the expansion, actually of the Taylor series, then how that error appear. But otherwise, the round off error and all this would form and then we do the relative error. So, we look at that truncation error and all these in the next session.