Introduction to Finite Volume Methods - II
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Lecture - 1
Linear solvers – I

Welcome to this Finite Volume Series. This is part II. And the previous semester you have probably enjoyed the course part I, and now this is the series continuation up to that and this is the part II. And as you know the finite volume is one kind of CFD tool which has been used widely and in industry for solving large scale of problem and also it is quite popular to use as in CFD tool in the academic community.

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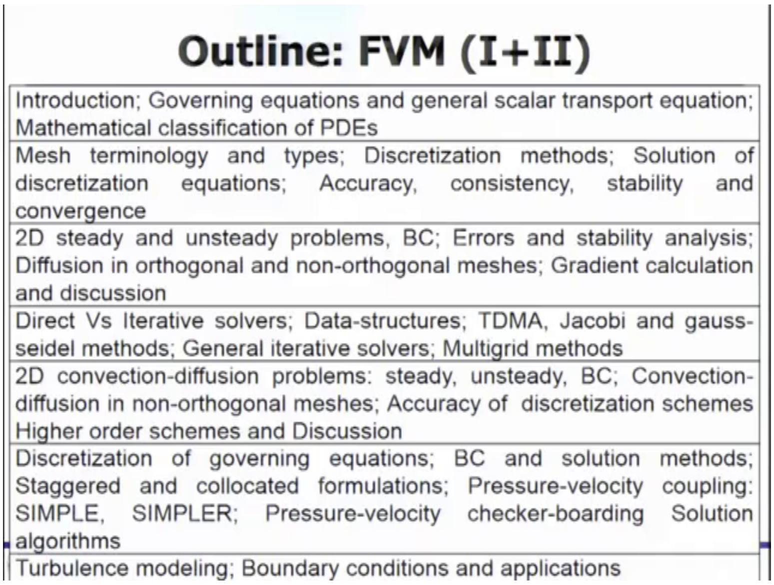
Outline: FVM (I+II)

Introduction; Governing equations and general scalar transport equation; Mathematical classification of PDEs
Mesh terminology and types; Discretization methods; Solution of discretization equations; Accuracy, consistency, stability and convergence
2D steady and unsteady problems, BC; Errors and stability analysis; Diffusion in orthogonal and non-orthogonal meshes; Gradient calculation and discussion
Direct Vs Iterative solvers; Data-structures; TDMA, Jacobi and gauss-seidel methods; General iterative solvers; Multigrid methods
2D convection-diffusion problems: steady, unsteady, BC; Convection-diffusion in non-orthogonal meshes; Accuracy of discretization schemes Higher order schemes and Discussion
Discretization of governing equations; BC and solution methods; Staggered and collocated formulations; Pressure-velocity coupling: SIMPLE, SIMPLER; Pressure-velocity checker-boarding Solution algorithms
Turbulence modeling; Boundary conditions and applications

Now, coming back to this particular one, what this is if you look at it, this is the outline of finite volume which includes both the part I and part II.

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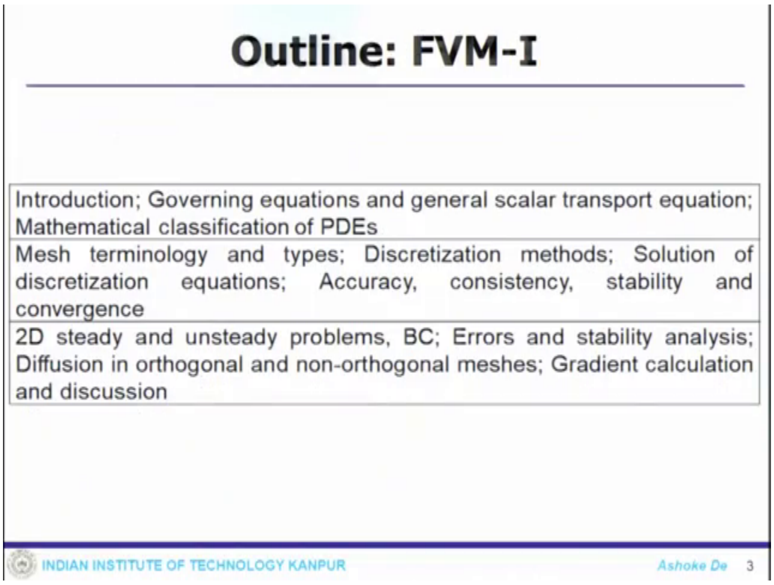

And that if you go this is the part I which has been offered in the previous semester where you have been introduced to the governing questions and the introduction of CFD, and everything, and how you deal with the classical partial differential equations which govern the problem, fluid flow problem.

And then we talked about mesh or the grid and finally, what you have looked at the two dimensional steady and unsteady problem with respect to the diffusion problem where you have looked at the different calculations of this things.

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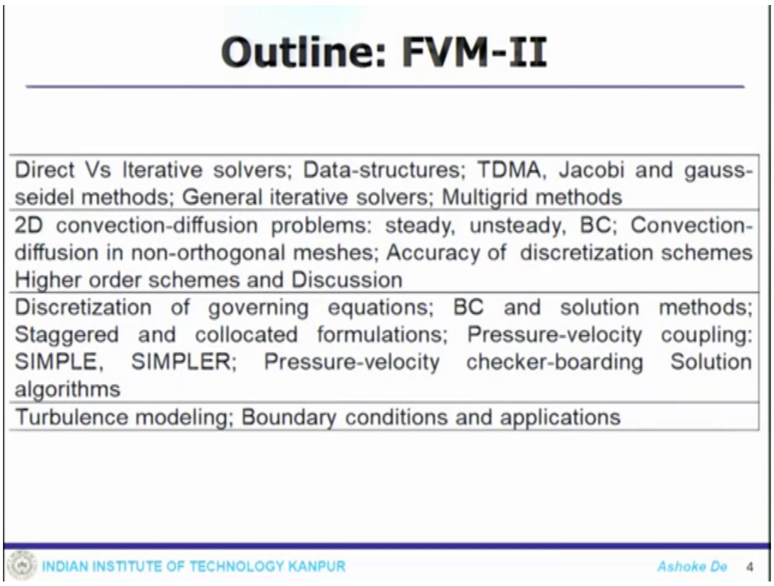

Now, continuation to that where we will be looking at this is the outline of this particular series part II, with this particular semester you will be introduced to the linear solvers. So, we will start with the linear solver where you look at the data structure, different kind of linear solvers, and we talk about that and moving ahead we look at the convection diffusion problem, and where will start with steady, unsteady, and talk about different boundary condition and orthogonality everything which will lead to your higher or a discretization also.

And once you do the convection diffusion equation, that would take you to the fluid flow problem and then we talk about different kind of solution methodology, and we talk the incompressible calculation, compressible calculation, and finally, with touch upon certain things special topics like turbulence modeling and its application. So, this is the overall content of this particular part which would be covered in this particular semester.

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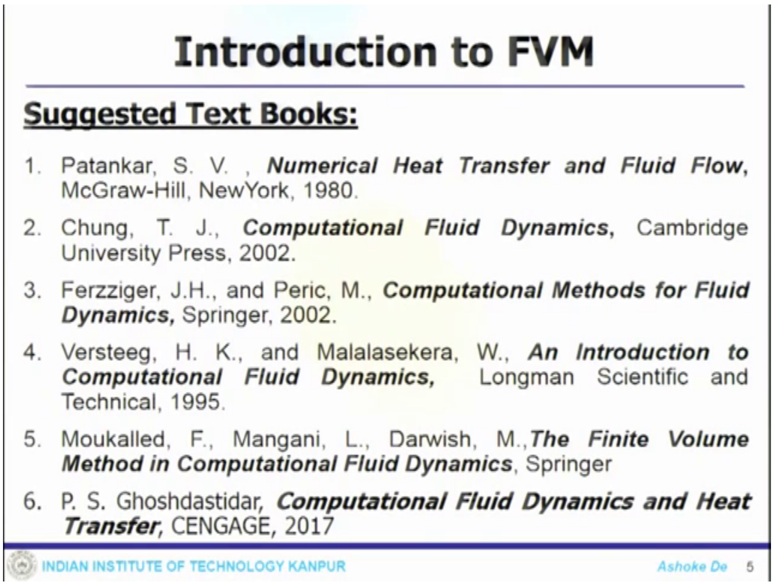

And the text book which are suggested one of the classical book is the Patankar's book, and one can look at this one as a reference book, also the Ferzzinger book is a reference book and these two book are also essential because the course material which are covered primarily the combination of these three books which talk about the finite volume methods. And so, once you complete this part II will be able to solve a real life fluid flow problem and can handle using this kind of technique.

And, now we were discussing the solution of the linear system and while doing that there are different approaches like direct approaches and iterative process. Now, while talking about the linear system the key component of that is the matrix. And we have so for discussed about the matrix, its vectors, norm and certain properties and along with some theorems. Now, today we will discuss on the solution procedure.

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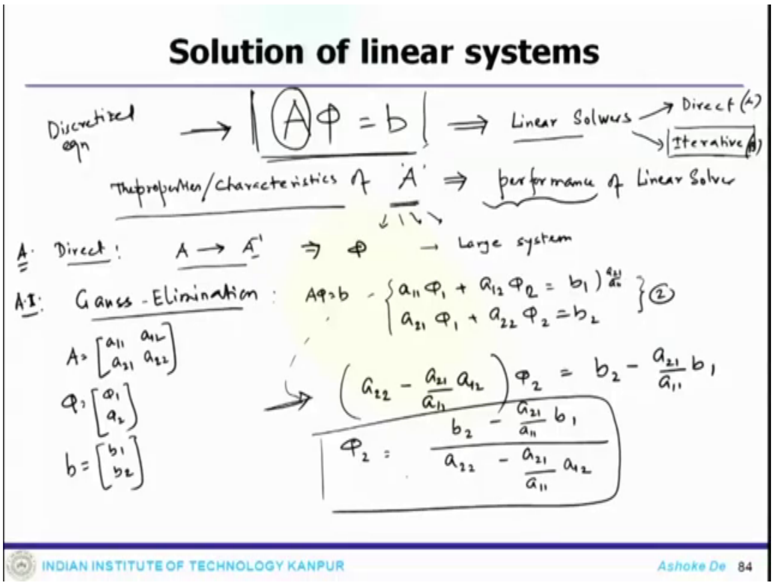

So, moving ahead, now this is on equation system or the linear system what we are getting it in. And where we are getting it? We are getting it from the discretized system. So, discretized equation we lead to the linear system. Now, here we need to use different solver, linear solvers. And when you talk about the linear solver there are methods, one is the direct approach and alternatively one can solve iterative approach.

Now, in both the cases whether it is in direct approach or an iterative approach, it all depends on this element A, how the behavior of the A that will dictate the performance of, so essentially the properties or characteristics of A would directly impact the performance of linear solver.

Now, when you say the performance, that actually includes the convergence, stability, norm, everything. So, everything is short of included in this particular terminology performance. So, what we need to do? In that context we need to understand this matrix very nicely and with that objective in mind we have done discussion on the property and characteristics of A. We have looked at norms, vectors, spannings, and other some theorems which could be important to look at. And the things which are always remain as and are going to plane pivotal role is that the properties of this A like whether its two sparse or bandage then the eigenvalues, spectral radius, condition number, so these are the some few things which are always going to come up specially when we talk about iterative solver.

Now, in the direct method if you come across the direct method, as we have discussed essentially you try to find out the A inverse or once you get the A inverse you find out the solution of phi. Now, while finding the A inverse the issues which are associated with this direct approach is that large system there is a restriction. So, if you have a large system and A is too large for a problem of interest; then, this going to be too expensive. Expensive in the sense, computationally expensive. Requirement of memory and other things are going to exponentially increase. So, that is why the alternative approach which is iterative process are often preferred in the large scale CFD calculations.

But, these direct approach or the direct solvers we will do some sort of a discussion because that will actually peb the way for introducing the effective iterative solver. So, its good idea to have some sort of a understanding of some of this direct solver which will have a platform for discussion of the iterative solver. And the simplest of that one which will start with is that if it is A, the direct process we call it A and this one is b then this let say A I. The one is that which is the simplest of the lot is the Gauss elimination. So, we talk about Gauss elimination and then move ahead.

So, let us start with an simple example of a linear system let say a 11 phi 1 plus a 12 phi 1 phi 2 equals to b 1 a 21 phi 1 plus a 22 phi 2 equals to b 2. So, essentially you got two equations and you have two unknowns in terms of phi 1 and phi 2. And if you put them together the coefficient of the matrix here would be a 11, a 12, a 21, a 22, and this is going to be the system which will lead to a phi equals to b. And phi is a vector phi 1 and phi 2 and b is another vector right hand side vector b 1, b 2. So, that is what it leads to.

Now, this system can be eliminated by one of the variable, because it is a two by two system. So, what you can do? You multiply the first term by a 21 by a 11 on this equation becomes. So, essentially this one you get a 22 minus a 21 by a 11 a 12 phi 2 equals to b 2 minus a 21 by a 11 into b 1. So, what we have done? Multiply this guy by a 21 by a 11 and then subtract the other equation. So, here you multiplied by a 21 by a 11 and then subtraction. So, essentially that is what you get.

So, now if you look at this particular equation, the two unknowns, now boils down to single unknown or here in this particular expression you got one unknown which can be directly obtained like b 2 minus a 21 by a 11 b 1, a 22 by a 21, a 11, a 12. Just an algebra which will get you back the phi 2. And once you know the phi 2 and you put it back you can always get the other expression for phi 1.

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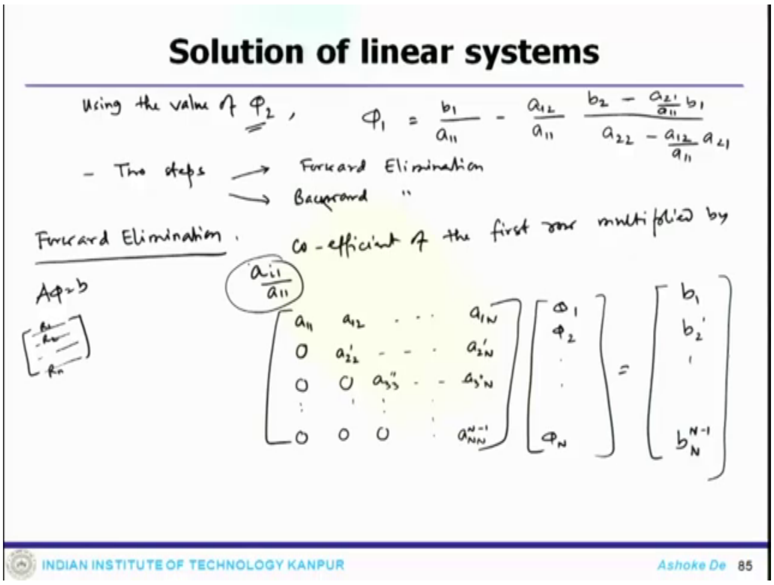

So, you using the value of phi two you get phi 1 equals to b 1 by a 11 minus a 12 by a 11, b 2 minus a 21 by a 11 b 1 a 22 minus a 12 by a 11 a 21. So, that is what you get, using phi 2 you get phi 1.

So, the procedure which we have done here or carried out its in essentially two steps. What are those steps? In the first steps equations are manipulated in order to element one of the variable and then we end up getting an one equation with respect to one unknown, and the second step the equation is solve to get back the variables.

So, one option is that, when we get this elimination process that is called the forward elimination. And when we obtain the solution and putting it back to get back all the unknowns that is where we do backward substitution. So, that is what the process is known for. Now, what you do in forward elimination? If you look at a generic system, then that will get to clear idea. So, in the forward elimination process. So, first row a refers to the discretized equations, for phi 1 and the second row correspond so if I have a phi equals to b and a are having this is row 1 this is row 2 this is like that R n. So, individual rows they actually points or represents to the equation of individual element like phi 1, phi 2 and so on.

So, what you do when you actually the coefficients of the first row. So, essentially the coefficients of the first row is multiplied by a factor a i1 by 11, and the resulting equation subtracted from those ith row this I can be 1 2 3 4 like that then the resulting equation would become like that a 11 a 12 so on a 1N. Then it should be 0, this is a 22 prime a 2 prime N, then it is 0 it will be 0 and so this is also 0 and third term could be a 33 double prime and so on N. And if you go and keep on doing these this will be all 0 and finally, you get a N, N minus 1 like that.

And here the variables are going to sit phi 1 phi 2 and n, and your right-hand side is also going also get modified so b 1 b 2 prime, so on b N, N minus 1. So, each of this row is multiplied with this kind of a factor the coefficients and subtracted from this. So, you get this result and equation.

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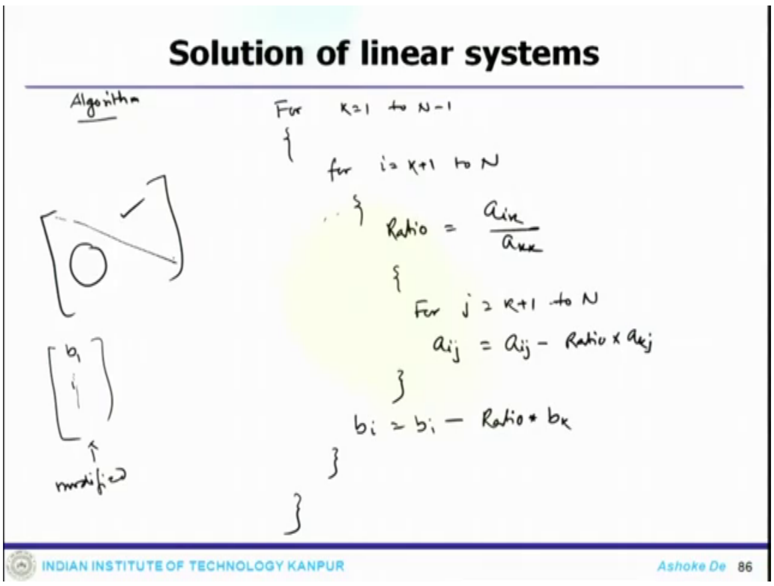

So, if one right that algorithm so that says you go by a loop for k equals to 1 to N minus 1. So, that is in loop. Then for i equals to k plus 1 to N you get this ratio that ratio is a ik divided by a kk. Now, again for j equals to k plus 1 to N you get a ij is equals to a ij minus that ratio into a kj. That is why it close and then you obtain b i, right-hand side b i minus ratio into b k. So, that closes this loop and the third one closes.

So, essentially what you do? You pick up this, this side you will have all the coefficients and this side become 0. So, you have all the elements here and right hand side vector is also going to be modified, and these are also modified vector. So, you multiplied the first coefficient and then subtracted from the respective rows then you get this kind of. Once you get this then you see it become sort of an upper triangular system.

So, you know that the last element here if you see this 6 here which will be connected with the variable at the Nth level and there is a; so the last one is connected with only one variable or one unknown and then the exact expression for this one can be obtained.

Once you get this one the last, but one will involve two equations and two variables or other two unknowns which includes phi N minus 1 and phi N since phi N is obtained then you can replace that and get phi N minus 1 and, so on you can move from the bottom to up and finally, you can get each variable like that.

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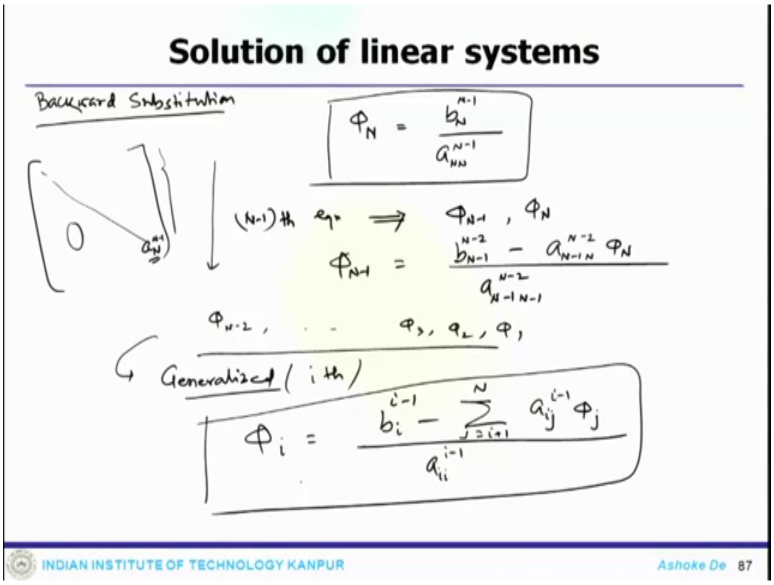

So, next step is backward substitution where you get the individual variables by computing directly. So, what happened? When you have modified that term then if you look at that system where you only get this is 0 and here is the coefficient which is sitting there, modified coefficient and connected with these variables. So, one can obtain phi N equals to b N N minus 1 divided by a NN N minus 1. So, using this you can obtain the phi N.

Similarly, the N minus 1 equation as I said which will involve two variables, one is phi N minus 1 and phi N and phi N minus 1 can be computed as b N minus 1, N minus 2 minus a N minus 1, N minus 2 phi N and a N minus 1 N minus 1, N minus 2, so on. If you go along this direction finally, we can obtain phi N minus 2 and so on phi 3, phi 2 and phi 1. So, all the variables can be computed by doing this kind of back substitution.

And when you come down to the, if you generalize this system and write down for one particular ith then one can write that phi i equals to b i i minus 1 minus summation of j equals to i plus 1 to N a ij, i minus 1 phi j divided by ii i minus 1. So, the general expression is that when you put this one for individual elements you can obtain the all the numbers.

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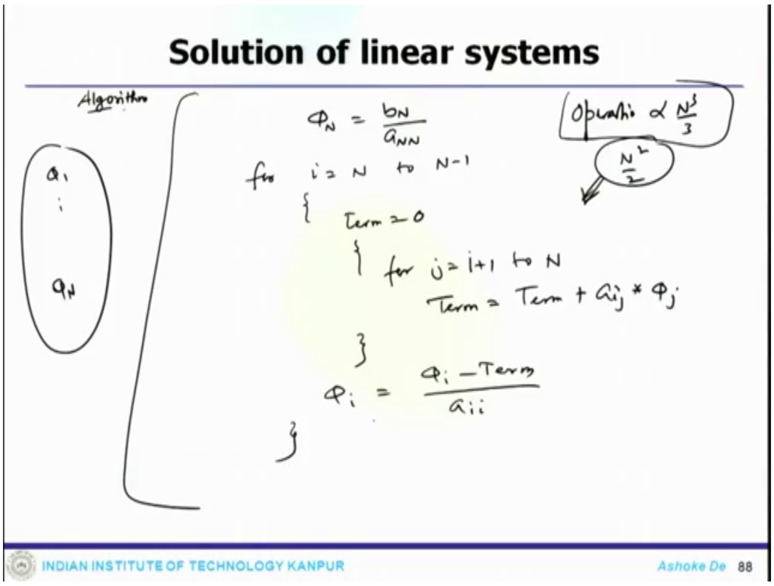

So, if you put them in the algorithm how it works? So, algorithm if you put them. So, you have a first you compute phi N which is b N by a NN because that is the term which you require then you go for in loop, where i goes to N to N minus 1 and let us say some term equals to 0. Then you go for j equals to i plus 1 to N you get term equals to term plus a ij into phi j then the substitution would work phi i minus term divided by a ii. So, that closes the system. So, that way you can obtain phi 1 to phi N. All these variables one can obtain.

Now, here this is perfectly and direct approach where you can first you eliminate the in the forward process and then it through the back substitution you get it. Now, this particular algorithm solve the linear system for N by N system it requires lot of calculations its and the number of operation required for this kind of system of N equation it require proportional to something if the operation proportional to N cube by 3 of which N square by 2 arithmetic operations are required for the back substitution. You can see this much is require for back substitution and the total operation count is this. So, this high computational cost has kind of limitation for the applicability of this kind of approach in the large scale problem.

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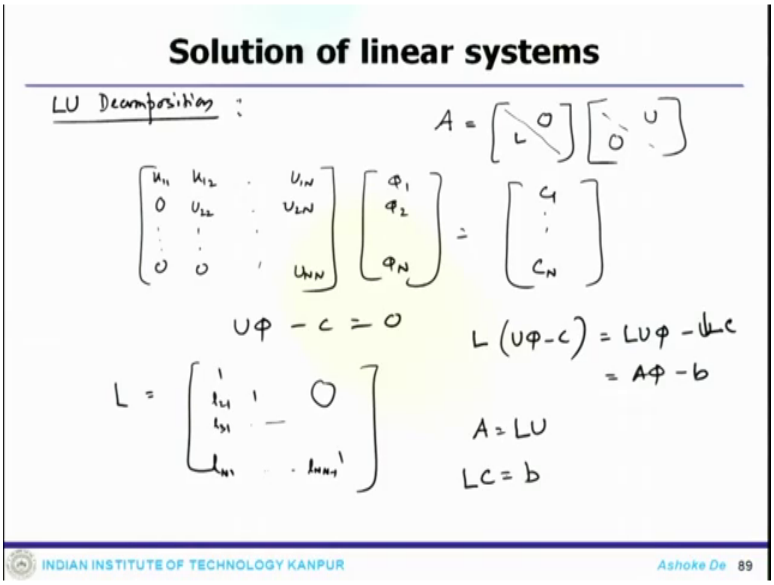

Now, one can look at another substitution called LU decomposition. What you do? You have a system like that and the whole matrix you decomposed in two system, one is the lower triangular system where this will be present another case is the upper triangular system where this is. So, the decomposition which get you is that the LU factorizations or the lower and upper triangular factorization. The advantage of this method over the Gauss elimination is that once the LU factorization is performed, the linear system can be solved as many as times as needed for different values of right-hand side vector v without performing an additional elimination. So, that is the advantage of using LU decomposition over Gauss elimination.

Now, if that is the case now if you perform the elimination process what you get at the beginning is that let say u 11 u 12 and so on u 1N, then 0 u 22, 2N, 0, 0, and so on you get u NN. So, this is obtained by doing the forward elimination and here is my phi 1, phi 2 and phi N and this is where the coefficient c 1, c N ok. So, in a compact form, so this has become my upper triangular system.

Now, this I can write u phi minus c equals to 0. Now, if you will be the unit lower triangular matrix and all the diagonal elements are set to 1 in order to make this factorization very unique then one can represent the L as 1, 1 and so on 1; these are all 0 and this would be l 21, l 31, dot dot dot l N1, dot dot dot l N, N minus 1

Now, this is a very unique factorization then one can write L U phi minus c equals to LU phi minus L L c equals to A phi minus b. Now, what the properties of the matrix says? A equals to LU and then L C equals to b. So, if I use this how do I get the decomposition step.

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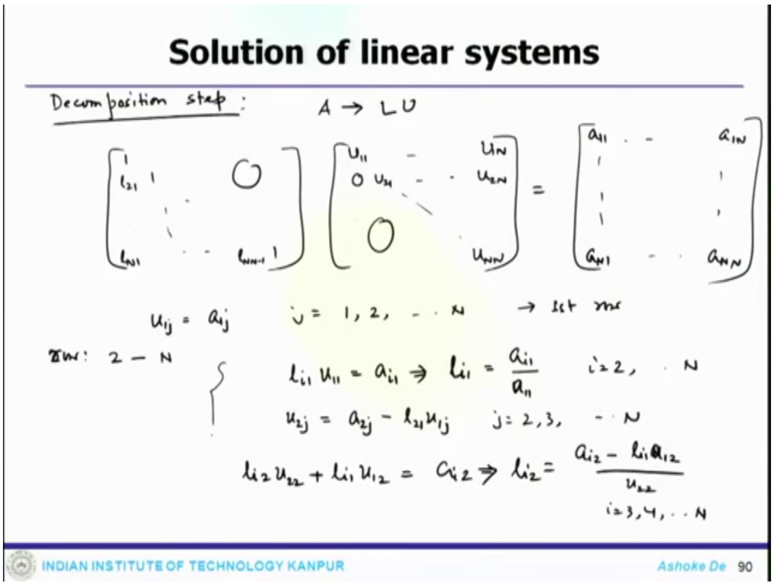

So, now I would find out the decomposition steps to obtain that LU. Now, one of the efficient procedure to get LU coefficient would be getting some demise procedure. But once you obtain from A to LU the whole system would be looking like this equals to essentially this, this is starting for a 11 to a 1 N and this goes on N 1 to a NN. These all the term which are there and when I do lower triangular it would be all one upper side is

0 21 to l N1 and this is NN minus 1, and this side it would be u 11 to u 1N, 0, 21 2N, so on this would be u NN and all 0.

Now, how to get the coefficients for L, the first L by all columns of U. So, what one can get u 1j equals to a 1j, for j goes on 1 2 3 to N. Then the second through Nth rows this is for the first row, first row. Now, for row second to N one can find out by L multiplied the first column on U, so which will lead to l i1 u 11 equals to a i1 which will get you back l i1 equals to a i1 by u 11, where i goes from 2 to N.

Now, this process is repeated by multiplying the second row of L by the second through Nth columns of u to get u 2j equals to a 2j minus l 21 u 1j, where j goes from 2, 3 to N. And similarly like that third through N, so that will get me back l i2, u 22 plus l i1 u 12 equals to a i2 which is l i2 equals to a i2 minus l i1 12 divided by 22 for which case i goes from 3, 4 like N.

So, each of these. In general, so now, this is how you get now if you want to generalize that expression then the generalized equation what one can write is that ith row of L getting multiplied by ith by the ith through Nth columns of U.

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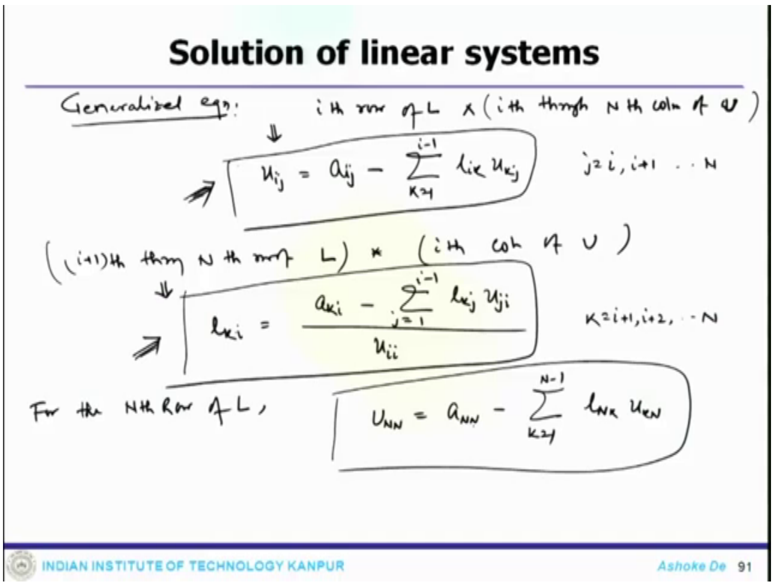

So, this is multiplied by ith through Nth column of the U which get you the result and equation u ij equals to a ij minus summation of k equals to 1 to i minus 1 l ik, u kj, where j goes from i, i plus 1 dot dot N. So, that is the generic expression one can write.

And i plus 1th through Nth rows of L getting multiplied by the ith column of U get you l ki equals to a ki minus j equals to i minus 1 l kj, u ji divided by u ii, where k goes from i plus 1 to i plus 2 and so on to N. So, that what you get so this is where you get the component of upper triangular matrix and the lower one get you the component of lower triangular matrix.

Now, for the Nth row of L, its coefficients are multiplied by the coefficients of Nth column of U which will actually get you the U NN, which is a NN minus k equals to 1 to N minus 1 l Nk u kN. So, Nth row you obtain like that. So, one case you get all the coefficients of upper triangular system using this you get all the coefficients of the lower triangular system and then finally, you get the Nth row.

So, we will stop here today, and will take from here in the follow up lectures.

Thank you.