Advanced Numerical Analysis
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Lecture – 49
Methods for Solving System of Differential Algebraic Equations (contd.) and Concluding Remarks

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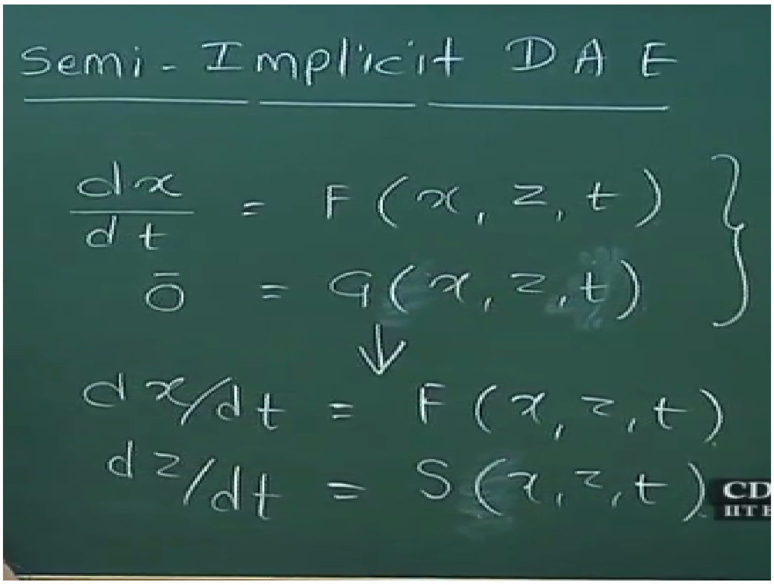

So, we have been looking at differential algebraic systems or DAEs and in my last class, I gave some examples of semi implicit DAEs, we also define what is called as index of a DAE, so we have been looking at semi implicit differential algebraic systems, so these can be written as dx / dt, so these equations are typically written by this coupled differential and algebraic system of equations.

So, this is zero vector and x, typically we call as differential variables and z, we call as algebraic variables. So, these are differential equations which have to satisfy certain algebraic constraints and not all the variables appear with their derivatives okay, very, very common situation in chemical engineering models in chemical engineering linear operations, so you have algebraic constraints which typically define the phenomena which are occurring at a very fast time scale.

Whereas, the differential equations would represent phenomena, which are at a slow time scale, so, in a distillation column for example, this would be thermodynamic equilibrium and this would represent dynamics of compositions, temperature on each tray, okay. So, we also looked at what is called as index of a semi implicit DAE, so index is minimum number of times you have to differentiate this equation to get into; okay.

Minimum number of times you have to differentiate to get into a system of pure ordinary differential equations. Now, remember this is G here and I am writing another symbol here, S, which means that when you differentiate and get a new system of equations, this would be different okay. The new system will be some function of G of course but it will be different. Now, we will look at a specific example and then understand this

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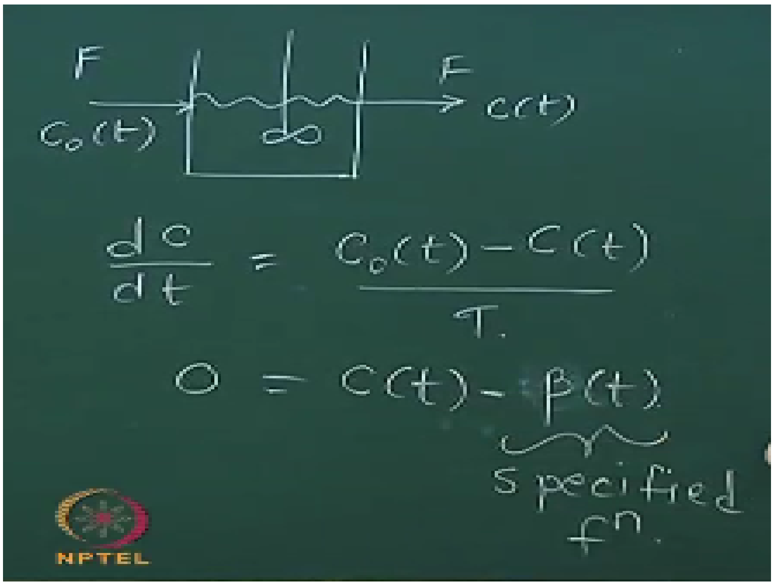

Last time, I talked about a mixing tank example, so this was a simple mixing tank okay, so this was the example that we looked at dc/dt is = C0 – Ct/ tau and C of t is specified that means beta t is unknown specified function okay, so this is my G of z and G of z and x. Now, note one thing here this equate the first equation contains both algebraic and differential variable that means, what is the differential variable here; C, okay.

Algebraic variable by; you know this is a semi implicit DAE, algebraic variable will be Co t, right, algebraic variable will be Co t, now the second equation does not contain the algebraic variable and this can be a troublesome part. The second equation does not contain the algebraic variable, you can get into difficulties while solving because Ct, the algebraic constraint is an implicit is a function of you know; is an implicit function of C0t.

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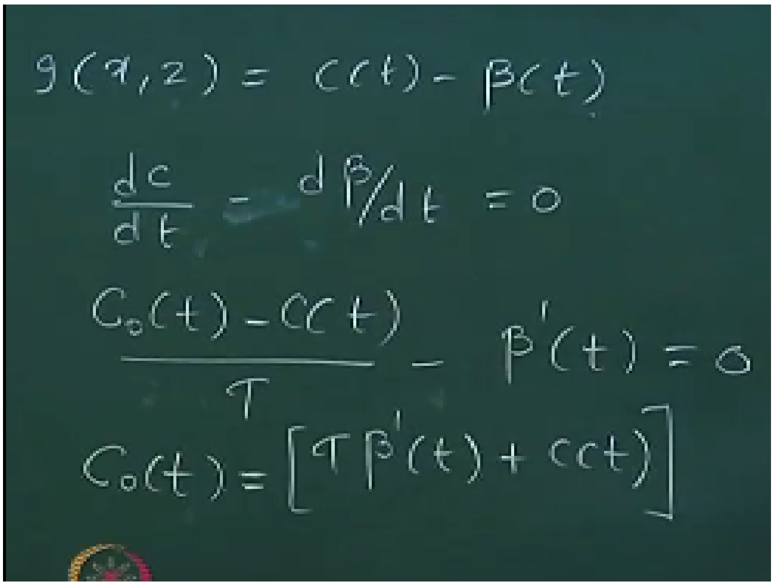

And the first derivative here with respect to Co t is not =; is = o, so it is not nonzero, so we have a problem. What is the problem I will just elaborate that, so this simple example actually turns out to be an index 2 system okay? Let us go and see why this is an index 2 system, so what is g; x, z; g, xz corresponds to Ct - beta t, right. Now, if I differentiate this; okay, if I differentiate this with respect to time, then I will get dc/ dt - d beta/ dt is = 0, okay.

But beta is a specified function, what is dc/dt? Dc/dt, if I substitute from here, I will get C0 t – ct/tau beta prime t is = 0, this is still an algebraic equation; we have not got a differential equation yet because I could substitute for dc/dt in terms of this okay. I could substitute and so I still have an algebraic equation, I want a differential equation okay. To get a differential equation, I will further differentiate this, okay.

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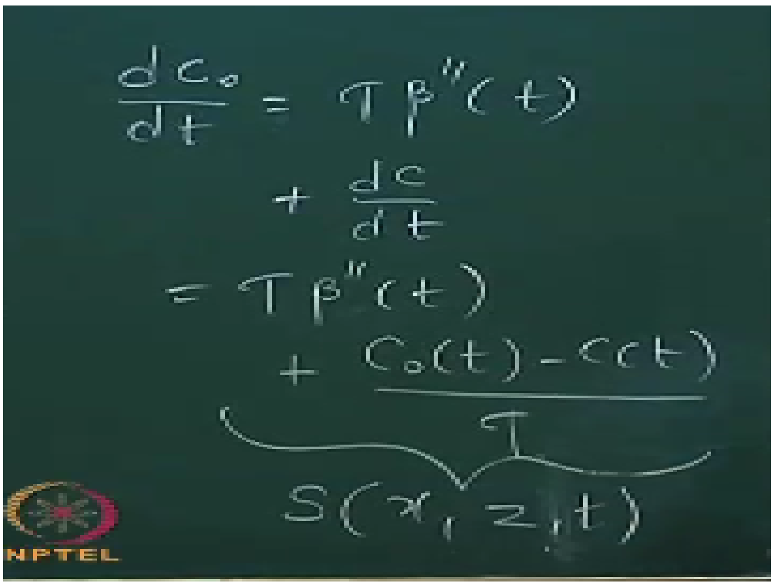

So, from this what we get is C0 t is = tau beta prime t + Ct, if I just rearrange C0 t is tau beta prime t + Ct and then I can now differentiate this. I want another differential equation, which is; now, look at this equation, I finally have eliminated algebraic constraint, I have one differential equation in C, another equation differential equation in C0 t okay. So, now this is my S of x, z, in fact S of x, z and t of time because beta double prime comes okay.

So, this is my system with index 2, I had to differentiate twice to get a set of consistent differential equations; first order differential equations. So, how will you use this index business we will come to that soon okay? Now, what is the problem, why do we have to worry about, why is it important to have index? So, let us look at this particular problem well, when you have a high index system, there are 2 difficulties.

One difficulty is that it is difficult to specify or it is tricky to specify I would say the initial condition, what you will notice is that C0 t cannot be arbitrarily specified for a pure differential equation, which is not coming from an algebraic differential equation okay, you can specify initial condition arbitrarily and see evolution in; of course, the initial condition should make sense from the physics.

But once you specify initial condition with that makes sense from the physics, you have a unique solution as long as dou F/ dou X is differentiable and so we had talked about this continuity right in the beginning about the existence of a solution, those things are not true here because of the algebraic constraint particularly for index; higher index systems, there is a problem, so there are 2 problems okay.

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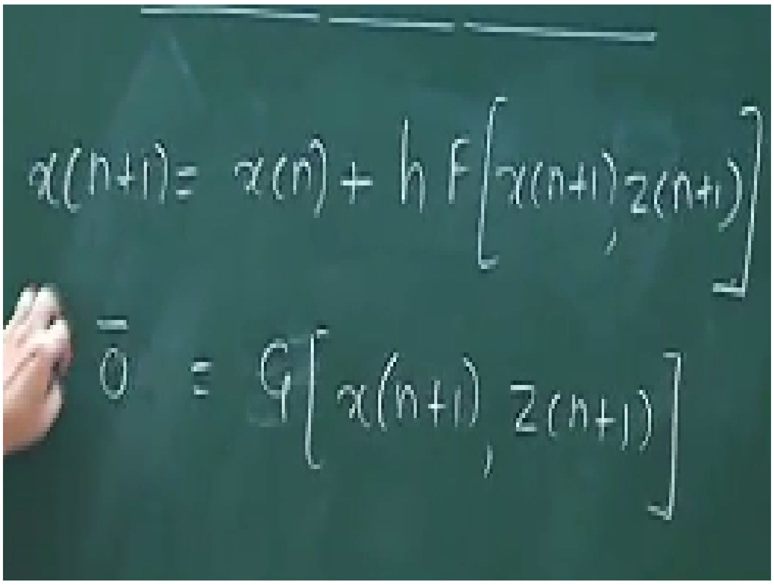

Now, let us see where this the problem come from, let us look at; let us look at solving this particular set of equations using implicit Euler. So, implicit Euler would mean that you know x n + 1 is = Fx n + 1, I am just dropping for the sake of convenience the time argument and oh sorry; this is my implicit Euler would be; this is my implicit Euler okay, this is my; I have to solve these 2 equations simultaneously.

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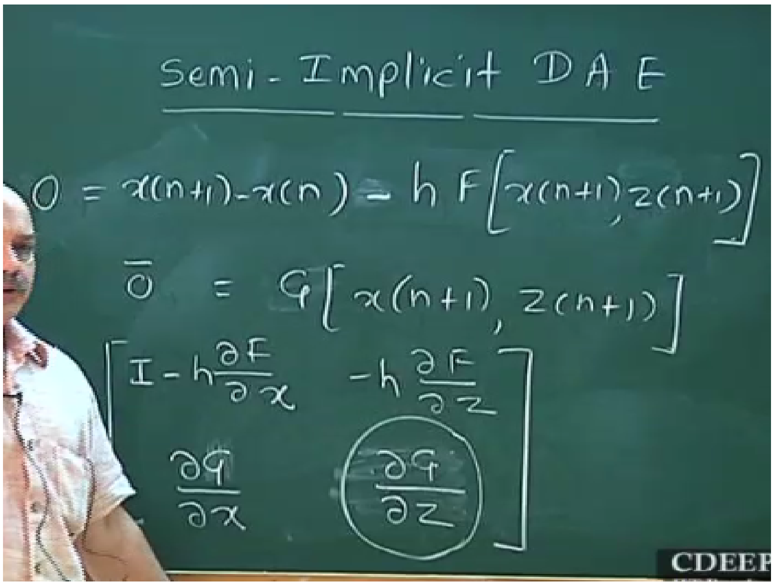

Or rearranging this; you know, you can write 0 = ; so you have to solve these 2 equations simultaneously, if it is implicit Euler and if you are solving it using Newton-Raphson for example, if you are solving it using Newton-Raphson, then you will get this matrix; Jacobian matrix. When you are trying to solve this using Newton's method, these 2-couple algebraic nonlinear equations using Newton's method, you will get this matrix.

This is Jacobian matrix that you know that you have to compute during each iteration, if we rearrange and then differentiate, you will get this okay. Now, the trouble is with this dou G /dou Z okay, if dou G/dou Z; if this is = 0 okay, then you have trouble solving this problem, when h goes to 0, for small h, okay. If this is 0, you can land up into trouble, okay, so this nice thing about index 1 systems is that dou G/dou Z is not equal to 0, okay.

We saw that flash example; in flash example, if you write algebraic constraints and if you differentiate, then you can show that dou G/dou Z is not = 0 and then you can solve that problem simultaneously and get the solution without a difficulty. In this particular case, dou G/dou Z is 0 because if you look at here; if you look here, this is G of; this is my G of x, z okay that the differential variable only appears in G of x, z, algebraic variable does not appear.

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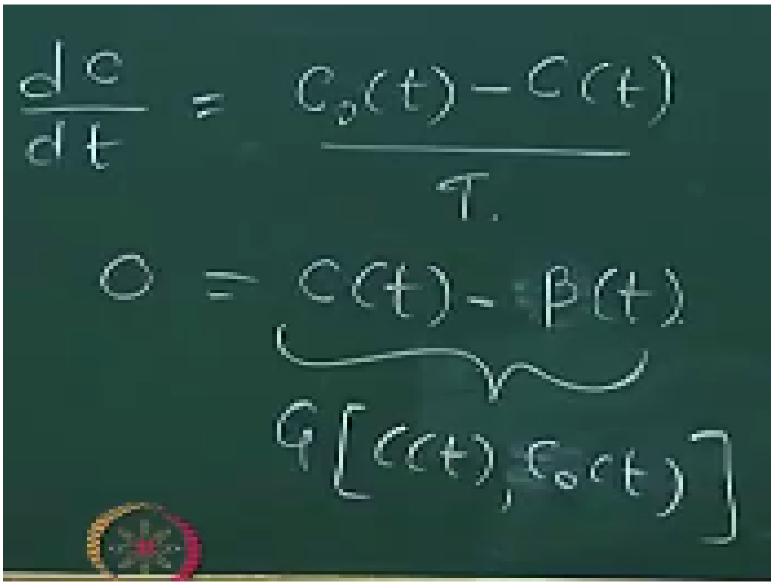

So, dou G/dou Z is = 0 okay and then because this is the high index problem okay, here this is my G of Ct, C0t and obviously C0t does not appear here, so dou G/dou Co t is 0, okay and then that is why you have a problem here okay. Now, what is very, very important is that when you have a high index system okay, this dou G/dou Z should be; when you have an index one system, dou G/dou Z is not = 0, you can solve it for high index system okay.

If you want to solve it, it becomes very, very crucial then to be able to specify the initial condition properly. If you are not going to give the initial condition properly, your solutions can diverge okay. So, I will just continue with the same example okay, yeah, **"Professor – student conversation starts"** we have to use; yeah, yeah, so the solution is when you have higher order system; high index system okay, you should actually differentiate multiple times go towards.

And then you solve simultaneously all the; I will come to that so. but now you realize there is one more thing, you should realize now, you should be able to find that thing using automatic differentiation. See, now for simple 2 variables, 3 variable thing okay, I can find the index of the system by you know; by hand differentiation, then I can say this is order; second index 2 system, index 3 system, index 5 system.

Maybe up to 5, 6 variables, 10 variables you will do lot of hand calculations and do it. If you have 1000 equations okay, which is the case where you are simulating a chemical; dynamics of a chemical plant, section of a chemical plant, you have trouble, right because how will you decide the index? You should automate, if you want; just given a set of equations you are not able to see, what is the index.

So, you should have a procedure that automatically differentiates and calculates the index and then does appropriate initialization, okay. So, unless you do that you are going to get into trouble okay, so I will illustrate this and then give the solution which is; he has very rightly guessed that you know; you should use those differentiated equations to develop what is called as consistent initial condition but just to show what can happen.

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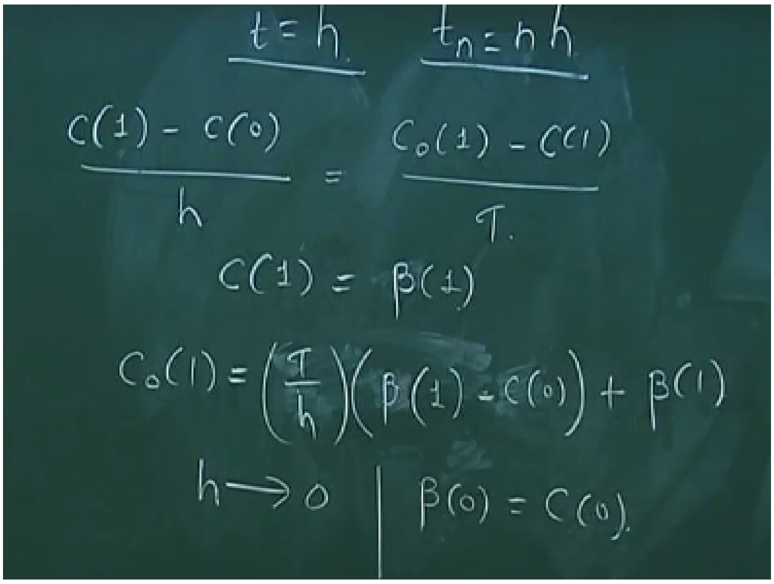

"Professor – student conversation ends" If the initial condition is not consistent, see this is; so C 1 – C0, I am just using for this particular system, I am just using the implicit Euler, let us say my h is my; this is how, way I will use implicit Euler for this particular system, right. On the right hand side at time 1, right, I am going from 0 to 1 at time 1, okay and then other equation that I have is C1 is = beta 1, right.

One is; you know, 1 here means t = h that is what we mean by 1. In our notation of time, we have taken tn = nh, so we use n right, to denote the time, so shorthand notation that we have. So, this C0 is actually Ch – C0, okay, so these are the equations at the first iteration; the very first iteration they are the equations okay. So, after you rearrange this, you will get C0 1 is equal to; okay.

Now, what happens for this equation to be consistent; see what will happen with, when h goes to 0, this beta 1 will actually tend to beta 0 because h is you know; ahead of time 0? If h goes to 0 okay what we require is that; if h goes to 0 for this equation to be consistent, okay we will require that beta 0 is = C0. We have to make sure when you start solving the equation that initial condition for C0 is given as beta 0, okay.

If you do not obey this constraint and start your integration okay, integration can blow up okay, so giving a consistent initial condition is very, very important for a differential algebraic system extremely crucial, okay particularly the high index DAE systems okay. Now, what do you do to deal with; how do you deal with this problem for high index systems, how do you generate consistent initial condition for a high index system.

"Professor – student conversation starts" No, no see beta 1 will tend to 0, as x tends to 0, as X tends to 0 okay, 1 will tend to 0, right because see, what is the meaning of 1? See, this is actually t = h, as h tends to 0, so the initial value has to be given correctly, you cannot arbitrarily; see in a normal differential equation, you can arbitrarily give C0 and it will work. Here, the constraint has to be obeyed that C0 is = beta 0.
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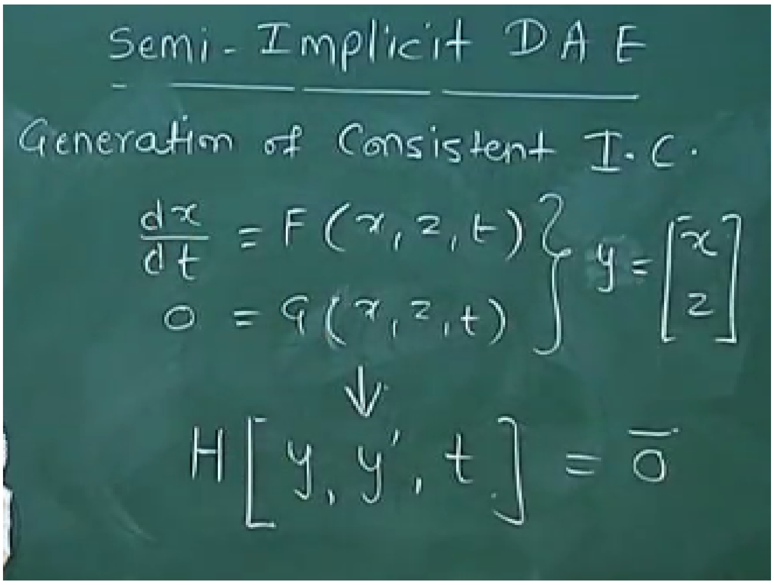

If it is not obeyed, you get into difficulty okay. **"Professor – student conversation ends"** Generation of consistent initial condition for a differential algebraic system, now this is a key thing particularly for the high index systems okay. So, what you do is; you write this, so we define a variable y or vector y, which is actually the x and z stacked up and then we translate this to some H of y y prime t = 0, okay.

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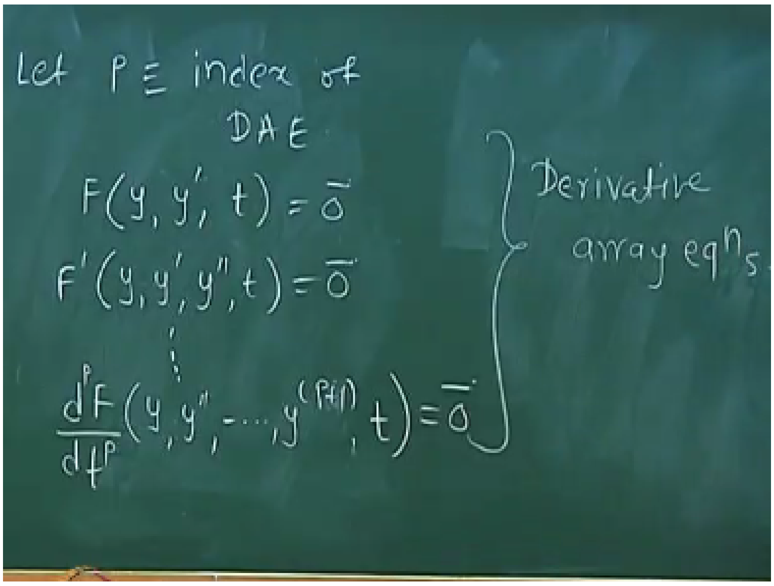

We translate this to y, y prime t = 0. Let P correspond to the index of DAE okay, then we differentiate this P times, which means; so this is F y, y prime t = 0, then df / dt, which will obviously have y, y prime, y double prime = 0 and so on up to differentiate this up to P times okay and these are known as derivative array equations. Yeah, **"Professor – student conversation starts"** P here means the order of the derivative; P + 1 not P – 1.

"Professor – student conversation ends" So, these have up to P + 1 derivatives of y, okay, so these are called as derivative array equations and to generate consistent initial conditions, we have to solve these equations simultaneously okay. So, higher index system, why it becomes difficult to deal with is because you have to solve these equations together to come up with a consistent solution.

In fact, if you solve it at time t = 0, you will get consistent initial condition, if you solve it any time in future at t = h, t = 2h, t = 3h, if you solve these equations together, you will get solution of the DAE, okay. So, if you know the index of the system, you can differentiate stack the equations together and then solve the stacked set of equations to come up with a consistent set of initial conditions as well as you can solve them in time.

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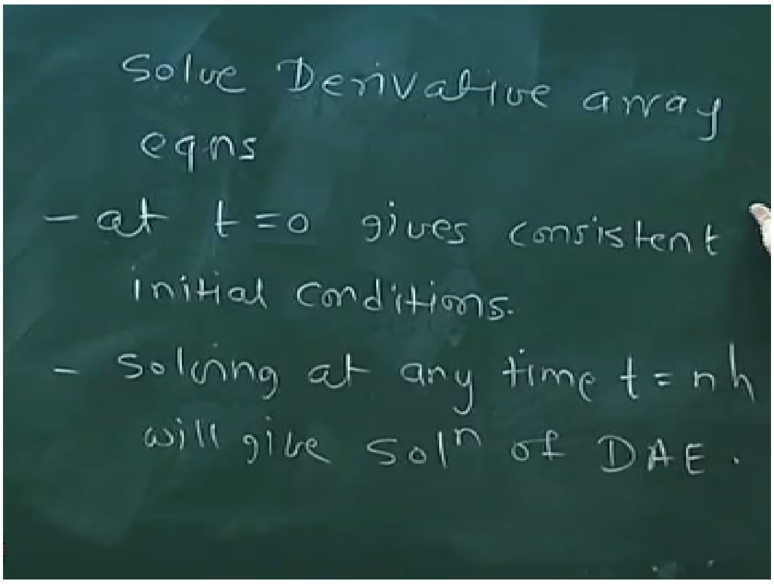

And then, you will get consistent solution of the DAE, high index t okay. To summarize; so I think what we shall was; you had guess, right that we have to solve them together that is the solution, you have to solve these differentiated equations together to get a consistent initial condition and then of course, there is one more way, you can go on eliminating high order; you can go on eliminating high order derivatives.

And finally you can convert it into a form, which is called as pure ODE + state any variant, I will just mention the form and then solve that, that is another way of doing it but solving it at t = 0 will give you consistent initial condition, okay. So, derivative array equations, you have to solve; you can see that why doing this automatically becomes difficult. So, developing dynamic simulators even though we have very, very advanced computers, even though we have a lot of knowledge now about solving large scale equations, dynamical systems;

It is still something, which is a difficult task because you have to do this business automatically, if you look at some of these commercial dynamics simulators, they do not ask you to specify what is the index of your differential algebraic equation. Obviously, when you are giving all kinds of constraints on the; you know a heat transfer, mass transfer, thermodynamic equilibrium and the dynamics associated with each of the units.

You are not expected to know as a chemical engineer, what is index, whether this is high index system or so you have to automatically internally find out what index it is, differentiate and create a stacked set of equations, which you can solve. So, generating consistent initial conditions or use some other way of generating consistent initial conditions, generating consistent initial conditions or consistent solutions is a big task; is a difficult task.

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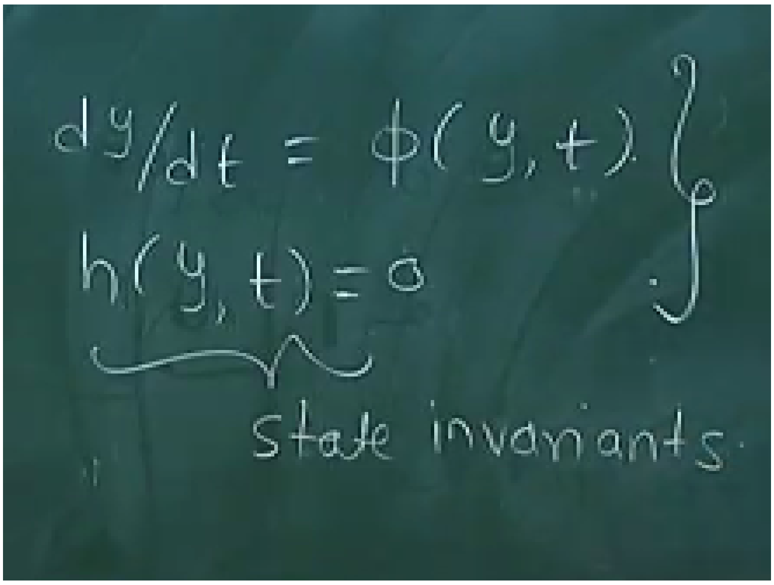

And if you make a mistake there, things can go wrong. The other approach is to reformulate okay. I think I will again move there because I want these equations, so the other approach is that you know; other approach is that this derivative array equation then can be written in this form, this is a pure ODE and this is an algebraic; these are algebraic constraints okay. So, you can reduce by eliminating higher derivatives, you can go on eliminating higher derivatives.

Now, this business might be pretty difficult for a very large system of equations but for some simple systems, you can obviously do this by eliminating derivatives, we just now did this for the; you know this mixing tank example, we eliminated the higher derivatives and so on. So, you can reformulate it like this and then solve it using a DAE solver which is; so these are called as state invariants; these are called state invariants.

And then you then you try to solve this set of equations using a DAE solver. So, with this I want to just close this very, very brief introduction to differential algebraic systems, my intention was to give you a flavour of what it is beyond you know, just differential or just algebraic systems. In reality, you get always a mixture and then solving it simultaneously is a difficult task, it is not that easy okay.

So, you need to develop expertise in solving these and beyond a point as I said working with numerical methods and solving the problem becomes an art, it is not just the mathematics, it is; you learn lot of tricks of the trade, which everything is not written in a book and cannot be written in the book. So, for example you know, when you start solving problems you will learn that making variables dimensionless or scaling the variables; all the variables help improving the numerical accuracy or stability of the algorithms.

If I have (()) (35:21), let us take a distillation column, you know you may have pressure, composition, temperature appearing in one huge vector okay, pressure might be you know Newton per meter square 10 to the power 5 something, temperature is in you know, kelvins 300 and concentration is in fractions, mole fractions. Then, you know you have a trouble the numerical integrating such things.

Because the vector has imbalanced you know; numerical values, so it helps to scale them on a similar scale and then work to the scaled variables and these things are something, which you have to learn by experience okay, these things. Unless you are hit by situation, where everything is fine and you do not get a good solution and you have to start thinking about now what to do.

So, that is where you start thinking, making dimension, defining dimensionless variables and all kinds of other tricks, so it is not enough just to know the mathematical background, it is also important to know all these tricks, which you can learn only through experience and as I keep saying in every of my instance of teaching this course is that the good part is that it cannot be automatic, you know that is why we are in business.

We keep getting jobs you know, because you have to know some tricks and that is where; you know you can still; otherwise, you know MATLAB or some software would be sufficient to solve all these problems but even though, you have very, very sophisticated solvers and software, you still need chemical engineers who know numerical analysis to go, you know make fixes or make things work that is because everything still you cannot automate it.

You have to have some kind of human intervention, (()) (37:26) or chemical engineer's intervention to make the problems solvable okay. So, let us have a quick look at what all things that we have done in this course, I would like to summarize this course by saying that it is not a course on computational or numerical methods but it is a course on numerical analysis. We learn to do analysis here than just learning the methods.

The aim was just to make you learn methods, I could just go on writing recipes and you know, you will not see the threads that connect them and then it just becomes you know, you memorize it and forget about it after some time. The reason for developing it as an analysis course is that you should remember the; you should understand the fundamentals behind how numerical recipe is concocted or is cooked or is developed.

And then you should have this confidence of coming up with a new recipe, if you are encountered with a new problem, every problem will be different, every problem would require different way of thinking, which will not be given in any of the numerical methods book because the real problems are very, very complex, you will have partial differential equations, differential equations, you will have algebraic equations all coming together.

It could be partial differential equations in time and space, some algebraic equations because you are lumping and saying that the spatial variation is not important okay, you know and some algebraic equations because of some constitutive laws or thermodynamic equilibrium and so on. So, you have a very complex system of equations, which you have to solve and solving mathematically modelling and solving it is becoming very, very popular in industry in academics in research everywhere.

Because you know, you can do an experiment without actually having to go to the; you can do a virtual experiment, you can develop a model, play with it, understand how the model behaves hopefully the model at least represents in a respectable way the reality and then if you learn something from the model you know, when you go and design your experiments or design your equipment or do control of a system, you will have some a priori knowledge about how to go about doing it okay.

That is what we hope when we do modelling and so modelling is becoming very, very important tool and then to develop models you should be able to solve them and get some reasonable solutions, which makes sense. Now, most of the models that we encounter in chemical engineering cannot be you know; their solutions for under different situations cannot be constructed analytically.

Though we do study a lot of methods for analytical constructions of solutions that is more to look at some idealized problems, simple situations okay and of course, analytical solutions typically which you can find for linear differential equations or linear partial differential equations, they give you a lot of insights, they help you understanding how things behave. They also have helped you numeric analysis to benchmark your approximate solutions to see whether approximate solutions are close to the 2 solutions.

So, there are different ways where you can use analytical solutions and in some simple situations, analytical expressions can be generated but even if the differential equations, partial differential equations are linear not that every time you can generate analytical solutions. If the geometry is nice okay; if you have cylindrical you know, something, which can be modelled as a cylinder, it can be modelled as a perfect you know; sphere or some tube some nice geometry, then you know it is easy to solve those problems.

But if you have some weird geometries even if you are linear partial differential equations, you still have to go for numerical solutions, you cannot construct analytical solutions with some weird geometries and the real problems are with weird geometries okay. So, computational modelling or computational fluid dynamics very, very important part nowadays, in design of chemical systems.

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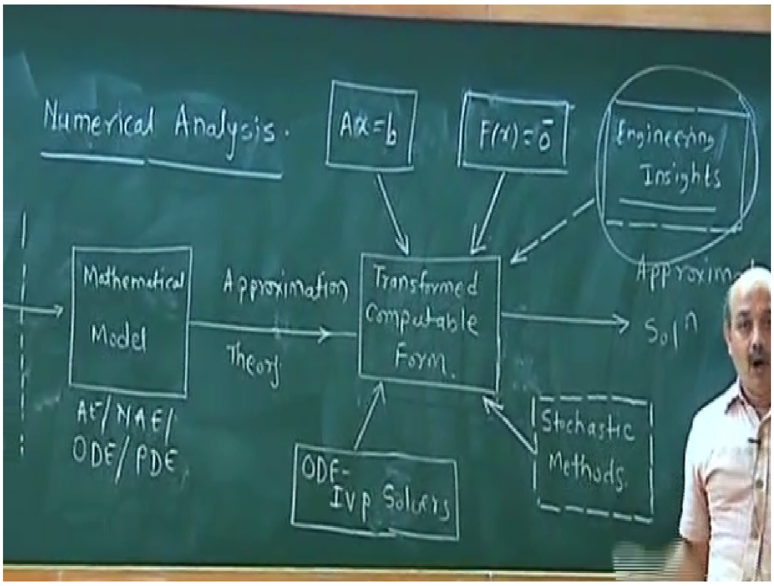

Now, the way we looked at it; the difference about this course and most of the other books, which present course on numerical methods for engineers, is that we did not; we did not look at the methods based on the types of equations. We looked at methods from the viewpoint of tools okay. So, the basic idea was that you have; for a real system, you develop a mathematical model.

This mathematical model typically would be you know, algebraic equations or nonlinear algebraic equations or ODE or PDE, some kind of you know; some kind of algebraic differential, partial differential or their combinations that kind of an equation. Typically, for the situation for which we would like to study this coupled set of differential algebraic partial differential equations cannot be solved analytically unless very, very rare situations, okay.

So, then we said that this you have to transform the problem, so we spend a lot of time in understanding how to do problem transformation, so using approximation theory, you get a transformed computable form. This transform computable form in terms of its structure could be completely different from what you started with; you may have started with a partial differential equation, you might get you know, algebraic equations; nonlinear algebraic equations.

So, what; the transform problem could have completely different structure from a mathematical viewpoint than the original problem okay. What you end up solving is the transform problem typically and not the original problem except for some very, very rare situations, where analytical solutions can be constructed okay. Now, then we said that to solve this transform computable form, we only have you know, 3 or 4 tools.

So, one tool that we said is solving linear algebraic equations, so solving Ax = B, this is one tool. So, this tool is used, then the other equation or other tool, which is very commonly used is solving nonlinear algebraic equations, so this is F of x = 0, okay, then the fourth tool; third tool is; the third tool is ODE IVP solver, so this is my third tool and a fourth tool that we did not discuss would probably form part of advanced course, stochastic methods, okay, random sampling based methods.

So, we have 3 or 4 tools, it is like you know; it is like you are a doctor with you only have 3 or 4 tablets with you and you have to create a concoction, you have to create a recipe that will cure the patient, so you have to use some combination of these 4 tools okay and then what you get finally is approximate. Now, is it sufficient that this 4 tools are with you, it is not okay. You also have to give inputs.

If I think in terms of another input that goes is; to solve a problem, you have to have some engineering insights from physics, chemistry, thermodynamics whatever because you have to give good initial conditions, which make physical sense okay, so this component cannot be ignored. This is in fact the most vital component, it is not enough to have these 4 tools, you should know limits of this 4 tools.

You should know about you know, things like stiff differential equations, you should know about you know, ill condition problems and well-conditioned problems and condition number and Eigen values and a relationship to convergence and so all this analysis that we looked at should be there in the back of your mind, when you are solving these problems. One of the focus of this course was analysis.

We looked at how to do convergence analysis, how to use eigenvalues particularly for solving linear algebraic equations iteratively, we could use you know, the theory of behaviour of difference equations; linear difference equations and understand under what conditions the error will go to 0. Same, you know, the theory of linear difference equations; qualitative behaviour of venial difference equations based on analysis of eigenvalues.

Also came to our help, when we looked at you know, different numerical solvers for OD IVP, we looked at convergence of error; error between the true solution and approximate solution when with it and how do you choose integration step size, all that was you know analysed using linear difference equations okay. So, these are tools that help us; well, for Newton's method, I just touched upon contraction mapping principle, though we could not go deep into it.

So, the idea was to give you flavour okay, it is not possible for this; this is a course that would prepare you for research, it is a course that is between your undergraduate course and advanced course; really advanced course, it is somewhere in the middle okay, what we are doing is a course which is fixed in middle, where you know, you are introduced to various things like sparse matrices, sparse linear systems, then how you can speed up your calculations.

Finally, we came to you know, combine things like differential algebraic systems together and what are the complications okay. Now, things like solving partial differential equations, boundary value problems all was dealt by approximation theory okay. If I go back and see what plays most crucial role in this is; how do you approximate, what are the tools for approximation?

Taylor series approximation then collocations or interpolation polynomials okay or interpolating functions in general and least squares polynomials or least square functions, least square approximations, now what is the origin? Origin comes from Weierstrass theorem that any continuous function can be approximated with arbitrary accuracy using a polynomial function of a suitable order okay.

So, this one idea, which was discovered more than a century back you know, it actually forms the CD of what has happened later on, okay, entire structure actually critically depends upon this fundamental idea. So, basically we cannot really solve most of these problems exactly, we have a real system there is a level of approximation when you develop a mathematical model.

A lot of simplifications, when you approximate reality using mathematical model okay, the mathematical model that you construct and situations that you develop again you know, you cannot solve them exactly you have to further approximate if you want to compute numerically. When you are computing them numerically, there are further difficulties, there is an error committed when you go from reality to the mathematical model, from mathematical model to the computable form.

Because typically, we looked at these different spaces associated and we said that the original problem is typically in the infinite dimensional space we are approximating with a finite dimensional approximation so you have limitations. So, there is lot of error committed when you approximate problem in finite dimensions with problems infinite dimensions because finite dimension problems are computable.

Further, when you solve using computer; computer has limitations, you cannot represent every number in the computer, it has a finite precision, whatever bits you use, 128 or 256, you have a limitation at some point and then that is where there are errors coming because of limitations of your computer okay. So, what you actually want to do and what you finally see, there is lot of difference, you have to use this part.

This is the most crucial part, which I cannot teach in the class, this you have to develop by solving many problems using all this theory, using the analysis, which I taught you. Unless you start using it you know, it is like you have been given tools, if you do not keep using them, then they do not remain sharp you know and then you will not understand why;

So, hopefully you know, you understood why behind most of these methods and then you will be able to carry it with you and so it was enjoyable teaching this course for your class and I hope you have learned something. So with this, I would like to close this course on numeric analysis, just remember this entire diagram and do not forget what is most important is your engineering insights and physics, which you cannot forget.

All these are tools, which will help only if you give correct initial guesses, only you make correct choices, there is no unique way of solving the problem okay, each one will come up with a different recipe or a different concoction, you should have confidence to make a new bhelpuri when; or a new concoction okay, when a new problem comes that is important that is what I wanted to learn through this course.