Computational Science in Engineering
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Lecture – 01
Computational Science in Engineering

Hello all, welcome to this particular course, which is designed for Computational Science in Engineering just to give you an idea about this particular course we will just talk about what is preliminary planned for this course and what about. So, myself is Ashoke De, currently working as Associate Professor in the Department of Aerospace Engineering at IIT, Kanpur. So, I will be the instructor for this course and what is Computational Science and Engineering?

Essentially this is an evolving field, which actually explodes the power of computational tool or computational methodologies to solve or to address issues in practical problems, whether it is in engineering or social sciences or such kind of field. So, the whole idea or the primary idea is that to use the computational science techniques or the methodologies to solve the problems, so in a nutshell or essentially, they should talk about or try to frame and framework for solution methodologies for large scale problems.

And now, when you use the power of computation, obviously it is based on certain primary things and like a linear algebra or differential equations. So, these are sort of the building blocks towards those devising those kinds of methodologies.

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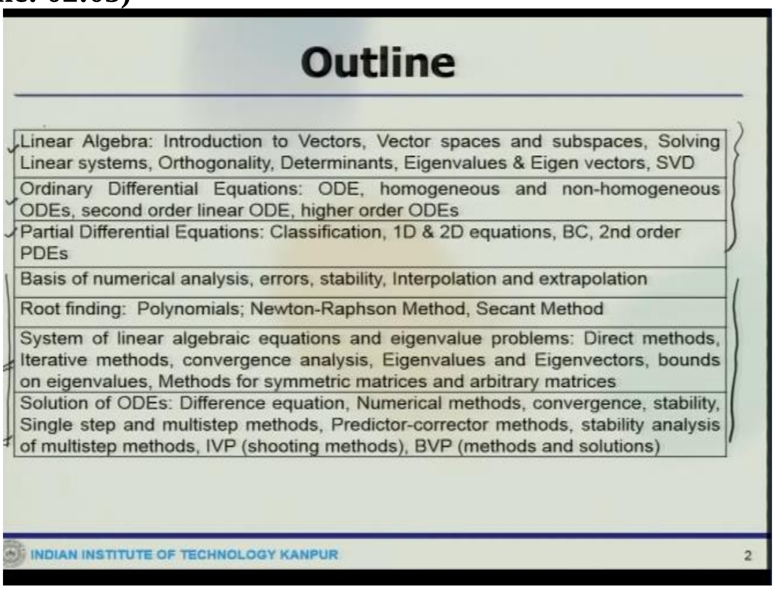

So, what we are going to cover in this particular course that you can see here, so as I said the primary focus actually lies on developing the problem-solving methodologies or robust tool for numerical simulation. And here the idea of the goal is to present the fundamental of numerical techniques or scientific computing with sort codes, wherever it is required to sort of establish the key concept.

So, obviously, it includes some frameworks of the applied mathematics such as linear algebra, what we see here, then differential equations, whether ODEs or PDEs. So, these are the sort of building blocks, which will allow to look at this computing methodologies and then to solve a problem or address the scientific or engineering problem. So that essentially, it would lead to some sort of a skill set, which you will develop for mathematical modelling based on computational technique.

So, as you see that initial part, we will be talking about like some of these applied mathematical algebras, which will include linear algebra and where we will talk about all these different vectors, vector space, Eigen values, orthogonality, single value decompositions and all such things. Then talk about little bit of ODEs and then PDEs, but then we will move to this part, where we will be talking about all these numerical methods.

And as you see that we will talk about in details about solving solution of the linear system, and different issues related to that here, when you will come to here and then ODEs. One may immediately think about that is nothing mentioned about PDEs, we will just talk about a little bit but not too much, because when you talk about or devise some techniques for PDEs, these actually lead to a typical some of the dedicated core future in terms of computational fluid dynamics CFD or compressible fluid mechanics whatever it is, to that short will not go into the detailed discussion of any formulations for PDEs.

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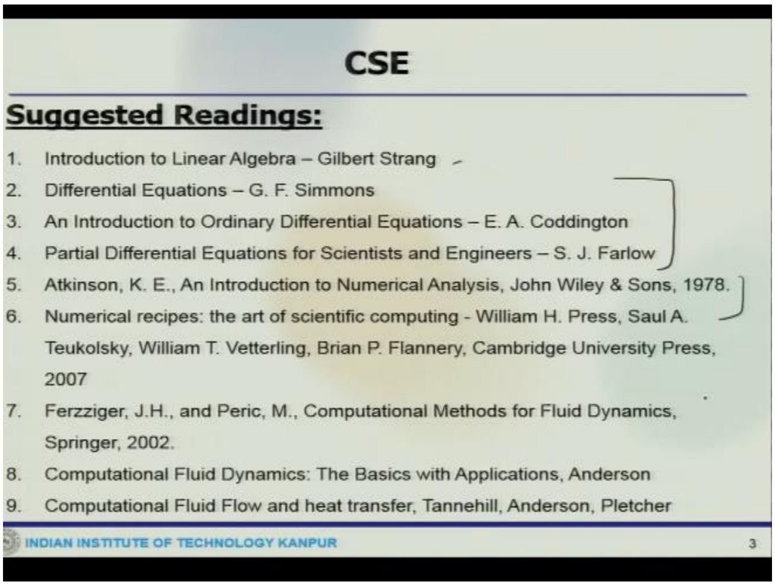

And these are some of the suggested books which would be kind of useful like the linear algebra part is very much, one can follow the Gilbert Strang or any engineering mathematics book. Then these are for differential equations and then the couple of numerical techniques, books or scientific computing books and then some computational fluid mechanics books which we will talk about and all these. So, that is what pretty much what you can expect that what we will be talking about in this particular course.

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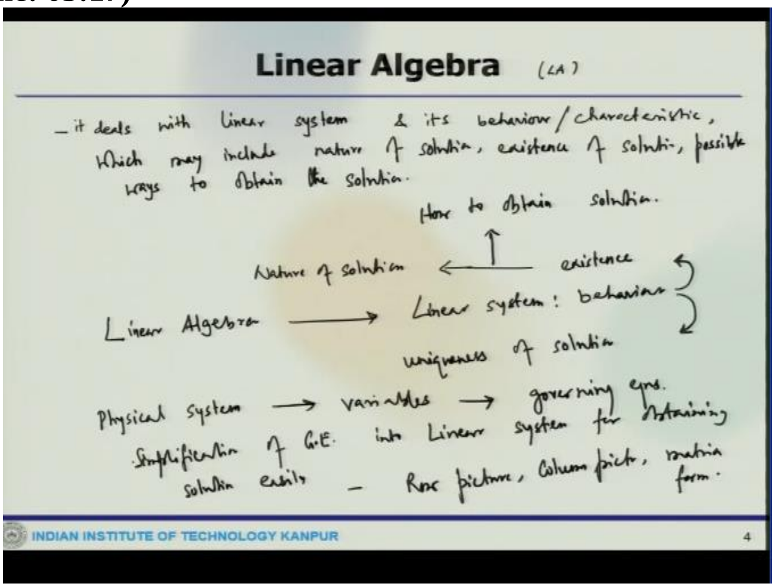

So, let us start with the discussion and first thing that as we mentioned that we will start with the linear algebra. So, what linear algebra does that it actually deals? So, one can say linear algebra it deals with linear system. So, which is not essentially a linear equation and its behaviour or characteristics which may include nature of solution, existence of solution and possible ways to obtain the solution, so that is what linear algebra does.

So, what if you look at that, if my linear algebra if you talk about so, this will deal with some linear system so, let us say the behaviour of that and then one can look at the uniqueness of solution or other way one can look at the existence of the solution. So, which will lead to like nature of solution and obviously then how to obtain solution? So, how you deal with the things, so essentially what you have is a physical system.

So, that means, there are certain quantities or variables which are associated with that, which will lead to some sort of and governing equations, which are kind of going to represent that problem. So, here now simplification of governing equations into linear system for obtaining the so, basically one can think about the simplification of governing equation into linear system for obtaining solution easily. So, what do we look at it that we will look at different things like row picture, column picture, matrix form so, these are the things which will come on the way.

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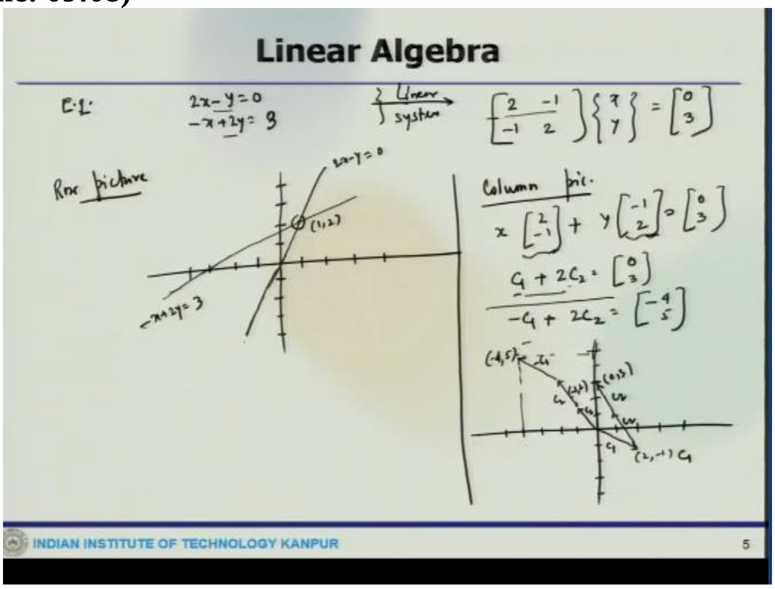

Now, let us start the discussion within simple example so, let us take an example so, let us say my system is $2x - y = 0$, $-x + 2y = 0$. So, now, if we convert that to a linear system, so the linear system of this one can write like

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{Bmatrix} x \\ y \end{Bmatrix} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$$

So, if we change that, then we can write in that way now, what we can look at first is the row picture as we mentioned. So, how do we look at it so that means we are going by this is the row, so we will go as a row picture.

So, let us draw this and so when I do that what it happens that this is (2, -1) and so they should be going through 3 and then so like this, this guy will pass through. So, this is $-x + 2y = 3$.

So, this is what it goes through, then the other guy goes through from here, which would be show through this line, which is $2x - y = 0$. So, this should be (1, 2) so we will go by that means this is first row, this is second row so this is how it looks like.

Now, if you on the other hand look at the column picture, so column picture we can rewrite this guy as

$$x\begin{bmatrix} 2 \\ -1 \end{bmatrix} + y\begin{bmatrix} -1 \\ 2 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$$

So, from column picture, it says that from some linear combination of two left hand side columns will give the columns of the right-hand side. So, what it is that

$$C_1 + 2C_2 = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$$

Again

$$-C_1 + 2C_2 = \begin{bmatrix} -4 \\ 5 \end{bmatrix}$$

So, you can see this is C_1, should these guys C_1 this is C_2, so if it is $C_1 + 2C_2$, so that gives me (0, 3).

And if I take in a different combination, so these are the column vectors, which are going to do like this. So, when I plot this guy in a column picture, so this would be interesting to see like when we do that, so the first column is (2, -1), so this is (2, -1). So, this is (2, -1) or sort of C_1 or this is the vector of C_1 and the second one is (-1, 2), so this is C_2 so (-1, 2) that C_2. |Now what you say $C_1 + 2C_2 = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$

So that means comes here, so this is C_1 and then $2C_2$, if we go that means we will go parallel to this, like this and then we go another C_2, so this is C_2 this is C_2. So, we come here, (0, 3). So that means when I add this column vector, this is C_1 then $2C_2$ along this direction that gives me (0, 3). Similarly, when you do this guy $-C_1 + 2C_2$, so this is (-4, 5), so it should be here. So, C_2 it goes like another C_2 then $-C_1$, so it goes like that.

So, this is $-C_1$, this is C_2 so this is (-4, 5) so this is how the column picture actually behaves. So, the column picture does basically deal with the linear combinations. For 2D case, this solution was available through both row and column picture, but when you go to 3D, so that things become a bit complicated. So, let us take an example on 3D.

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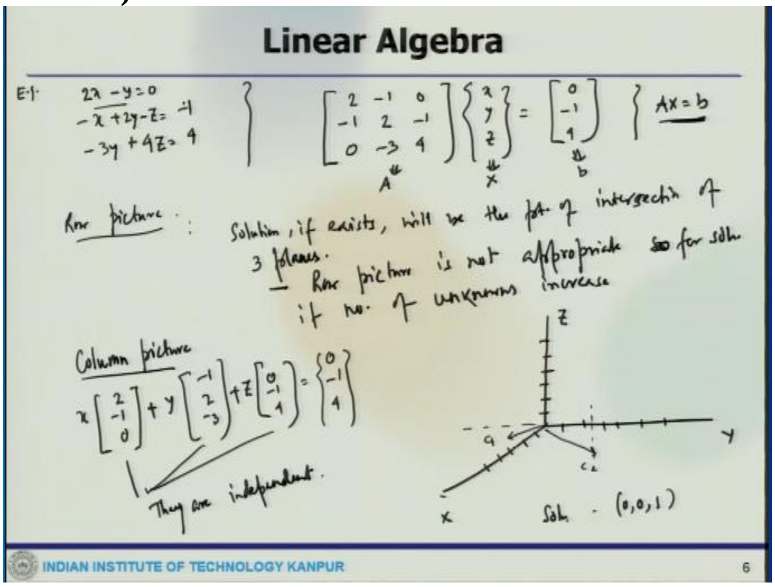

So, let us say we will consider

$$2x - y = 0$$

$$-x + 2y - z = -1$$

$$-3y + 4z = 4$$

So, now if we write this, this should be written as

$$\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -3 & 4 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 4 \end{bmatrix}$$

So, essentially, one can think about this is A, this is x, this is b, so, that gives me Ax = b. Now here the row picture if we see the row picture, so, each of the 3 equations denotes 3 planes, so these are planes. So, each row is 3 planes and if the solution exists it will be the point of intersection of 3 planes. So that means so the solution if exists will be the point of intersection of 3 planes.

Thus, however, it is hard to visualize, so this is in 3 dimensions so, it would be have to visualize. Hence, row picture is not an appropriate solution essentially that is what it is that row picture is not an appropriate for a solution if number of unknowns increase or row increases. So, this is not a sort of and easiest way to look at things, so rather to try to look at from the column picture.

Now, what column picture tells us that this guy can be written as

$$x\begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix} + y\begin{bmatrix} -1 \\ 2 \\ -3 \end{bmatrix} + z\begin{bmatrix} 0 \\ -1 \\ 4 \end{bmatrix} = \begin{Bmatrix} 0 \\ -1 \\ 4 \end{Bmatrix}$$

So, here again if someone at least in 3 dimensions draw it, so, this is x y, z. So, this would be essentially you somewhere 2, so somewhere C_1, somewhere this would be C_2, we somewhere here like this. Now another important thing is that these column vectors are not parallel and also, they are not arranged as 1 as the sum of the other 2.

So, hence these guys, these, these and these they are sort of independent vectors. there also important to look at, they are also not in the same plane. Here the solution will be the final solution would be (0, 0, 1). Now, these kinds of graphic visualizations become impractical for more than 3 dimensions because that is where you cannot visualize, but the unknowns if they are more than 3 or it increases, then even the column picture or graphical visualization become difficult.

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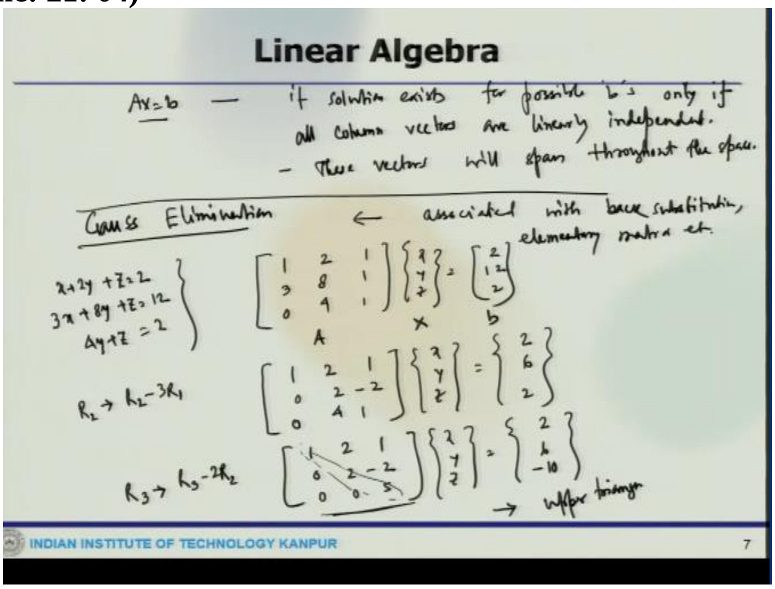

So, the point here is that we have to come up with other ways to find out so, now the point Ax = b, now if a solution exists for possible b's. So, this system Ax = b will provide a solution or the solution exists for possible b's only if all column vectors are linearly independent and also these vectors will span throughout the space. Now, the b column vectors produce 3 different planes in a 3D space and hence, have solution for any b.

However, if number of planes produced is less than the space dimension, then the solution may exist only for specific b's, so that is a very important thing to note. Now, we will look at how we do so the Gauss Elimination, what we does? In the Gauss Elimination, so this would be also associated with back substitution elementary matrix. so, these are sort of associated with that substitution elementary matrix etcetera.

Again, here also we will try to look at the things through examples again, we will take an example

$$x + 2y + z = 2$$

$$3x + 8y + z = 12$$

$$4y + z = 2$$

So, if we write them down

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 8 & 1 \\ 0 & 4 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 12 \\ 2 \end{bmatrix}$$

so this is here A, this is x, this is b. Now here in the Gauss elimination process, we will do or it is done by row elimination. So, what we will do here? We will do

$R_2 \rightarrow R_2 - 3R_1$

so that will give us

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 4 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 6 \\ 2 \end{bmatrix}$$

Now the second stage, what we will do,

$R_3 \rightarrow R_3 - 2R_2$

and we will get

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 0 & 5 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 6 \\ -10 \end{bmatrix}$$

So, here what we get here this if you look at you have the diagonal elements setting here, now, this is a 3×3 matrix and the below diagonal elements are missing or kind of eliminated. So, this is an upper triangular matrix and what we get the solution is received by the back substitution.

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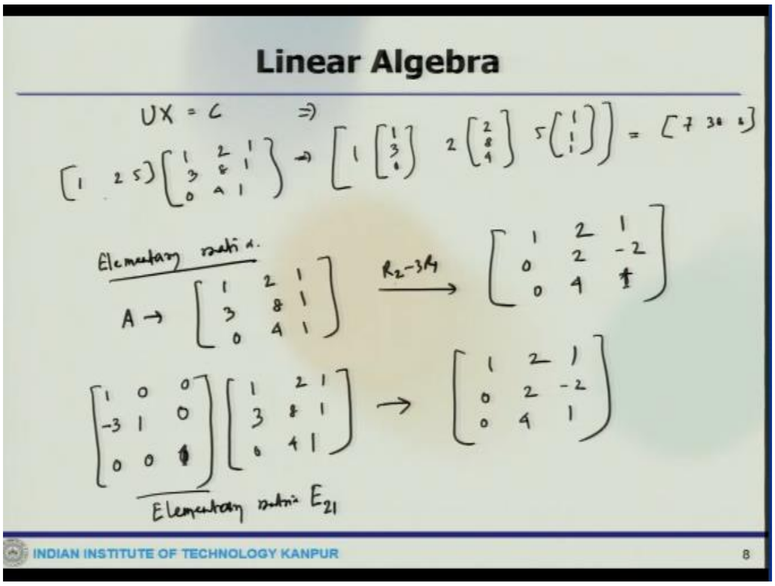

Now, the point is that if the first pivot, so this is the first pivot, if the first pivot is 0 then rows are exchanged, Gauss elimination fails to give solution when all pivots are 0. So, this is one of the limitations that one has to keep in mind that if that happens then no one would be do. Now upper row operations what do we get we get an upper triangular matrix UX equals to let us say C, so this is what you get this is a new vector C.

So, U is upper triangular matrix here what we get that this will now the row vector multiplied with the matrix will give a row vector for example, we do like for example,

$$\begin{bmatrix} 1 & 2 & 5 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 3 & 8 & 1 \\ 0 & 4 & 1 \end{bmatrix} \rightarrow \left[1 \begin{bmatrix} 1 \\ 3 \\ 0 \end{bmatrix} \quad 2 \begin{bmatrix} 2 \\ 8 \\ 4 \end{bmatrix} \quad 5 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right] = \begin{bmatrix} 7 & 38 & 8 \end{bmatrix}$$

Now, we come to the elementary matrix, what is that now we have this A which is $\begin{bmatrix} 1 & 2 & 1 \\ 3 & 8 & 1 \\ 0 & 4 & 1 \end{bmatrix}$, so here after row operation we got $\begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 4 & 1 \end{bmatrix}$. So, this is what we got to the first-row operation that we did. So, this could be multiplied with like then what we can say this is my original system $\begin{bmatrix} 1 & 2 & 1 \\ 3 & 8 & 1 \\ 0 & 4 & 1 \end{bmatrix}$ which got into this $\begin{bmatrix} 1 & 2 & 1 \\ 0 & 2 & -2 \\ 0 & 4 & 1 \end{bmatrix}$. So, here is the matrix which got multiplied and this is called the elementary matrix of E_{21}.

So, what did that we have done R_2 - $3R_1$, so here this would be

$$\begin{bmatrix} 1 & 0 & 0 \\ -3 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

So, this is what it does the elementary matrix, so when you do that, this is row operation so this should be 1, so you get back these things. So, we will see that when you have this row operation instead of doing that you can have an elementary matrix which is multiplied with this original matrix and you get the other one. So, we will continue this discussion in the next session.