Mathematical Modelling and Simulation of Chemical Engineering Process
Professor Doctor Sourav Mondal
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Lecture 37
Block Tridiagonal Matrix

Hello everyone. In this lecture we are going to talk about how we handle the Block Tridiagonal matrix and how essentially this Block Tridiagonal matrix can be solved. As this in the last class we have seen that this block tridiagonal matrix is obtained as a result of the 'simultaneous correction method'.

So, it is very important to understand that how does this block tridiagonal matrix can be handled or essentially solved, solved means essentially we need to work out its inverse. And then I mean this is a requirement for the calculation of the simultaneous correction method. Now, in the block tridiagonal matrix, the idea is very similar. It is very close to the situation where we have seen for the case of a normal tridiagonal matrix except that the elements of the block tridiagonal matrix are itself small matrices.

So, it is like a matrix inside a matrix. So, the idea of solving or handling this block tridiagonal matrix is similar to the in case of normal tridagonal matrix where we will be essentially trying to reduce or simplify this matrix structure in a way such that all the A elements are gone, all the B elements convert to unity and then we have non-zero C elements.

That is the principle of the Thomas algorithm that we have seen already for normal tridiagonal matrix. And the same thing we will apply to the case of block tridiagonal matrix also. And all these operations on the individual elements will also be some sort of matrix operation that we will be doing here. So, the idea the inspiration is same except that in the case of handling individual numbers we will be handling small matrices, okay.

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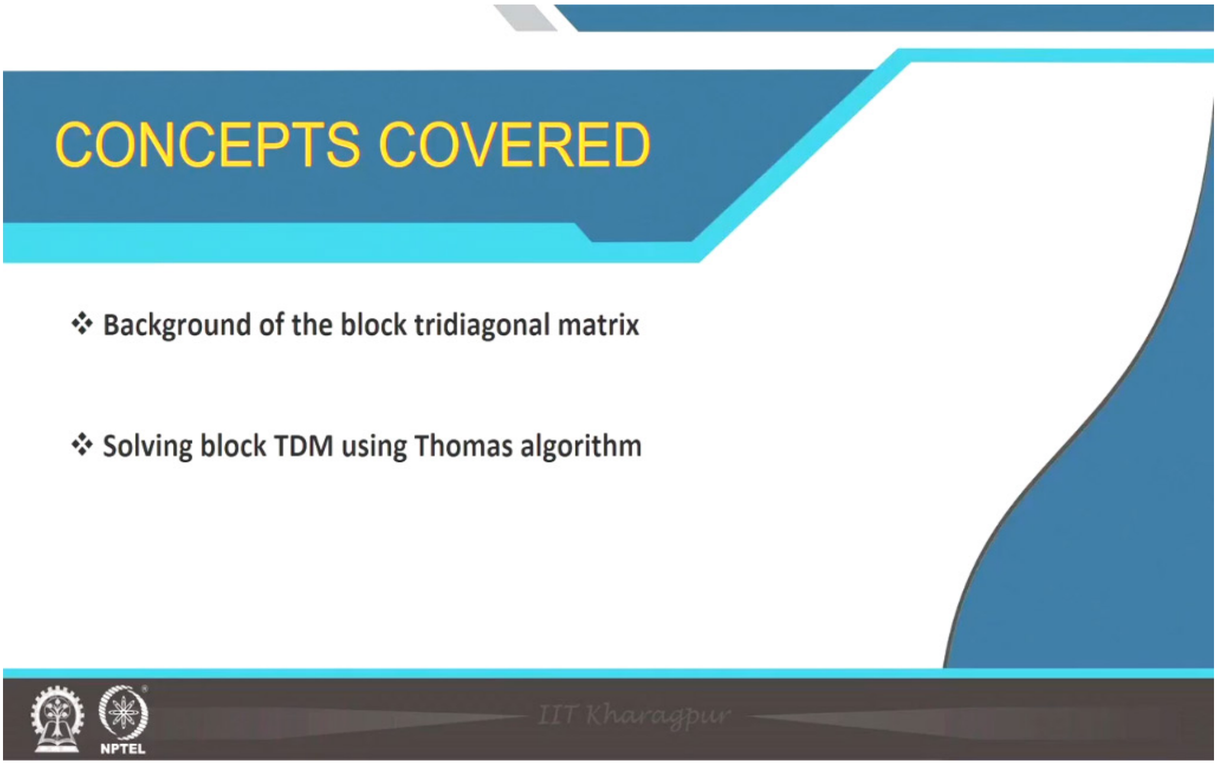

So, with this idea, let us move forward and as I have said here in this class we are going to talk about this block tridiagonal matrix.

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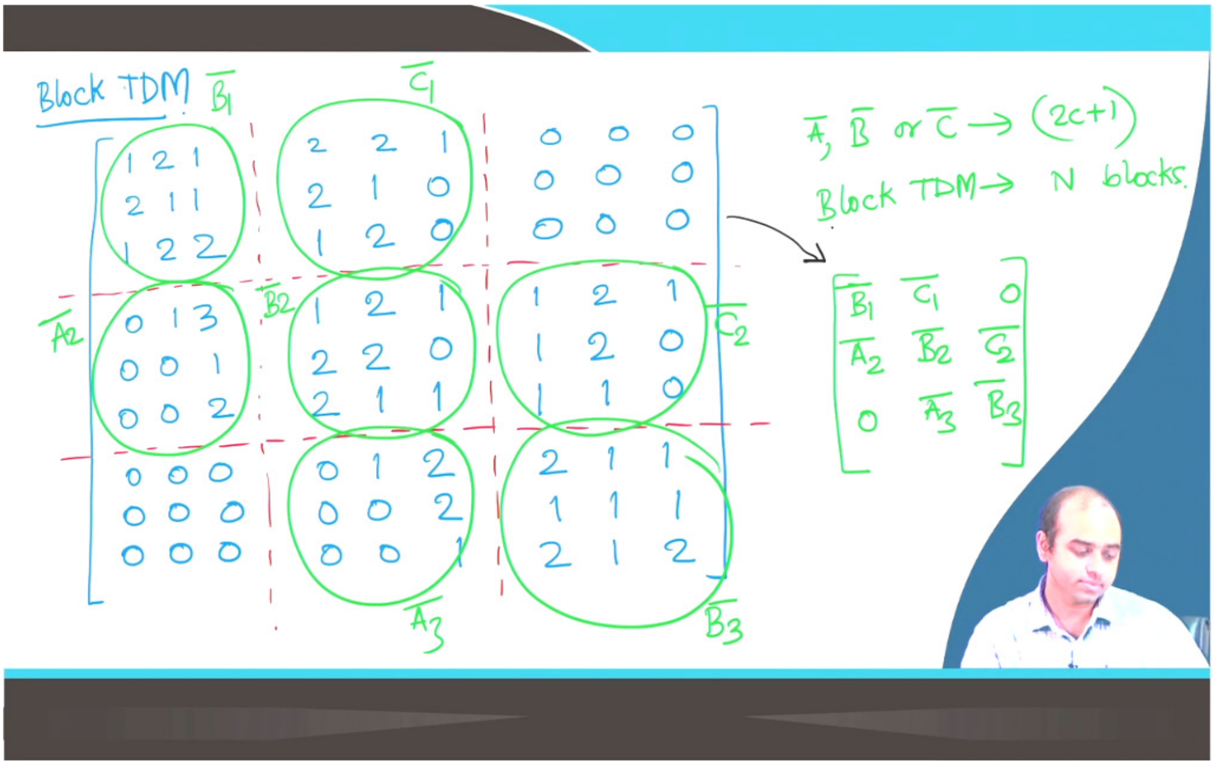

So, let us see how the block tridiagonal matrix actually looks like. So, I will first, this is just a example situation where we have a block tridiagonal matrix and this block tridiagonal matrix we consider like three blocks, 3 by 3 row blocks. So, essentially, we are having something like this. So, this is you can consider it to be one block, this is another block and here is the third block.

Similarly, let us write down the second column block and if you look carefully you will very soon realize that each of these blocks here, so, this is another block, this is the third block we are talking about. So, this element, I mean this block is essentially zero which gives you the idea of the block tridiagonal matrix where you have only the diagonal elements and one column after, I mean there is only the diagonal elements and one before and one after which are non-zero elements. So, here these are non-zero, I mean rest are zero.

So, in this case, these are zero blocks or blocks of zeros that we are getting. Just bear with me as I finish writing this block matrix. First consider this as a big block of the matrix where essentially these are the blocks we are talking about. So, this is divided into 3 by 3 blocks. So, you can designate, I mean essentially, we designate this is as one block.

So, I can designate this as B 1 block. This is another block, I can call that a C 1. Similarly, this is like our B 2 in this case. I am writing is a bar because these are matrix and not single elements. This is C 2 and this is A 2. And this is A 3 this is B 3. This is something I can always designate to, so, essentially this matrix, I mean this whatever this matrix that we have all these elements, I mean all these blocks B 1, C 1, A 2, B 2, C 2, A 3, B 3 these are all blocks are each of small elements, each are having small elements of 3 by 3 matrix.

So, essentially this number of blocks in the matrix represents the number of stages in the column. So, in this case, it is having, we are having it to be total number of blocks here as three. So, essentially, we can say that this is a three, there are number of stages is three in this case. And each blocks contain three by, each block is of 3 by 3 matrix.

So, essentially, you can think of this to be like 3 by 3 matrix means it is having one this, I mean these are X. So, this is essentially, one liquid, so, it is only a single component we are talking about, one is the liquid flow rate one is the vapor flow rate of that particular component, another one is the T A, T.

So, at least for a binary system, you will be having five elements in each block and number of blocks can be depending on the number of stages in the system. So, each of these blocks or each of these matrix is essentially 2 C plus 1 depending on how many number of components we are having.

So, in this case the number of components is one, as you can understand. Because it is only 3 by 3 matrix. So, with one component is essentially not a possible to do distillation. But this is just to give you a glimpse about how does the block matrix or what is the superstructure of the block tridiagonal matrix that we can think of.

And of course, this is not a realistic picture. Because at least, the realistic picture you need to have two components. So, each blocks will be having, will be of size at least 5 by 5 that is the minimum size we are talking about, even for a binary system. But 3 blocks are possible I mean the block tridiagonal matrix have three blocks.

So, that is depending on the number of states in the column. So, this means one reboiler one condenser and one is the physical stage. So, that is how you can think of in this way. So, then size of this A B C matrix or whatever this A B C matrix is whatever A B or C matrix that we are having is 2 C plus 1 and this block TDM generally having this number of n blocks, n is the number of stages in this case.

So, this is how the block tridiagonal matrix look like and you can always represent this as, sorry, this starting one is B 1, B 1, C 1 then zero then A 2 B 2 C 2 and 0 and then we are having A 3 B 3. So, this is how the big block can be translated here into this form of B 1 A 1 B 1 and say I mean A B and C block of matrix.

So, this is very similar the tridiagonal matrix except that the elements are individual blocks. So, with this block matrix the right hand term that we are having here is does exist. I do not know whether it is appropriate to write it here or maybe I should write it in the next page. So, let me write it down in the next page.

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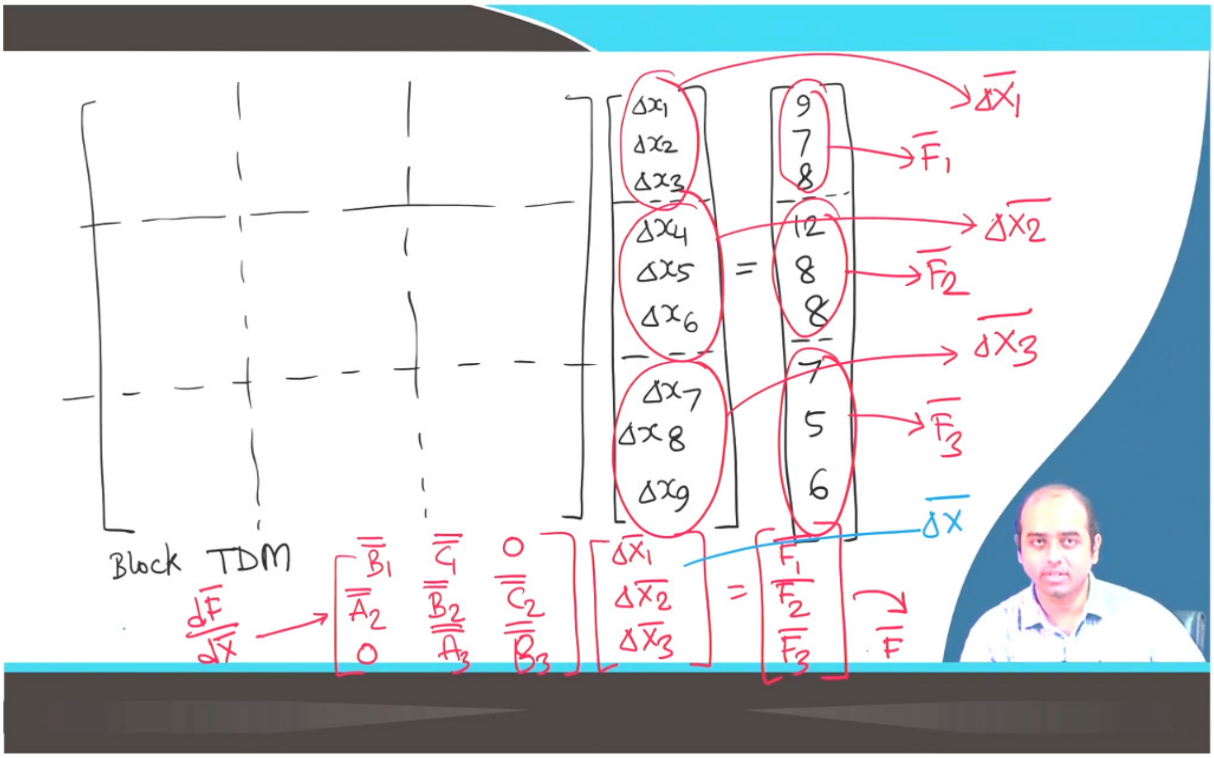

So, let us say this is our block. I am not going to write that block again. This is our block TDM and here I am having delta x 1, delta x 2, delta x 3, and on the right hand side I get similar such matrix blocks and Vector blocks. So, let us see the top is nine we put some numbers here. So, each of these blocks of delta x these can be written down as delta, I mean these can be written down as delta capital X 1 where capital X is a vector.

Similarly, this can be written down as delta X 2 and this part can also be written down as delta X 3 and these components whatever we are having is like capital F 1 this is capital F 2 and this is capital F 3. So, overall this entire thing boils down to this sort of scenario. This is a block tridiagonal matrix.

Then we have delta X 1 delta X 2 delta X 3 is equal to F 1 F 2 and then we are having F 3. And you can easily relate what do I mean by this delta X and F. So, these are essentially the from the Newton-Raphson this is the equation that we got that new this f of x is equal to 0 and then essentially when we differentiate d F d X I am going to get this block tridiagonal matrix. And this is I mean solving this equation out will give me the inverse of the d F d X. So, these essentially is d F d X and this is the capital delta X matrix and this is the F matrix.

This is F matrix and this is the delta X matrix. So, this is what we are trying to write down that F is, I mean, I mean d F by delta X into d F d X into capital F this is what we are trying to solve out, so that we get the new correction factor, I mean everything should be multiplied with alpha then we get our new correction factor. the solution of this will give me the inverse of d F d X. Now, how do you calculate this blocked tridiagonal matrix?

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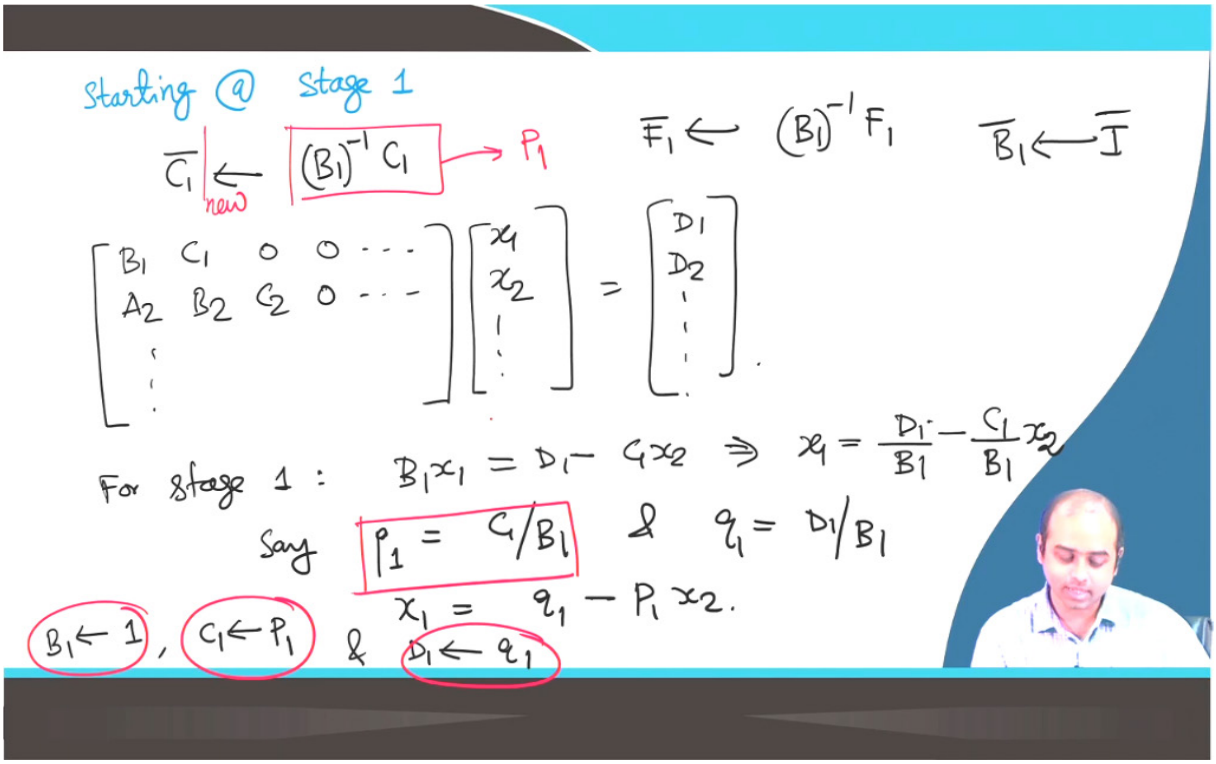

So, the inspiration is very similar. So, starting at stage 1 which is the first block, row of blocks, what we are trying to do is that we try to substitute whatever the C 1 that we have we are trying to substitute as B 1 inverse C 1 and F 1 we are trying to substitute by B 1 inverse F 1. And of course, B 1 will be substituted by the identity matrix.

So, if you are having this TDM where I am having, sorry, this B 1 C 1 zero zero like this then I am having A 2 B 2 C 2 0 0 and like this it is going on and on the right hand side I have this whatever this x 1 x 2 like this and then right hand side if I am having this. This was the normal tridiagonal matrix I am talking about.

Then if you recall for stage 1, we had the equation was V 1 x 1 is equal to D 1 minus C 1 x 2 and then we substituted x 1 is equal to this D 1 by B1 minus C2 by, sorry, C 1 by B 1 x 2. And then we said this P 1 is equal to C 1 by B 1 and q 1 is equal to D 1 by B1. So, we said that x 1 can be replaced as q 1 minus P 1 x 2. So, what does this essentially means that my B 1 is replaced by 1.

That is what the conclusion that we got that time from here, just a quick recap I am trying to give you that B 1 is replaced by 1 C 1 is replaced by P 1 and D 1 is replaced by q 1. These were the replacements or substitutions we made. And what is P 1? So, P 1 is C 1 by B 1. So, same thing we are trying to replace here and P, and ultimately P goes back to the position of the C 1. So, this new C 1 that we are talking about.

This is the new C 1, new C 1 will be, I mean this C 1 by B 1 should, I mean whatever this value will be replaced as the new C 1 and that is nothing but. So, this quantity in the old version is nothing but equivalent to P 1. And that is why we are trying to substitute.

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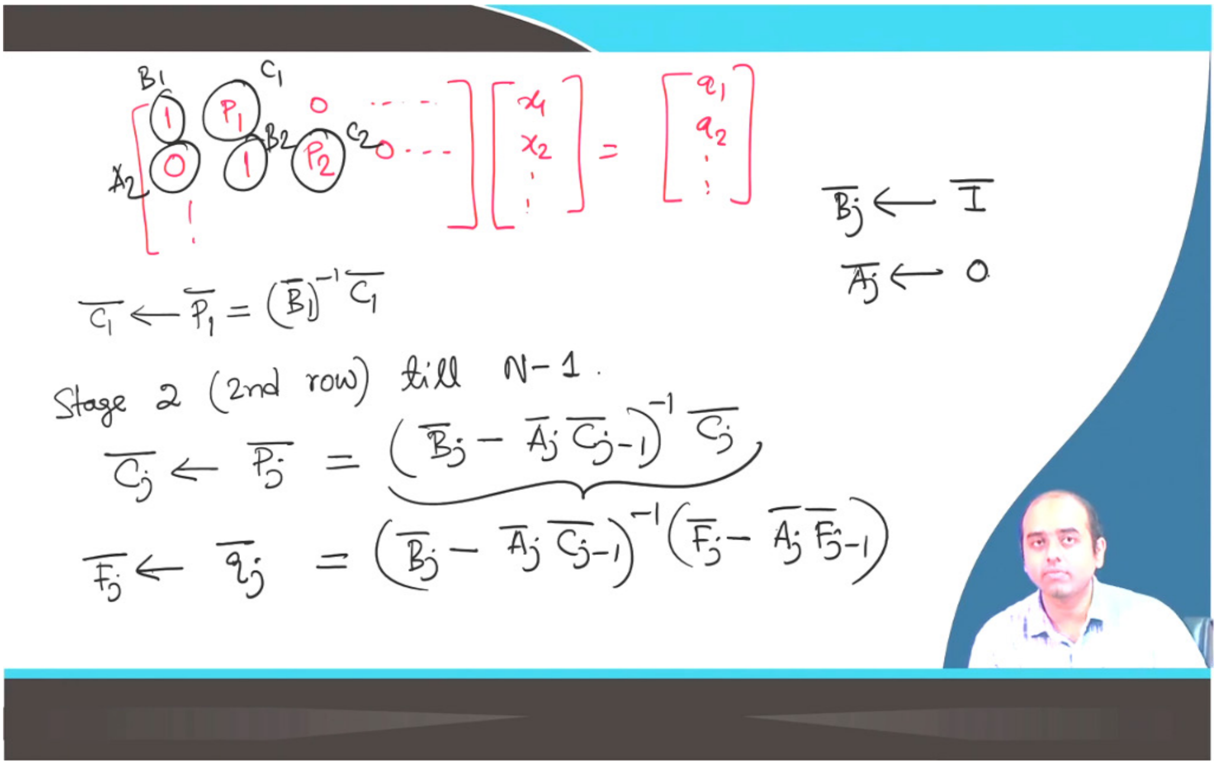

Because ultimately if I do the substitution, I am going to get something like 1 then P 1 0 0 0 like that. Then I am having 0 1 P 2 like that the tridiagonal matrix get transformed to. So, in the original equation this new position, I mean originally this was our B 1, this was our C 1, this was A 2, this was B 2 and this was C 2.

So, all the C are replaced by the value of their P and all the B are replaced by 1, in this case, block tridiagonal matrix the same thing happens here. Instead of writing 1, we write the identity matrix. So, this whatever this new C 1 I am getting that should be replaced by P 1.

And this is equal to B 1 inverse by your inverse C 1. Because please note, now, we are having all these as matrixes. So, now, it is like something divided by has to be done in inverse way.

Similarly, for stage 2, stage 2 that is the second row onwards till this N minus 1 all the C j are the placed by P j. And what is this P j here? This is B j minus A j C j minus 1, these are all matrix and this has to be taken inverse. Because ultimately, it is C by, divided by this quantity. So, this will be. So, this entire thing is P j in this whatever this is the normal tridiagonal matrix, this was ultimately the scenario.

Similarly, F j is converted into q j and which is B j minus A j C j minus 1 and in the numerator, this is in the denominator and in the numerator you had F j minus A j F j minus 1. So, these are all block matrix. So, instead of the normal multiplying numbers and division here, we are doing matrix multiplication and matrix inversion, now in this case. And B j is 1 and 1 we write as identity matrix and A j is now converted to zero. Everywhere it is zero. This is the conversion we are talking about now.

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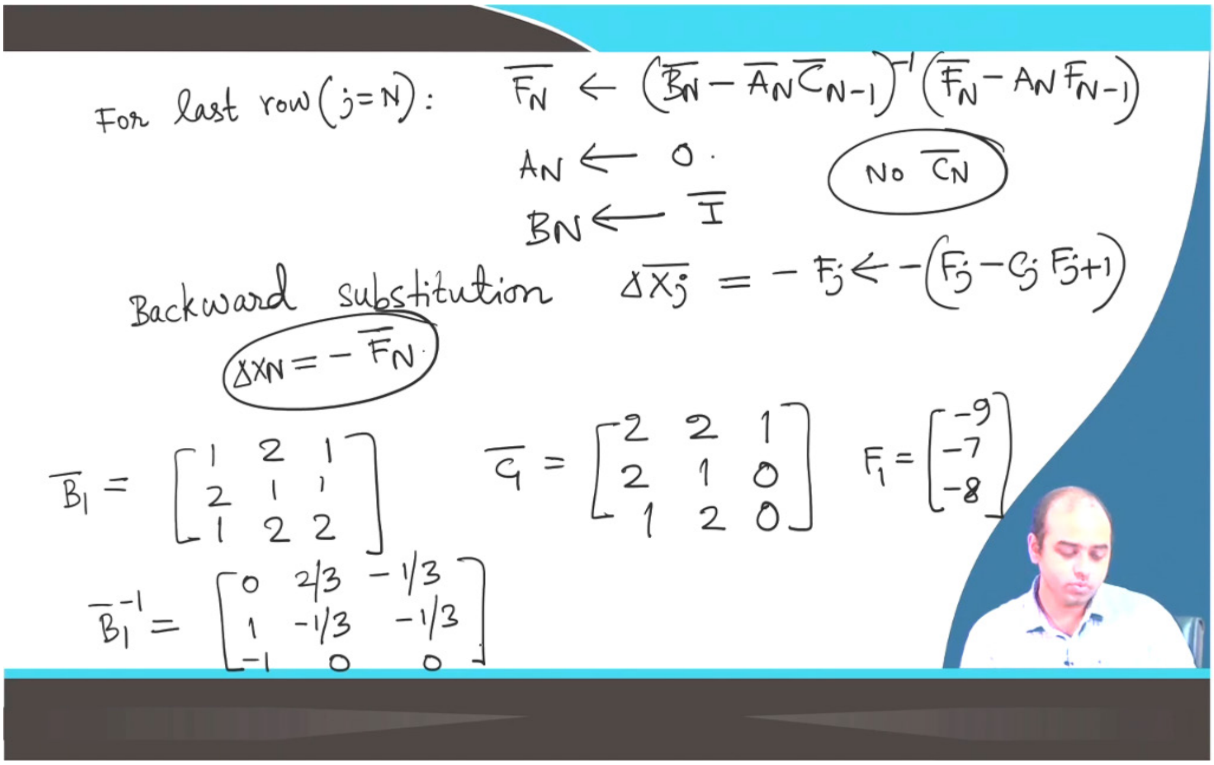

So, for the last row or j is equal to capital N, we have this F N matrix as B N minus A N C N minus 1, all are matrix, inverse F N. So, this F this is same as F j formula only. Now, A N for the last row is equal to zero and B N is I (identity matrix). So, there is no C N, no C N component for the last row.

So, if I do this backward substitution, I mean if I do this backward substitution at the last row which is something we used to do in the normal tridiagonal matrix and this is what the Thomas algorithm is all about, you do recurse, you start from the backwards or from the last row and then recursively calculate the rest of the row.

So, if I do the last row, I will be getting something like minus F j which is replaced as F j minus, sorry, C j F j plus 1 is the replacement that we are getting and this is the final value of our F component that we are seeing. So, delta X N ultimately becomes minus F N in the last row. That is what we are seeing that we do the backward substitution from the last row.

So, now, let us look into this scenario with the different matrix, so, our B 1 matrix is, if you recall 1 2 1 then I have 2 1 1 1 2 2. C 1 matrix I have, so, let me check the C 1 matrix once again. 1 2 0. This is our B 1 and this is our C 1 and then also I have my F 1 as minus 9 minus 7 minus 8. Because this is minus on the right hand side. So, now, we have to work out this B inverse.

So, since I have already done the calculation, so, I am writing it out straight away. This is the normal matrix inversion you have to do. Because these individual blocks are not tridiagonal matrix. So, these are normal blocks with having having certain non-zero values of these individual blocks. And essentially, they are not block, I mean they are not triangular matrix.

So, it is not necessary, I think it is not important to apply this whatever we have the tridiagonal matrix algorithm in this case. So, let me write this properly. So, we can essentially, calculate this inverse using the classical techniques. And these matrix are 2 C plus 1 number of components.

So, this is a costly operation here. Because this has to be done normally by the normal mode of the calculations to find out these inverses. And if you have more components then this matrix size would be large. It is 2 C plus 1. So, if you have 10 components in the system this will be like 21 cross 21 matrix. But this has to be done by the normal matrix inversion methods. So, this is the matrix by inversion this is what I get.

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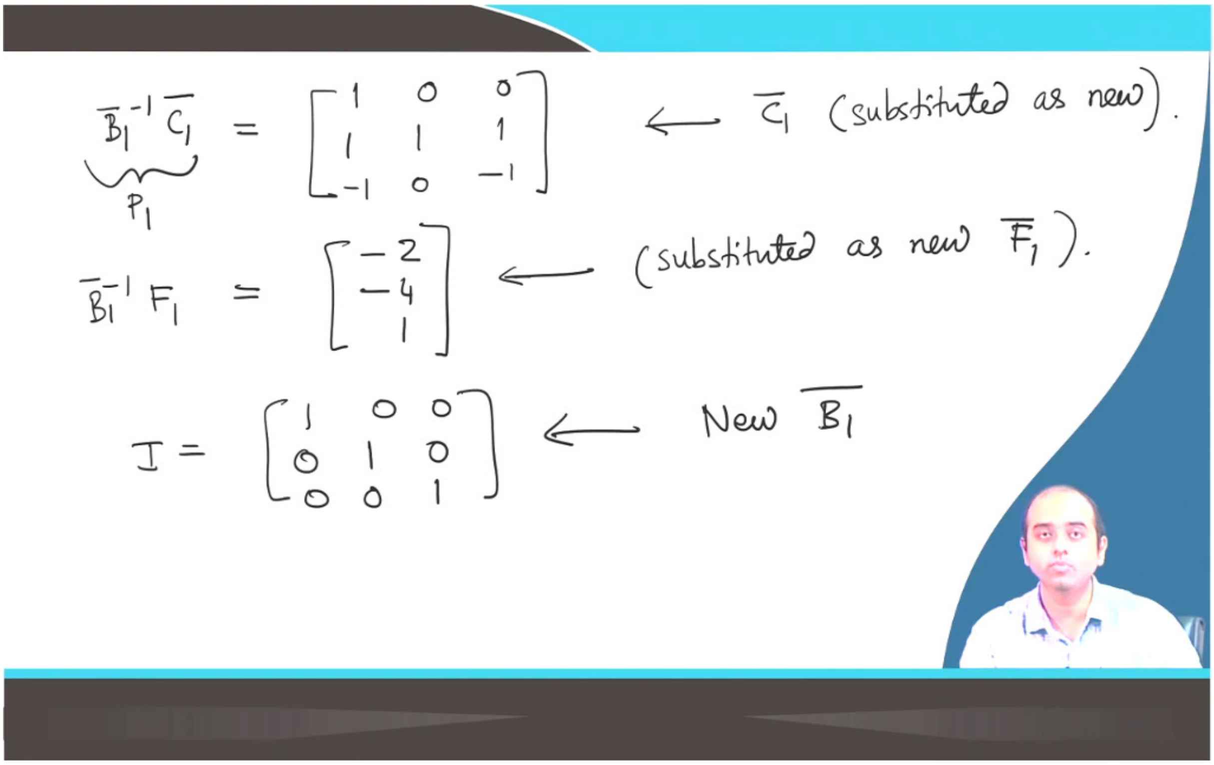

So, what I have to do, I mean I have to work out this B 1 inverse multiplied with C 1 this is my P 1 for the first row in this case. So, if I do the inverse multiplication of the inverse I will be getting like this, okay. So, this has to be replaced or substituted as new C1. Similarly, I can also work out B 1 inverse and multiplied with F 1 to get my new F 1.

So, this is my, this should be substituted as new F 1. And the identity matrix is only the diagonal elements are 1. So, this will be my new B 1. So, if you do this substitution in the first block row is complete for the new matrix.

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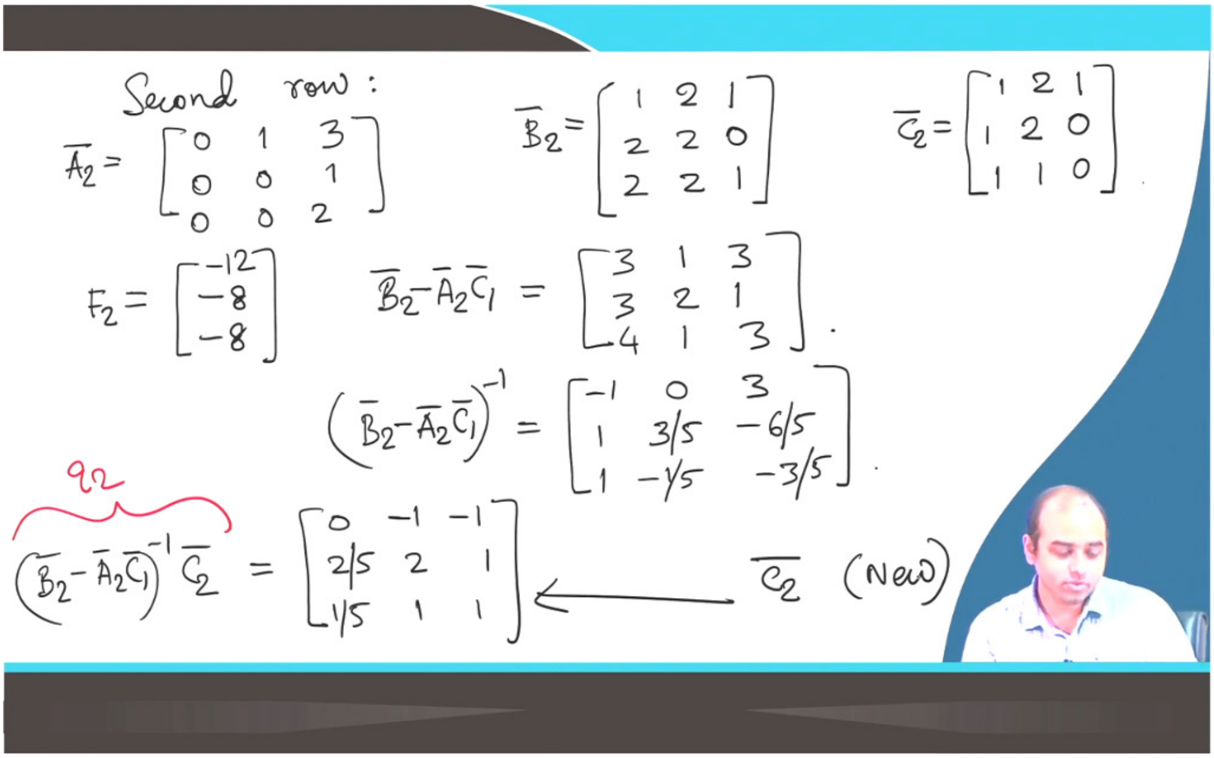

Now, the second row. From the second row, this little bit more operation. This is your A 2, this is the B 2 we have and this is the C 2 we have. And F 2 also is there minus 12 minus 8 minus 8. So, now, I want to do this quantity B 2 minus A 2 C 1. So, this is all matrix multiplication.

So, this stands out to be like this. You can also do it yourself and cross check the values. And the next subsequent thing is this B 2 minus A 2 C 1 inverse. We do it by classical inversion techniques. So, this B 1, sorry, this B 2 A 2 C 1 inverse has to be multiplied to C 2. These are all matrix and these C's are nothing but our, so, this quantity is same as q 2. I am just trying to relate everything from the normal tridiagonal matrix.

So, this number looks like this. And these we want to substitute as our new C 2. This is a new replacement or a substitution we are going to make into C2 over the existing value and this is the only non zero component or I mean rest are diagonal elements becomes 1, identity matrix. So, this block is the only non-zero block.

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And of course, new F 2 becomes like this in this case. So, next we try to write down the, I mean, similarly you can do it for A 3, sorry, B 3 and this F 3. Which is actually there is there is no C 3 in the last row and B 3 would be like just in identity matrix. So, if you work out this the total matrix now, it looks like. So, this is my first B 1 block. So, that is the identity matrix. So, 1 0 0, 0 1 0, 0 0 1 and below it all zero blocks. So, this is the first column.

In the second column, this is the having, we are having this new C 1. So, this is 1 0 0, 1 1 1, minus 1 0 minus 1. This is B 2. B 2 is 1 0 0, 0 1 0, 0 0 1, is identity matrix. And this is zero. This is A 3, all A 3 gone to 0 by this transformation. This is originally, it was 0 only, this because part of the tridiagonal matrix block. This is the new C 2 we are having. So, 0 minus 1 minus 1, then these are the values we got.

And this is our B 3. So, this ultimately forms the big block after transformation and this I write as delta X 1, delta X 2, delta X 3, delta X 4, delta X 5. And then this is the new F matrix which is also transformed or converted, minus 4 1. This is the first row. Then we have 1 minus 22 by 5 minus 16 by 5 and if you do the third one. It all comes out to be minus 1 minus 1 minus 1. So, now, what we have?

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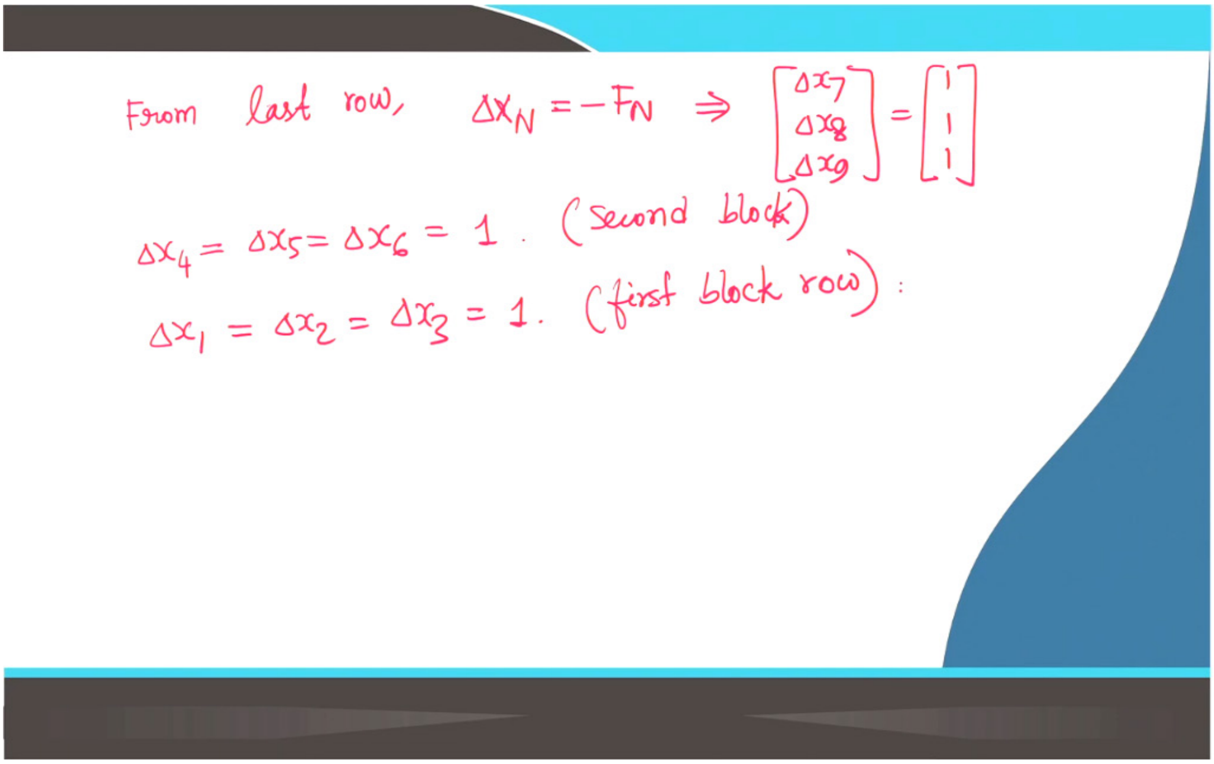

If we write down the last row, if I try to write down the last row, so, I get from last row based on this idea of the block, from last row I have this delta X N, sorry, capital N is equal to minus F N. So, this means that all my delta X 7, delta X 8, delta X 9 all are equal to 1. Because the last F was 1 1 1. So, similarly you can also work out. What would be your delta X 4. Sorry, this second block also delta X 4 delta X 5 delta X 6, you can also work them out. So, if you work them out you will also see that this also turns out to be 1. I mean it is just a coincidence in this case. And the last block delta X 1 is equal to delta X 2 is equal to delta X 3, this also will turn out to be 1. So, this is like the second block, from the second block. And this is the first block row by working out the first block row.

You can also find out this delta X. So, I hope, so, all of you got an idea or this overview of how this block tridiagonal matrix is actually handled. And this you can essentially solve both in the same way and the idea that you are trying to solve for the case of the normal tridiagonal matrix. So, I hope, all of you have liked this lecture. And in the next class, we will talk about the ‘simple batch distillation’ and ‘multi-component multi-stage batch separation processes’ in subsequent classes. Thank you.