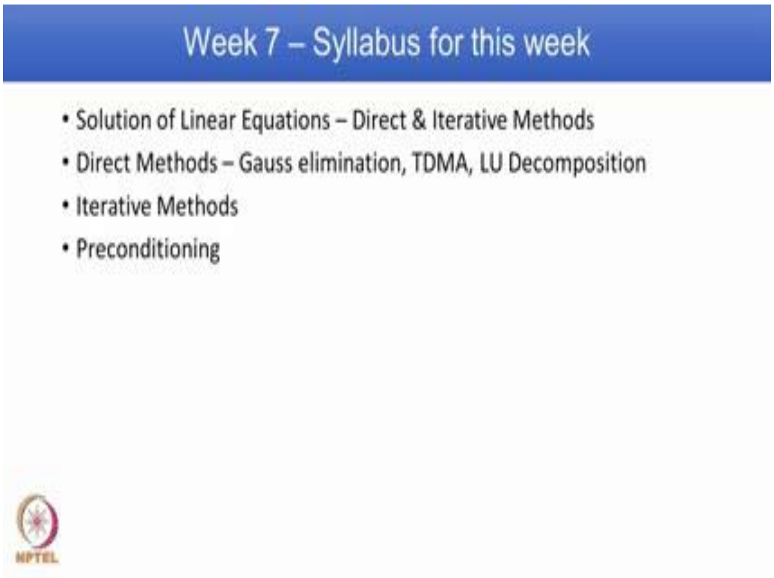
Foundation of Computational Fluid Dynamics

Dr. S. Vengadesan
Department of Applied Mechanics
Indian Institute of Technology, Madras

Lecture - 33

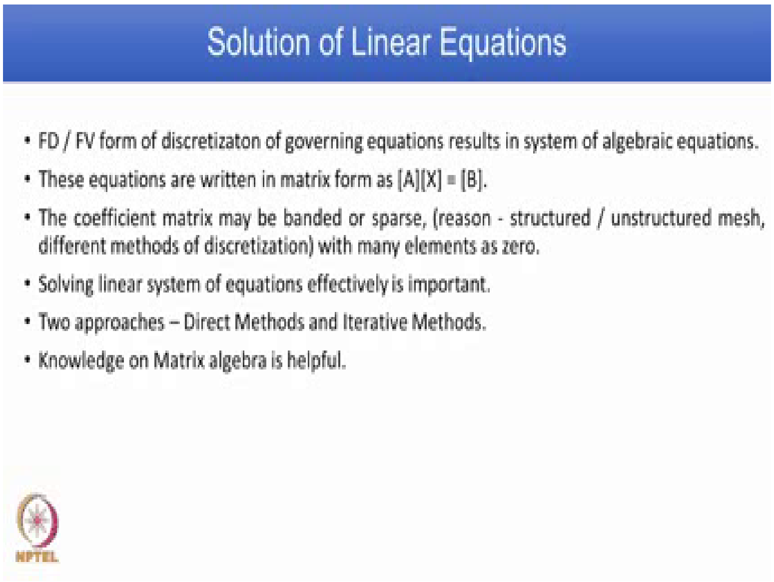
Greetings, welcome, and welcome again to this course on CFD. So far we have seen different discretization procedure, particularly finite volume in detail; turbulent flows and modeling, boundary condition implementation and how to arrive at generalized discretized equation. This week class, we will focus on how to get a solution of linear equations. There are two methods in particular direct methods and iterative methods.

(Refer Slide Time: 00:49)



In direct methods, we are going to see three methods gauss elimination method, a specialized form of gauss elimination method called tridiagonal matrix algorithm, LU decomposition. We will also talk about five different methods under iterative methods. Then there is a procedure called preconditioning; if the matrix is in ill-condition, difficult to get the solution then we do the procedure called preconditioning. We will talk about different procedures available under preconditioning.

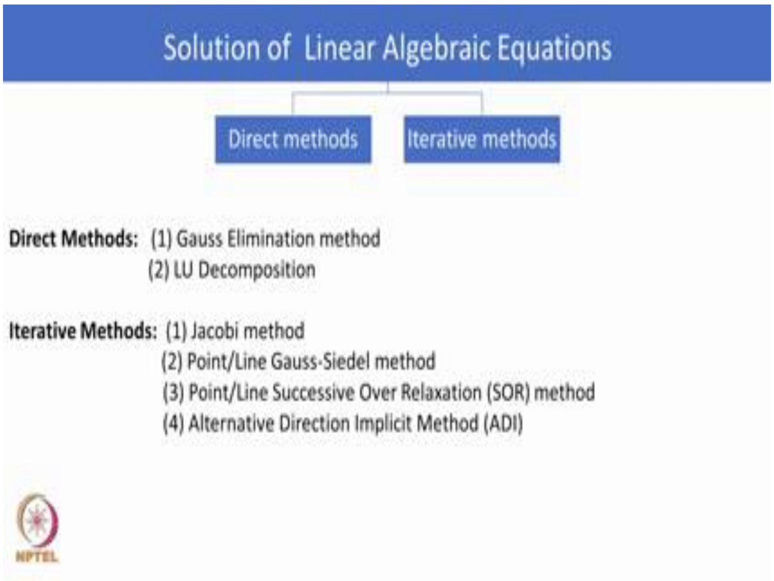
(Refer Slide Time: 01:29)



By now we know whether we follow finite difference or finite volume method, discretizing the governing equations will results in system of algebraic equation. These equations can be written in matrix form as A into X equal to B, where A is a coefficient matrix; X is a column vector of unknown and B is another known matrix. The coefficient matrix A, it may be banded or sparse; for sparse, it is sparse, because we use different structural grid or unstructured grid, we follow different discretization procedure. For example, when we talked about finite volume procedure for convection, we have different procedure pure upending, quick scheme or central type linear approximation and we have different procedure for diffusion term. So, we put them together then it may result in not a banded structure.

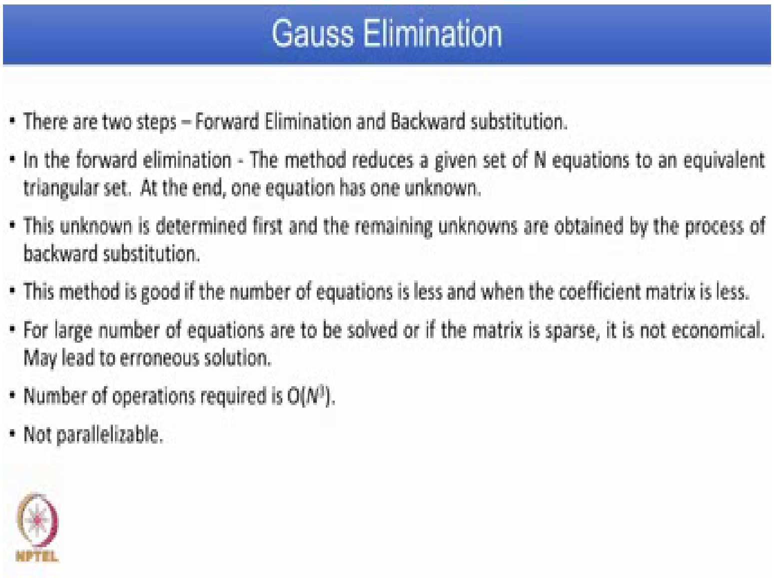
And you also observe the matrix coefficient matrix has many zero elements. Solving such a system is very important, because it affects solution accuracy and it takes computational time enormously. There are two approaches one is direct method, other one is a iterative methods. To understand this knowledge on matrix will be very helpful which would have studied in your basic undergraduate program. Matrix algebra in terms of Kramer’s rule, Eigen values, pivoting, singular matrix, rank of the matrix all those using this very helpful to understand the solution procedure.

(Refer Slide Time: 03:27)



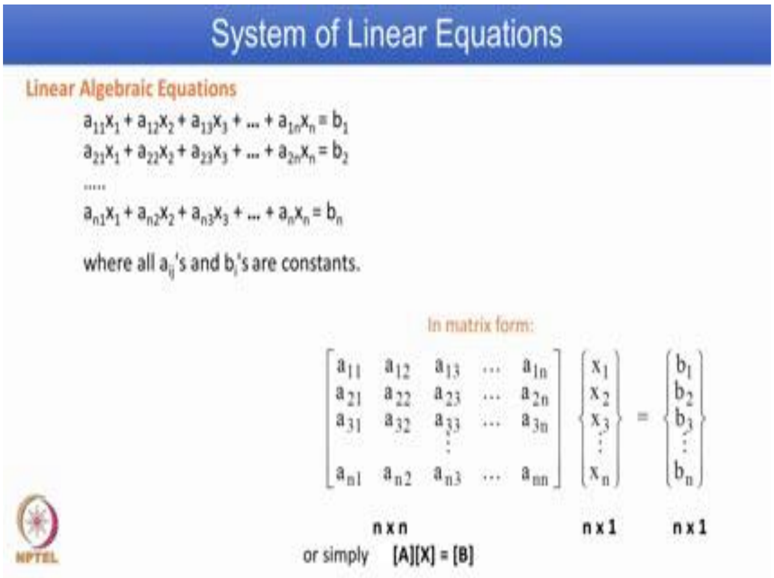
We will now focus particularly on direct methods. We are going to talk about three methods - Gauss elimination method, tridiagonal matrix algorithm, and LU decomposition. In iterative methods, we have Jacobi method, point or line Gauss-Siedel method, point or line successive over relaxation - SOR method, then there is an alternative direction implicit - ADI method.

(Refer Slide Time: 03:55)



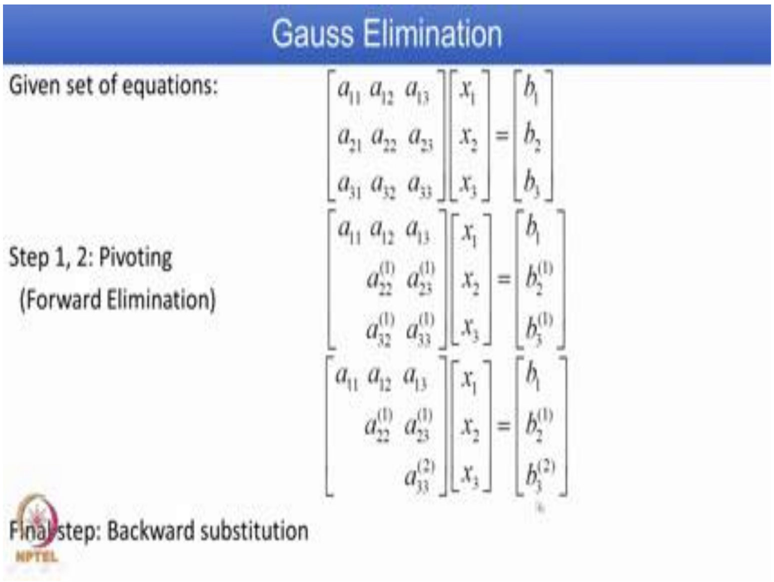
Gauss elimination method, it has basically two steps one is forward elimination and the second step is a backward substitution. In the forward elimination, the method reduces a given set of N equation into an equivalent triangular set. So, the coefficient matrix, at the end of the forward elimination step will result in the form of what is known as the upper triangular matrix. By doing so, at the end, the last equation will have one unknown and the unknown is directly computed then the remaining unknowns are computed by a step called backward substitution. This method is good, if the number of equation is less and when the coefficient matrix is sufficiently simple. And for large number of equation to be solved, which is the case for the example, say 3D calculation or if the matrix is sparse then this procedure of Gauss elimination is not economical. It may also lead to erroneous results. Number of floating point operation required in Gauss elimination method is of the ordered N cube. And we have today most of the programs are parallelized to get results quicker or turnaround time for computation to be as short as possible. In such case, we should have a matrix inversion procedure also parallelizable, the gauss elimination procedure is not parallelizable.

(Refer Slide Time: 05:43)



Let us look at in detail, a set of linear algebraic equation is shown here, where a as well as b are constants. Same equation in the form of matrix is written here, coefficient matrix a, it has elements a 1 1 for example, all the way up to a n n, then unknown column vector x from x 1 to x n. Then on the right hand side, we have the known column vector b 1 to b n. So coefficient matrix a has n by n size, and column vector unknown column vector has a size n by 1 in the final and right hand side b matrix has a size n cross 1. In simple form, it is written as A X i equal to B.

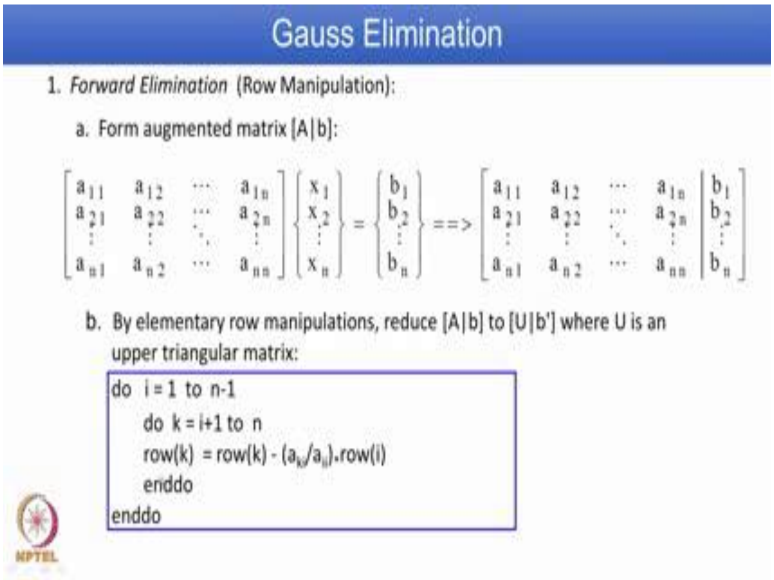
(Refer Slide Time: 06:41)



We will see the procedure for three by three combination matrix. So, here it is elements are given a 1 1 a 1 2 a 1 3 for example, and column vector is given unknown x 1 x 2 x 3 and the right side you have b 1 b 2 b 3. So, in step one and two, because there are only two steps in these because you have only three by three matrix; step one and two involved pivoting and that is stage is called forward elimination. So, in the first step, a 1 1 a 1 2 a 1 3 is not altered, whereas the second row and third row are altered; and altered coefficient is written with the superscript in the bracket one. Correspondingly coefficient matrix on the b is also altered and that is also written here b 2 superscript 1 and b 3 superscript 1.

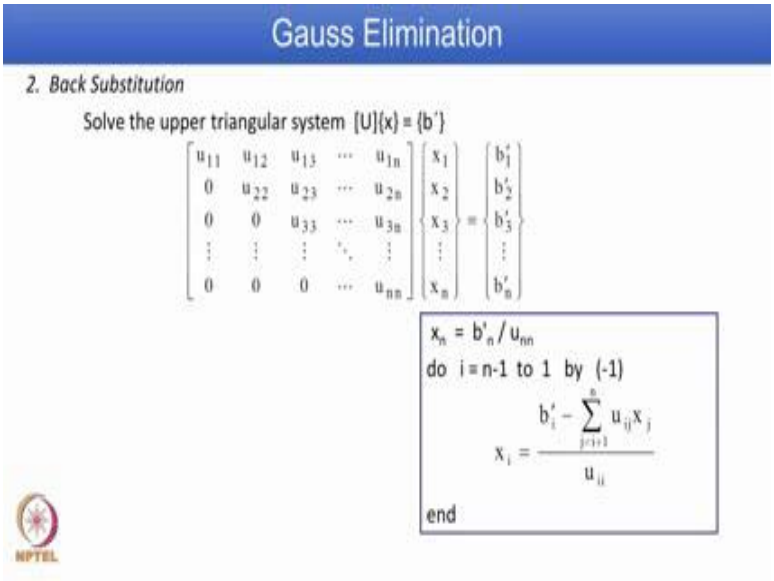
Now you do the pivoting for the second step also, and you can observe the third row is now altered as a 3 3 with the superscript 2 standing for that it is a second time pivoting, correspondingly coefficient b also changed b 3 with the superscript 2. Now we can immediately observe the coefficient matrix, original coefficient matrix a is now reduced to upper triangular matrix as shown here. The last row for corresponding unknown x 3 and you can immediately get x 3, then we follow what is known as the backward substitution in this direction to go x 1.

(Refer Slide Time: 08:25)



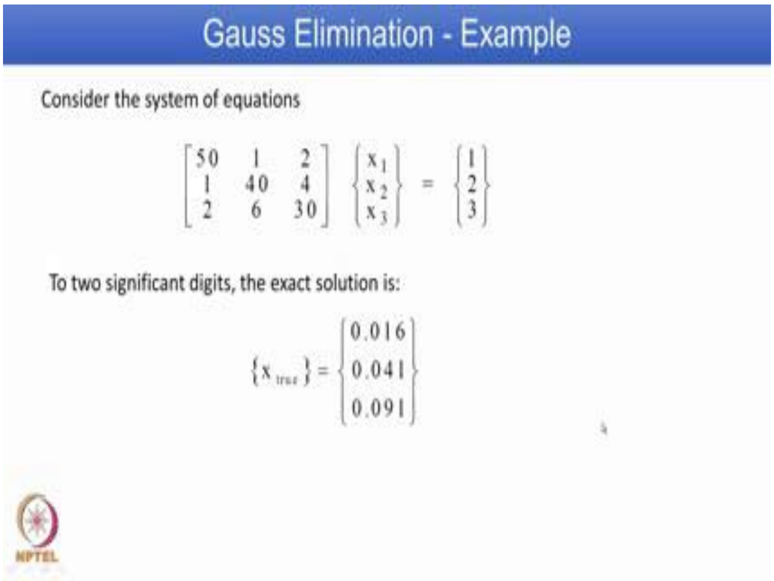
So in forward elimination, we do row manipulation, we also have a procedure what is known as the augmented matrix and which is represented here as A is the original matrix with the line and b is element to use for augmentation. So, a 11 a 1 2 a 1 n all the way up to a n n that the coefficient matrix is now augmented by including right side b matrix and that is shown in this. Now, we perform elementary row manipulation reduce that augmented matrix to U upper triangular matrix; with every time, we get the new value for coefficient matrix b also. What is shown here is the skeleton of the program used to perform this operation. So, do i equal to 1 to n minus 1, do k i plus 1 to n row of k is equal to row of k minus this is the pivoting operation and you end the do loops.

(Refer Slide Time: 09:36)



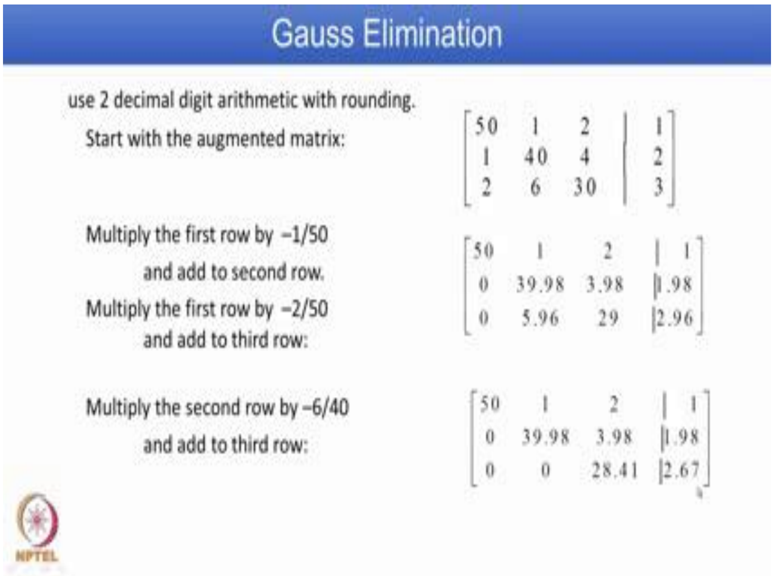
Now you do the backward substitution because all now becomes upper triangular matrix and you can immediately recognize the last row of that matrix u n n is the only element, all other elements are zero. So, if you write equation corresponding equations for this, it becomes u n n x n equal to b n prime. So, we directly get x n, then we use that to obtain other unknown coefficient in the reverse order from x n minus 1 to x 1. This is achieved by what is known as recursive relationship and that is what is shown in this formula x i is equal to b i prime minus summation j i plus 1 to n u i j x j by u i i. Now because that is a recursive relationship, it is also easy to program and this is the structure of the program which you might use to get the backward substitution.

(Refer Slide Time: 10:43)



We explained the gauss elimination procedure with the help of a simple matrix as shown here. So, 50 1 2 1 40 4 2 6 30 are the elements of that matrix, x 1 x 2 x 3 are column vector unknown values equal to the right side one two three. There is a exact solution available for this matrix system and that is also listed as shown here as 0.016 0.041 and 0.091. We explained Gauss elimination procedure for this system in the next two slides.

(Refer Slide Time: 11:25)

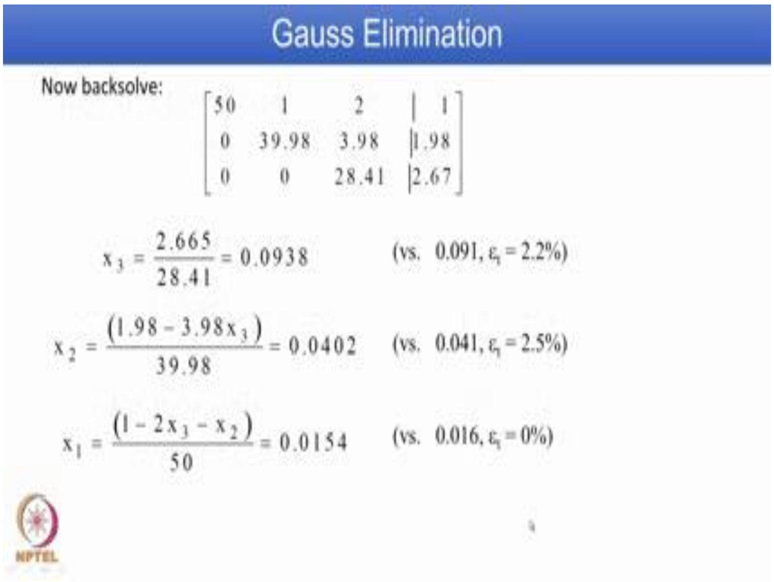


Coefficient matrix is written along with augmenting, considering the right side value 1 2 3 as shown here. So, we do few arithmetic operations, and we decide to have a two decimal accuracy. So start with the augmented matrix as shown here. First operation, perform multiply the first row by minus 1 by 50 factor and add to the second row. So, second row, first element is 1, first row first element is 50, you want to make the second row first element as zero. So, to do that we multiply first row by minus 1 by 50 and add to the second row and that will result in zero for first element in the second row.

Similarly, the third row, the first element is two, and we have to make it to zero; to achieve that, we have to do this operation; multiply the first row by minus 2 by 50 factor and add to the third row. So, if you perform these two operations on this matrix including the augmented column then it will result as shown here. The first row remains the same, second row first value goes to zero that is the intention, similarly the third row first value goes to zero that is again the intention, and remaining values gets adjusted because of this operation. So, 40 become 39.98, 4 become 3.98, and 2 becomes 1.98. Similarly, for the third row, because we are following accuracy up to two decimals, we have written here values up to two decimals.

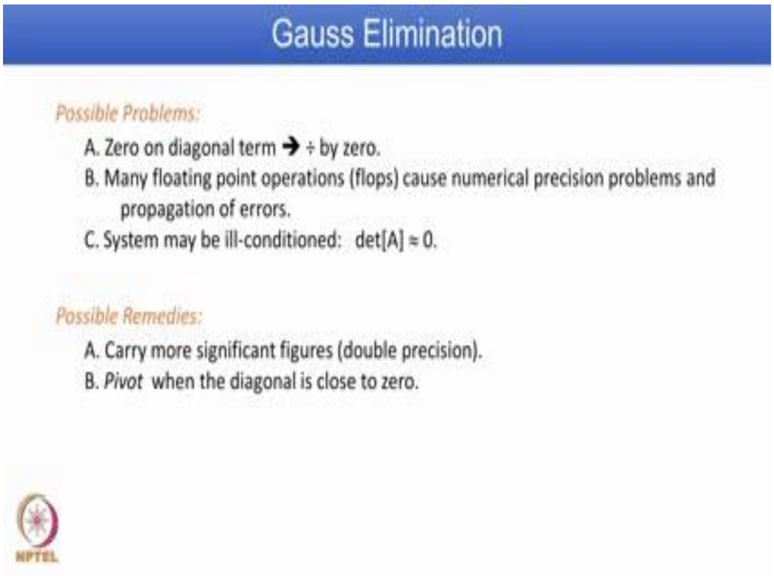
Please recall in the Gauss elimination, we have to make the matrix, upper triangular. So, the lower part has to go to zero that means, in this case, we have to make the second element third row also zero. So, to do that we have to perform one more operation as given here; multiply the second row by 6 by 40 and add to third row, and that will result in the second element the third row has zero, the remaining values gets adjusted as shown here. So, original matrix which is displayed here gets converted into upper triangular matrix as shown here, so 50 1 2 0 39.98 3.98 0 0 and 28.41and 2.67.

(Refer Slide Time: 14:28)



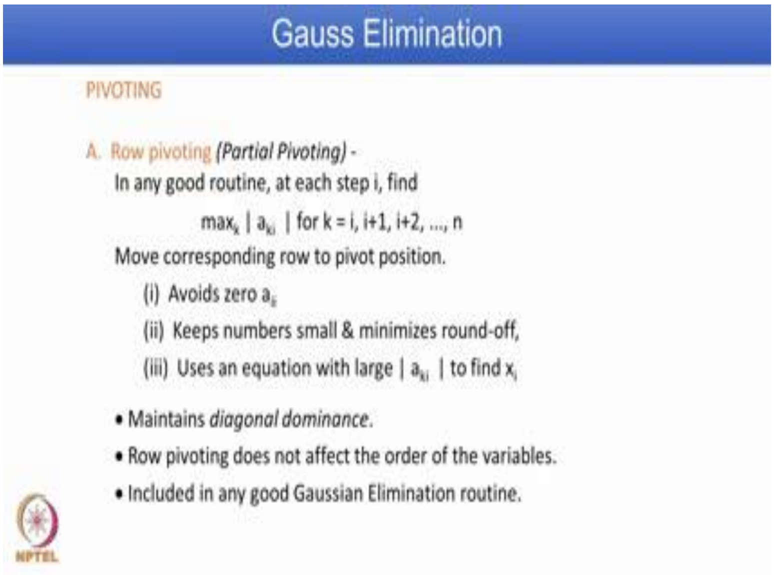
So, we do first forward elimination, and then backward substitution, the matrix is reproduced here. So, backward substitution is start from the last row. So, last row is 28.41 into x 3 equal to 2.67. So, to perform you get value as 0.0938. We compare this against the exact value that is 0.091, and the error is approximately 2.2 percent. We do the back substitution, so second row will give you the x 2 value and first row will give the x 1 value as shown here, and corresponding deviation percentage with respect to the true value is also shown here. So, they are within acceptable level that is 2 to 2.5 percent.

(Refer Slide Time: 15:23)



The possible problem in Gauss elimination zero may be there on the diagonal element and when we perform floating operation, we may end up a statement like dividing by zero. And we have observed, there are many floating point operation, in other words flops, and which may cause numerical precision problem because you are handling so many operations, and every time you are approximating. And any error introduced at any state will propagate and finally, you may get erroneous result and system may be ill condition for matrix condition determinant A is the approximately are very close to zero situation. There are solutions available for this kind of problem; one you can carry more significant figures. So, instead of limiting to three decimals, you can know as the double precision just handles up to 16 significant positions after decimals. Then it is also possible to have different pivoting strategy in the next few slides, we are going to talk about different pivoting strategy.

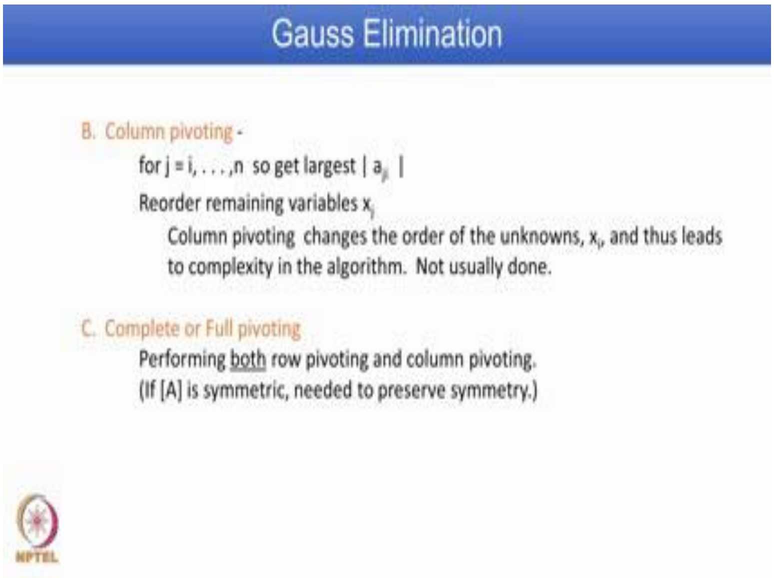
(Refer Slide Time: 16:39)



So, pivoting we have three different types, first one is what is known as row pivoting; it is also otherwise called partial pivoting. It is good for many situations; at every step at i, we find the max corresponding to k i to n and all other elements are adjusted for that maximum value. So, move corresponding row to the pivot position. It avoids any zero elements because you are finding out maximum value, and zero is automatically avoided and that helps to avoid dividing by zero error. And it keeps number of small and minimizes round off error, and it uses an equation with large element value to find x i. It maintains diagonal dominance, we already seen why it maintain diagonal dominance.

The row pivoting does not affect order of the variable. So, this is very important because we are dealing with the matrix, we are dealing with unknown coefficient, it should not change the order of the variable, and it is included because of these properties in any good Gaussian elimination procedure, so normally we do only row pivoting.

(Refer Slide Time: 18:06)



Next pivoting is the column pivoting for j 1 to n get the largest value. So, this is like row pivoting instead of row, we consider column. And reorder remaining variables x j, this column pivoting results in changing the order of the unknown x i, hence it may lead to complexity in the algorithm, and this is usually not preferred. There is another procedure what is known as the complete or full pivoting, where we perform both row pivoting as well as column pivoting. If coefficient matrix A is symmetric then we need to pay attention to preserve symmetry while doing this kind of pivoting. So, in today's class, we have particularly seen Gauss elimination in detail; tomorrow's class, we see a special form of Gauss elimination procedure, what is known as the Thomas algorithm for triangular system of matrix.

Thank you.