Computational Fluid Dynamics

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Module No. # 07

Dealing with Complexity of Geometry of the Flow Domain

Lecture No. # 41

Transformations of the Governing Equations

Illustration for the Laplace Equation

Appearance and Significance of Cross-Derivative Terms

Concepts of Structured and Unstructured Grids

We have seen the approach – the computational plane approach, where we solved the equations not in the physical plane, that is xyz, but in a transformed plane, the computational plane, where it is expressed in terms of the coordinates are psi, eta and zeta. So, this transformation, this need for solving the equations in the computational plane also requires us to transform the equations, which are described in xyz into the corresponding derivatives appearing in the psi, eta, zeta directions. So, this transformation of equations is done systematically like the following. We will illustrate it with the for a simple two-dimensional flow case. We will take case of heat conduction.

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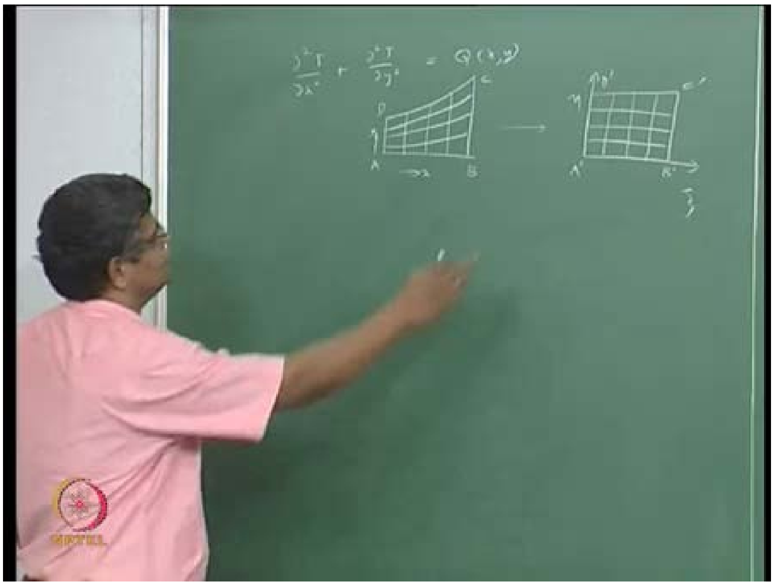

Let us say that we are looking at dou square T by dou x square plus dou square T by dou y square equal to Q x, y. This is the equation that we have, where Q is the source term and T is the temperature. And, of course, as a thermal conductivity and all that is included in this.

Now, when we are trying to solve this in a computational plane in two-dimensions in terms of psi and eta, then our physical domain may be for example, like this. This is x and this is y. This is transformed into the computational domain. And, here if you say that this is A, B, C and D, this is A prime, B prime, C prime and D prime. Therefore, there is this C prime, D prime corresponds to this and this AB corresponds to this; A prime D prime corresponds to this. And, lines, which are uniformly distributed here may correspond to lines, which are curvilinear like that; 1 2 3 4 5; 1 2 3 4 5. So, this is the physical plane; and, this is the computational plane. And, we do not want to solve the equations in the physical plane, because that is not a constant y line. But, since this is mapped on to the computational plane like this in which this is a constant eta line and this is a constant psi line here, therefore, we can think of doing it like this.

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Now, we have write dou T by dou x. We can write in terms of this as dou T by dou psi into dou psi by dou x plus dou T by dou eta into dou eta by dou x, because x is a function of psi and eta in two dimensions. And, this is dou T by dou psi into psi x plus dou T by dou eta eta x. And, what we want is dou square T by dou x square; that is, dou by dou x of dou T by dou x. And, dou T by dou x is given by this. So, this is dou by dou x of psi x dou T by dou psi plus eta x.

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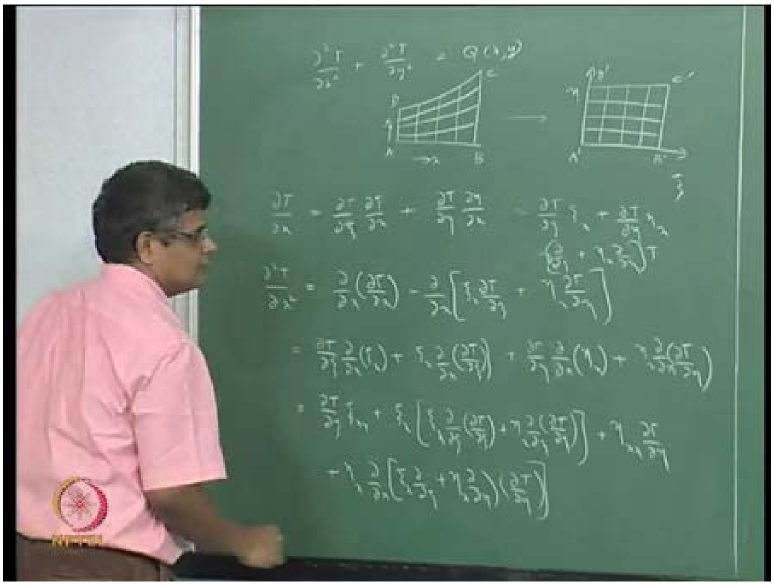

Now, we can write this as dou T by dou psi into dou by dou x of psi x plus psi x times dou by dou x of dou T by dou psi plus dou T by dou eta times dou by dou x of eta x plus eta x times dou by dou x of dou T by dou eta. And, each of these derivatives here, dou by dou x is like this and that will have two components; this will have two components and like that. So, we have to evaluate this as dou T by dou psi times psi xx plus psi x times dou by dou x of dou T by dou psi. So, this will be… Here we take this. So, dou by dou x of something is equal to… So, we can write this as psi x dou by dou psi plus eta x plus dou by dou eta of this T. So, this is the operator, which is acting on T. And, now, this is the same operator which will be acting on dou T by dou psi. So, we can write this as psi x dou by dou psi of dou T by dou psi plus eta x plus dou by dou eta of dou T by dou psi. And, here we have plus eta xx – second derivative dou T by dou eta plus here again we have plus eta x times dou by dou x of this operator psi x dou by dou psi plus eta x dou by dou eta of dou T by dou eta. So, we can see that this becomes dou square T by dou psi square.

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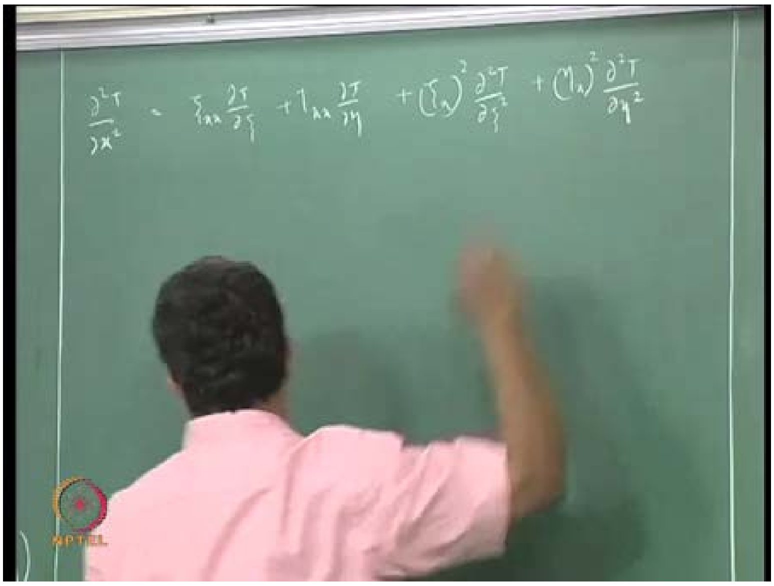

So, we can write this as dou square T by dou x square as psi xx dou T by dou psi and here we have this eta xx dou T by dou eta plus psi x whole square dou square T by dou psi square. And, similarly, we have eta x whole square dou square T by dou eta square.

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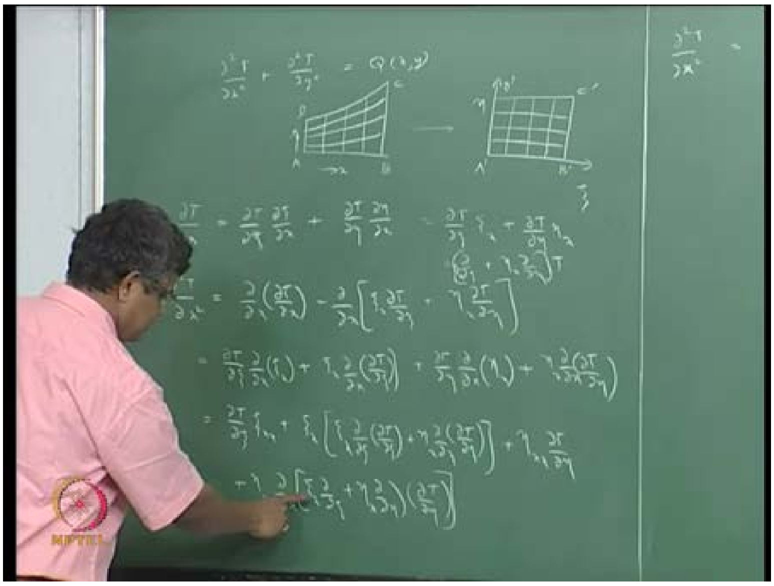

Then, we have psi x eta x dou square t by dou eta dou psi. And then, we also have psi x dou x dou square T…

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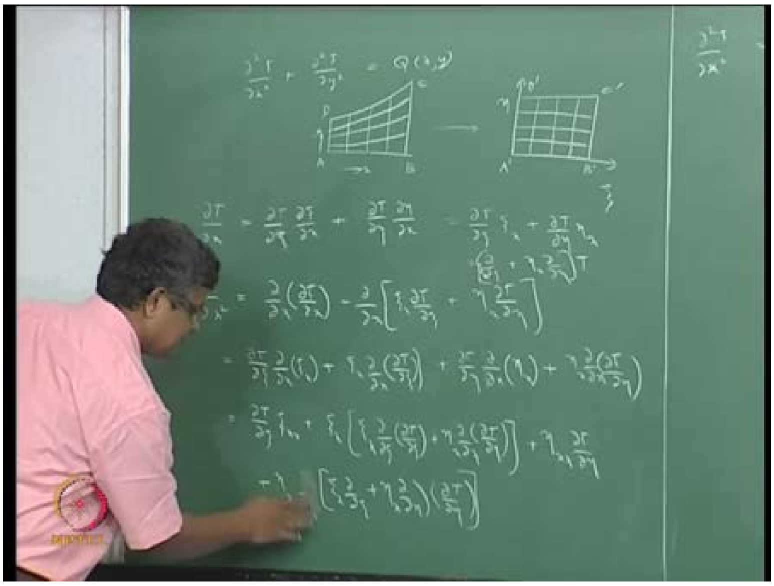

So, psi x eta x dou square T by dou psi dou eta here.

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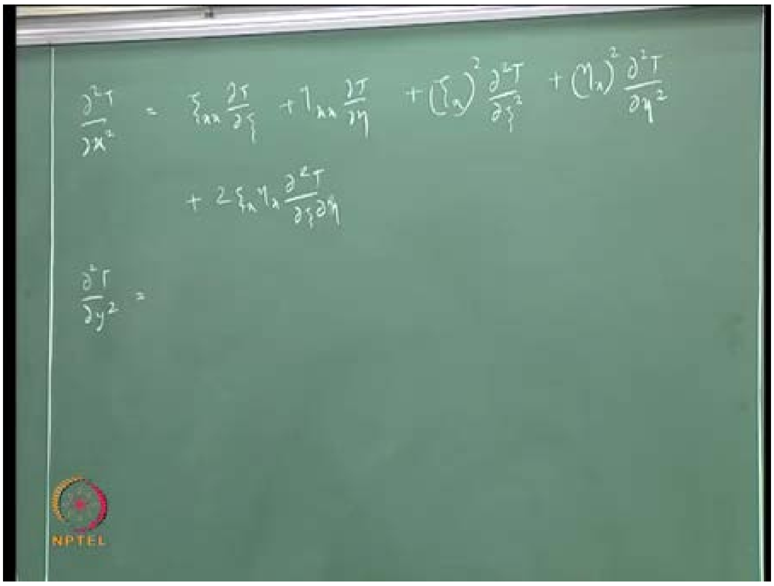

So, we will have plus 2 psi x eta x dou square T by dou psi dou eta. So, this is what we have for dou square T by dou x square. And similarly, we will have dou square T by dou y square.

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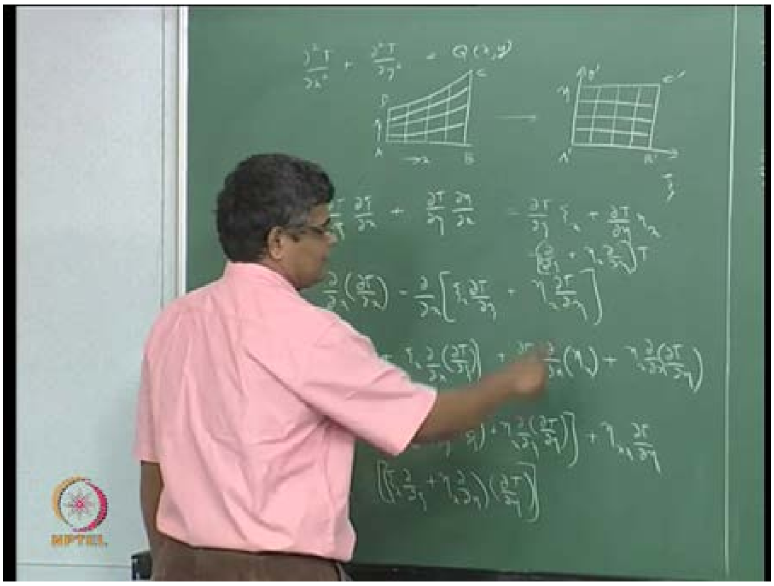

We will have dou psi by dou y here and dou eta by dou y. So, the operator here will become psi y dou by dou psi plus eta y dou by dou eta of this.

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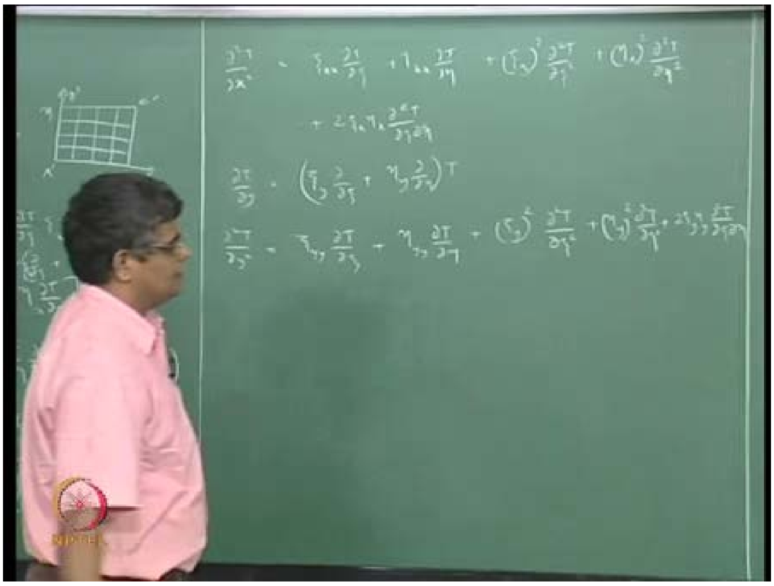

So, we can write dou T by dou y equal to psi y dou by dou psi plus eta y dou by dou eta of T. And then, we can again differentiate this and finally, we can get dou square T by dou y square equal to something similar – psi yy dou T by dou psi plus eta yy dou T by dou eta plus psi y whole square dou square T by dou psi square plus eta y square dou square T by dou eta square plus 2 psi y eta y dou square T by dou psi dou eta.

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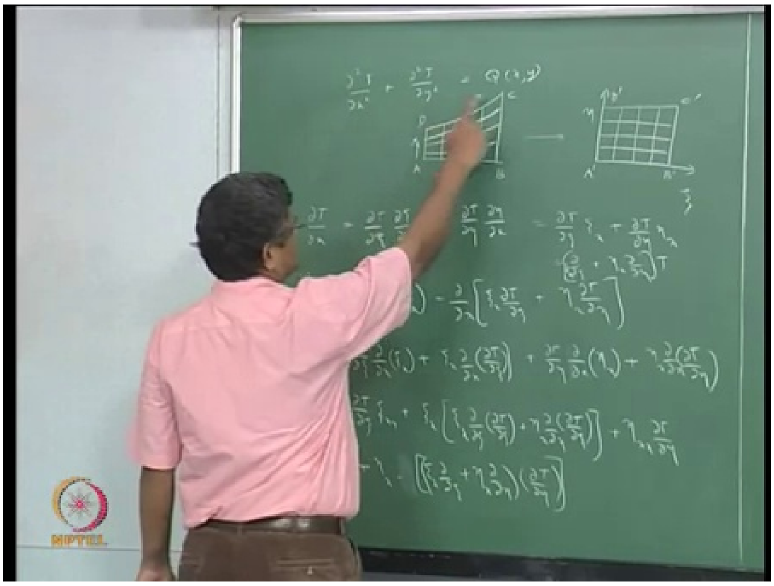

So, this equation Q, which is x and y here will now become Q corresponding to psi and eta.

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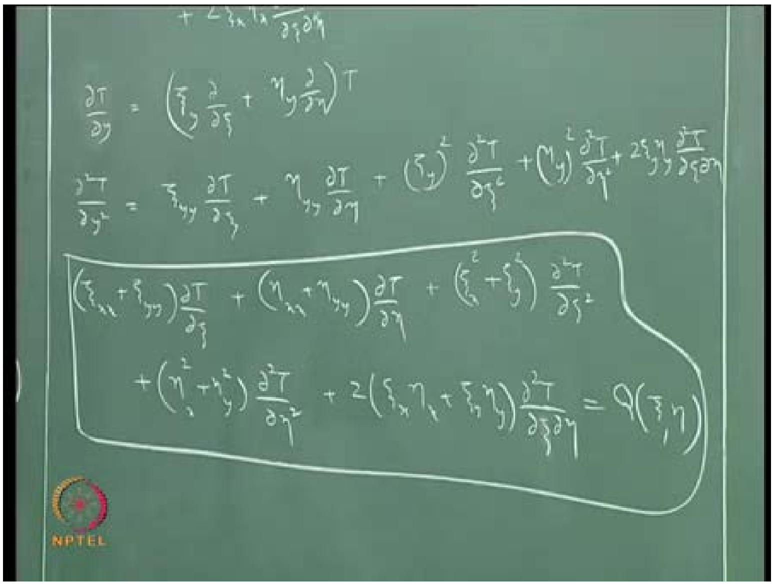

So, we can put up this whole thing here as psi xx plus psi yy dou T by dou psi plus eta xx plus eta yy dou T by dou eta plus psi x square plus psi y square dou square T by dou psi square plus eta x square plus eta y square plus 2 of psi x eta x plus psi y eta y dou square T by dou psi dou eta equal to Q of psi, eta.

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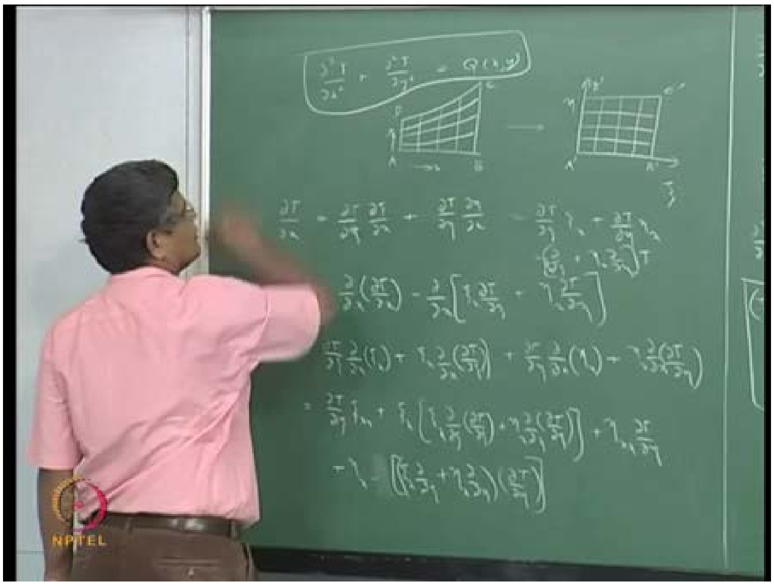

This is the transformed equation from here.

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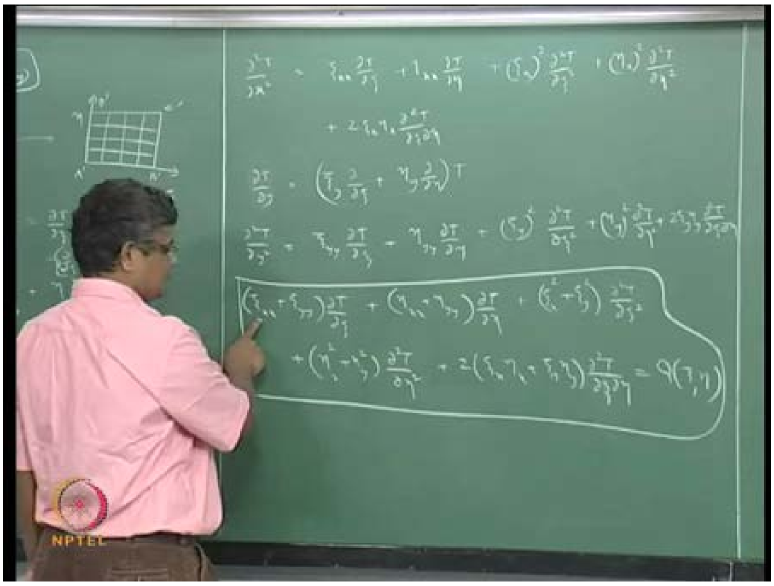

And, one can see that in the transformed equations, we have the metrics of the transformation; we have psi x, psi y, eta x, eta y. And, double derivatives of psi and eta – these are all coming.

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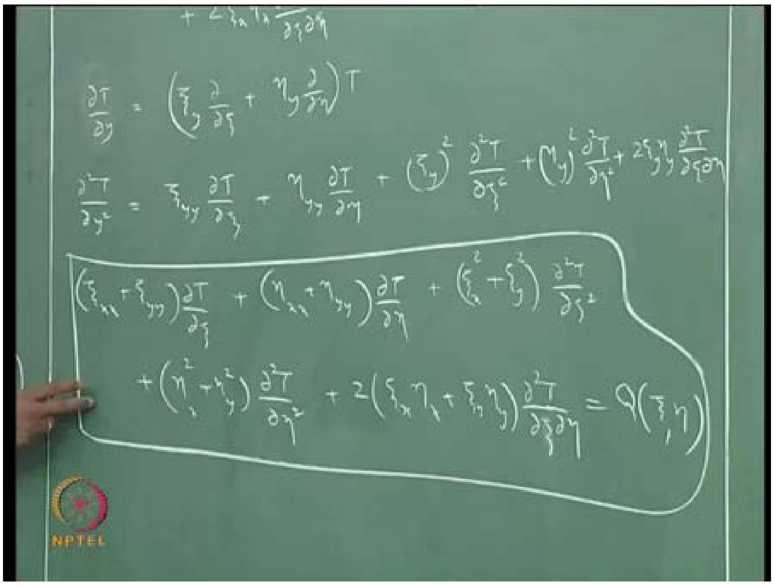

And, one can immediately see that this equation is much more complicated. There are many more terms that are coming here for the general case of transformation, where both x and y depend on psi and eta. In this particular case, it looks like x direction; there is no change, but y direction is obviously changed. So, some of the derivatives may cancel out. But, in the general case, all these things are present.

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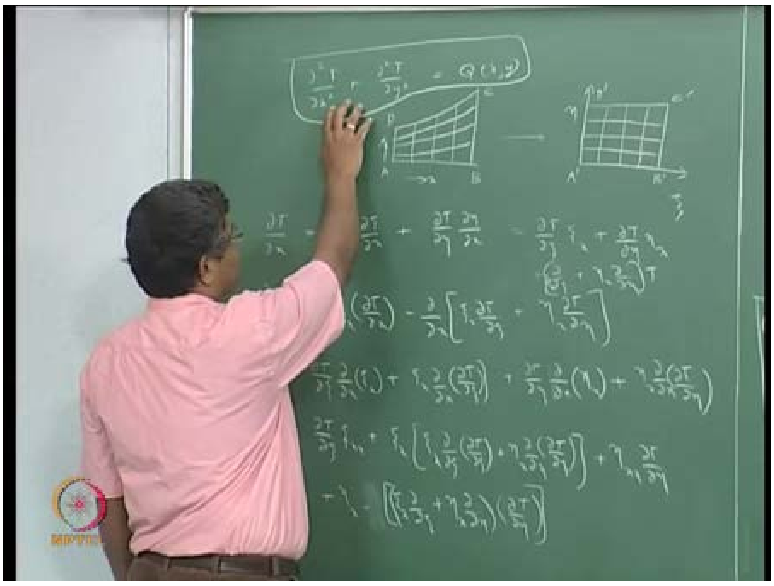

Now, what is also important is that… Whereas, this equation – we have only normal derivatives.

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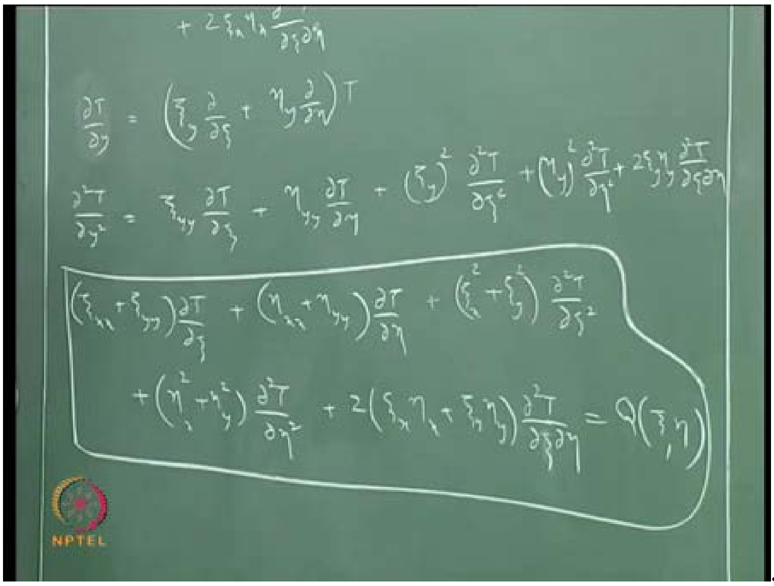.

Here we have cross derivative term, which is coming here. And, we have these terms – the first derivatives, which are not there in this. But, what is especially important is that we have the cross derivative term, which comes here.

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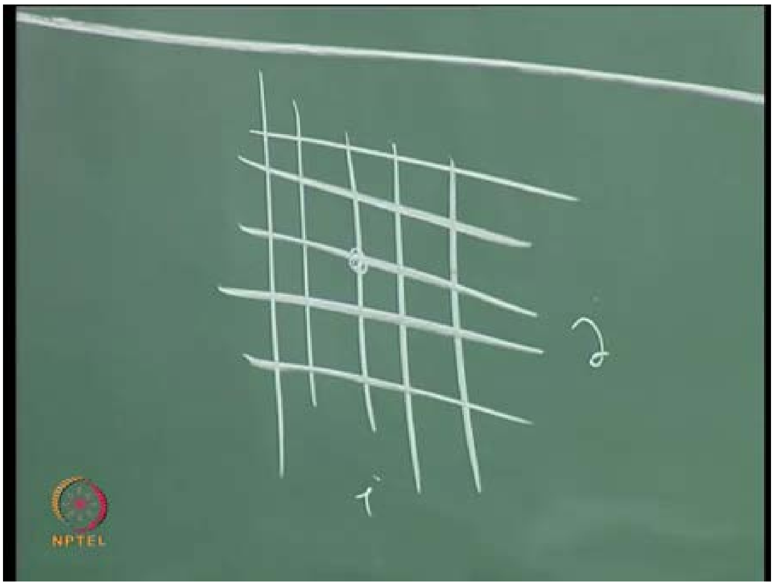

And, we have seen that if were to use a central differencing scheme for… Let us say that this point i comma j.

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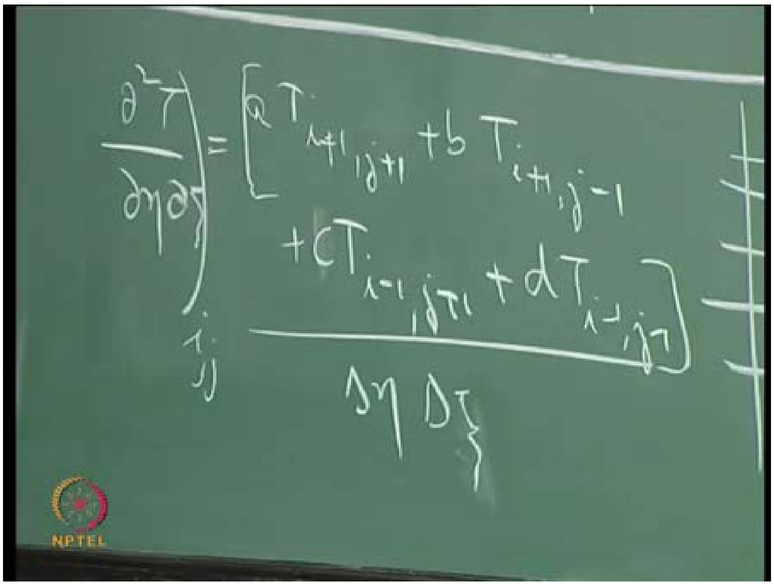

Then, if we consistently use second order approximation, then the second derivative dou square T by dou eta dou psi will be represented as in terms of this point, this point, this point and this point. And, it would not have any contribution coming from this. So, this will be T i plus 1, j plus 1; let us put it as a plus b tau i plus 1, j minus 1 plus c times T i minus 1, j plus 1 plus d times T i minus 1, j minus 1. This whole thing divided by some delta eta. This sort of approximation will come, where a, b, c, d are some numerical coefficients. And, especially, what is important is that this discretization around point i j does not have any contribution from T i comma j. So, when we put this together in the form of overall…

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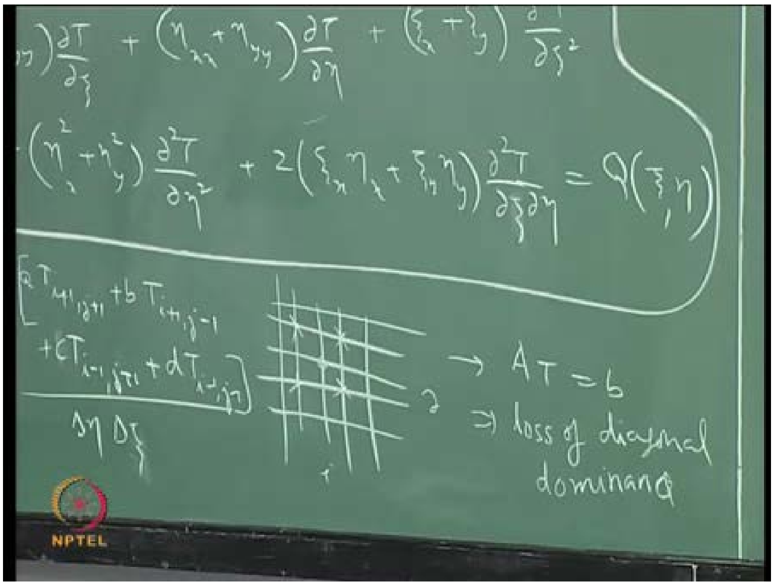

When we convert this into A T equal to b type of situation, the contribution to the central term, that is, i j from this derivative is 0. And, there is contribution term from half diagonal terms.

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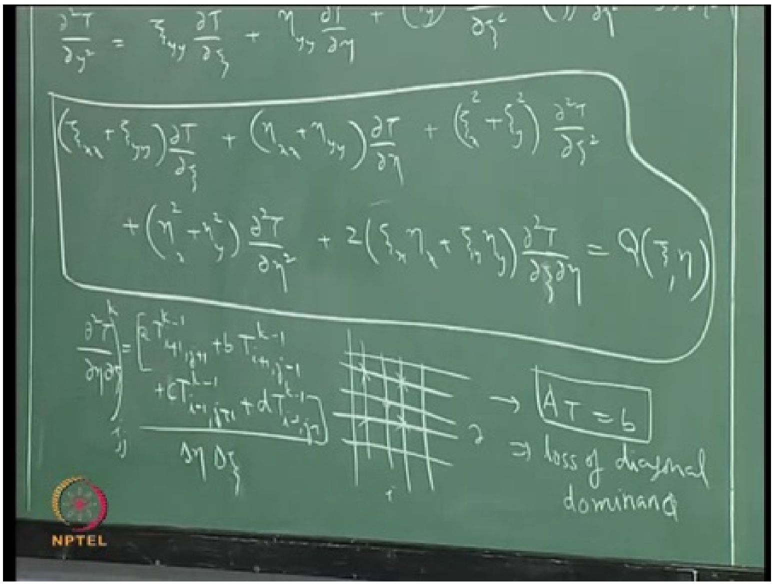

So, a direct discretization of this will lead to loss of diagonal dominance. This is an important factor when we deal with this. And, we have deal with… We will have to therefore use a method, which does not depend on diagonal dominance for the solution of this, for example, a direct method like Gaussian elimination or an iterative method like conjugate gradient method. These are all methods which do not depend on diagonal dominance. But, if you wanted to use Gauss-Seidel method for the solution of this or even the TDMA method, they depend to some extent on diagonal dominance for assurance of convergence. So, there is a problem with this. And therefore, one way of solving this is to take this term on to the right-hand side and evaluate all these (Refer Slide Time: 17:44) things for the kth iteration in terms of k minus 1 based on the previous values. And, since all these things – T k minus 1 are known at all i j from the previous iteration, this will go to the right-hand side. In the discretization here, we will have only terms, which will be contributing to i comma j.

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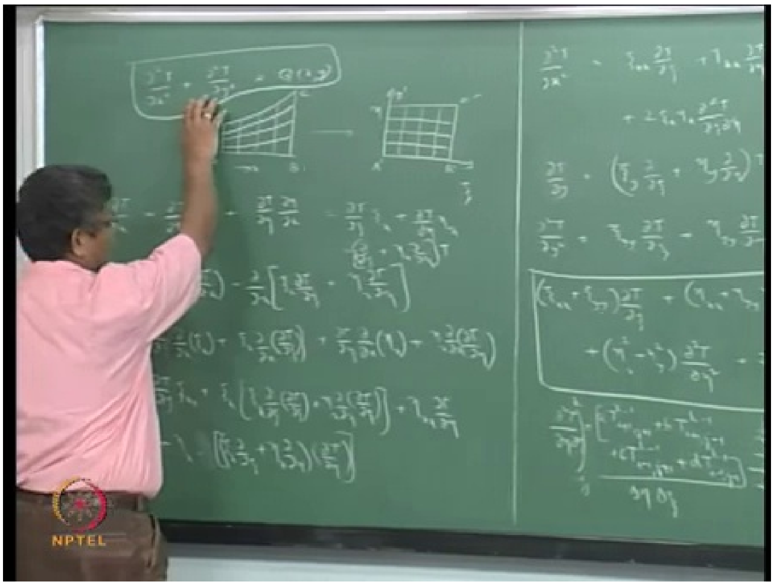

And, here we have normal derivatives appearing.

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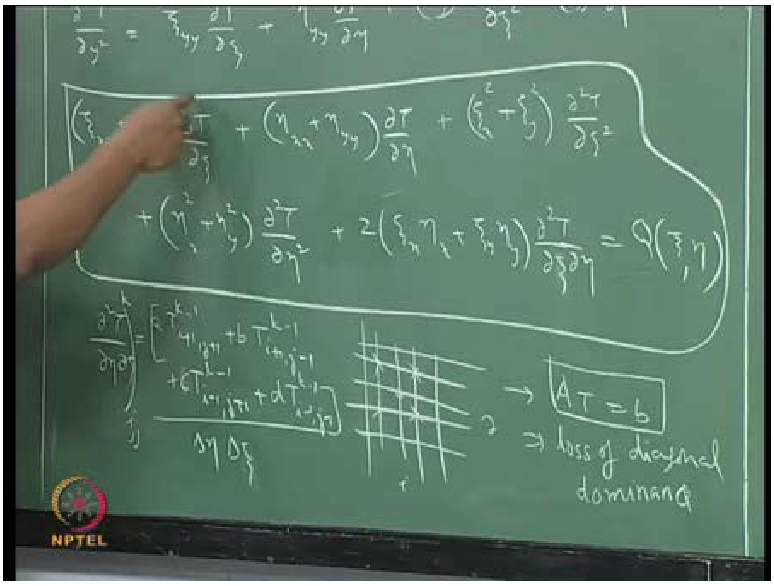

And, here we have something like the advection term also coming in this. So, this is the first derivative and this is the second derivative. So, if we were to look at it as some kind of generic scalar transport equation with advection and all that thing, there is a first derivative coming here. So, one has to do a proper stability analysis for a discretized scheme for this derivative and this derivative put together. So, that is another complexity that we have to deal with. And finally, what we also see is that there are derivatives –

first derivative or a second derivative of the grid coordinate transformation that is coming into picture. And, for these things to be faithful to the original equation, we should have a smooth grid – smoothness of the transformation.

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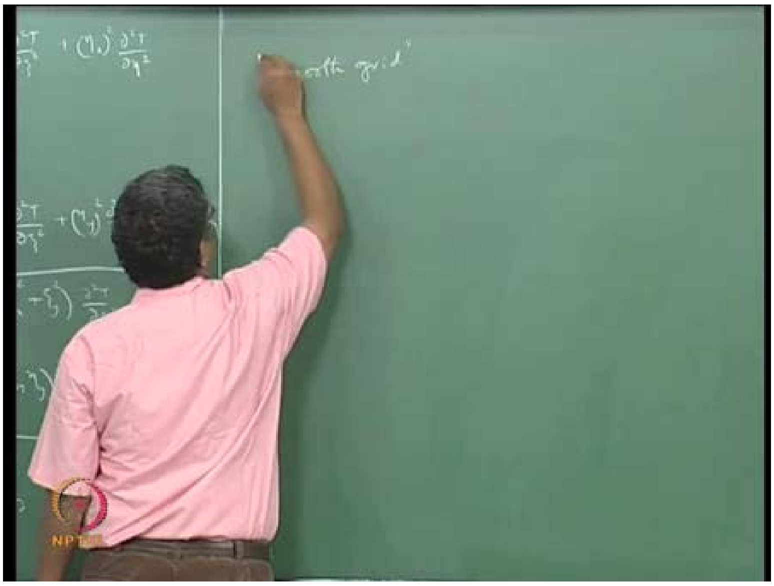

If the grid lines are smooth like this, then the second derivatives will be small; otherwise, these will tend to dominate the whole solution and you may get away from the visca, the diffusion type of solution that is expected for this. So, we would like to have a…

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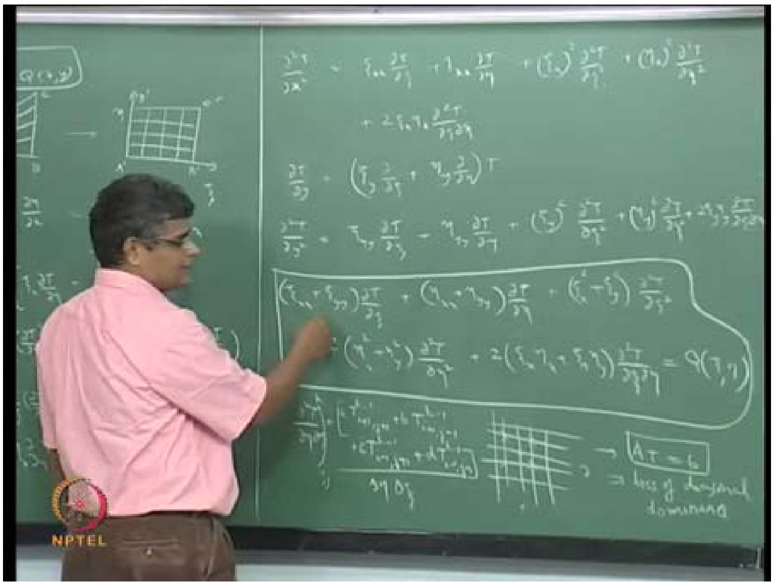

This is an artificial thing that is being introduced into the equations because of the transformation. One can show that because of the transformation, the mathematical nature of this equation does not change; that is, if we are starting with an originally elliptic equation like this, then even this transformed equation will also be elliptic. If we are starting with the parabolic, then this will be parabolic if… So, that criterion is… That condition is maintained; that assurance is there that we are still dealing with a parabolic or elliptic equation as we started out with… Therefore, the wellposedness is not affected.

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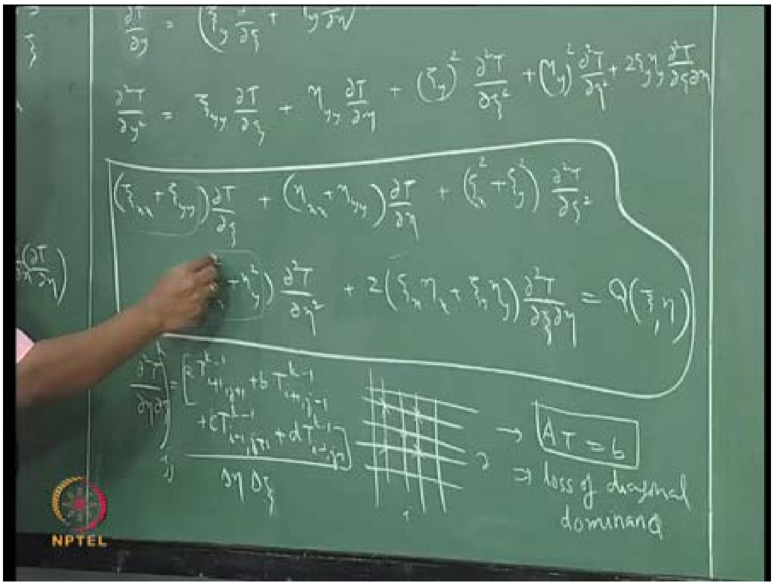

But, there are transformation dependent terms, which are coming here – first derivative square and then second derivatives. So, the influence of these things should be suppressed wherever possible. And, that is possible when we have a smooth grid. So, if we have a discontinuous grid, so that we have discontinuous things, where the second derivative becomes ill-defined and all that kind of thing, then we have problems.

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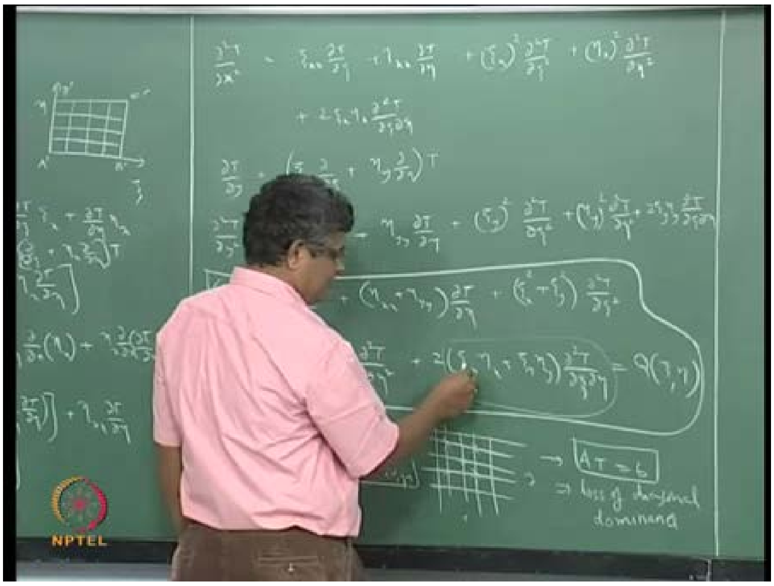

And, the most important problem is also with respect to the appearance of the cross derivative. And, this cross derivative is multiplied by these metrics here. And, the contribution of these metrics, these terms will be higher if you have a non-orthogonal grid. So, if the grid lines psi and eta are orthogonal and x and y are orthogonal, for example, these lines here (Refer Slide Time: 21:55) are orthogonal with each other, then this term will be identically 0 and it can be shown in that way. But, in the general case, we cannot expect orthogonality.

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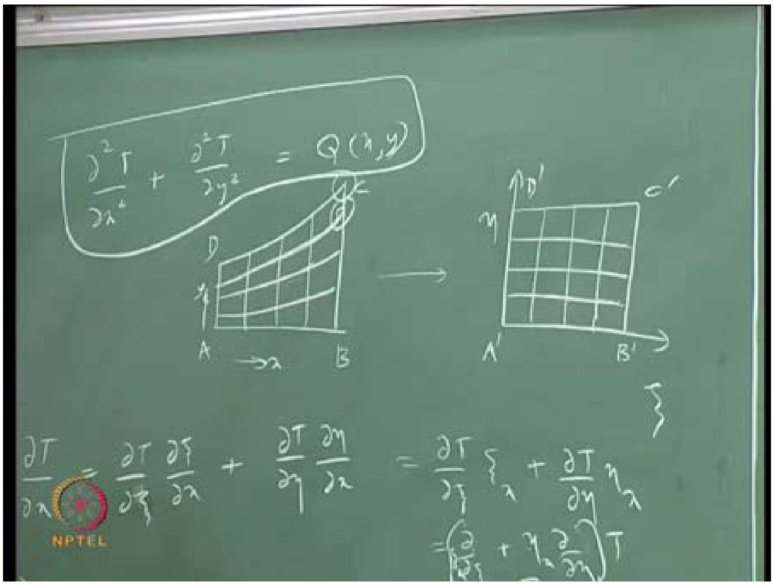

For example, this is coming like this and this is here. So, this is cleanly not 90 degrees at this point. And, this point here is not 90 degrees. So, that means that for a general case of transformation, when you go back to here to here, this transformation, the resulting grids are not necessarily orthogonal.

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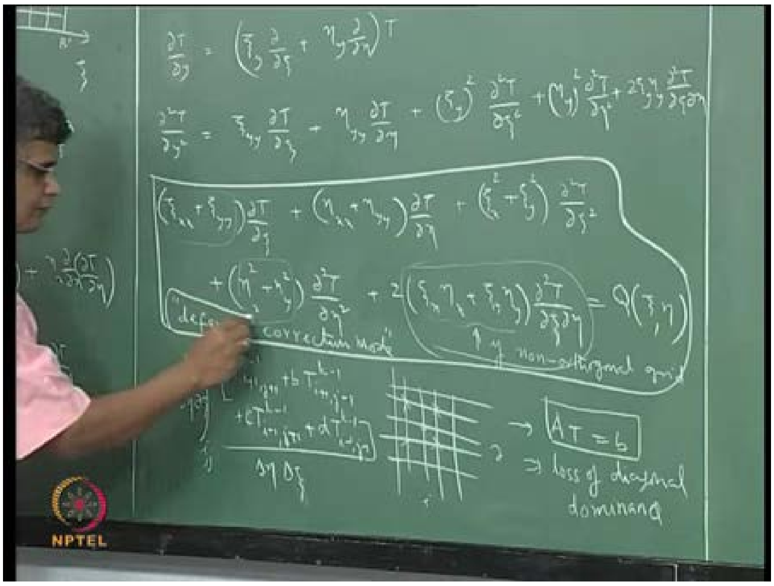

If they are not orthogonal, then this term, this contribution here is not 0; we will have to live with cross derivatives. And, these derivatives can be treated in this deferred correction mode. So, we call this as deferred postponed correction. Because there is one term here which is not evaluated at the current situation, but at the previous situation value, the convergence of this scheme is compromised, is delayed. And, the convergence, the correction, which is coming after some time is going to delay it more if the value of the magnitude of the correction is large. So, in cases where this term is large, that is, where we have highly skewed grid…

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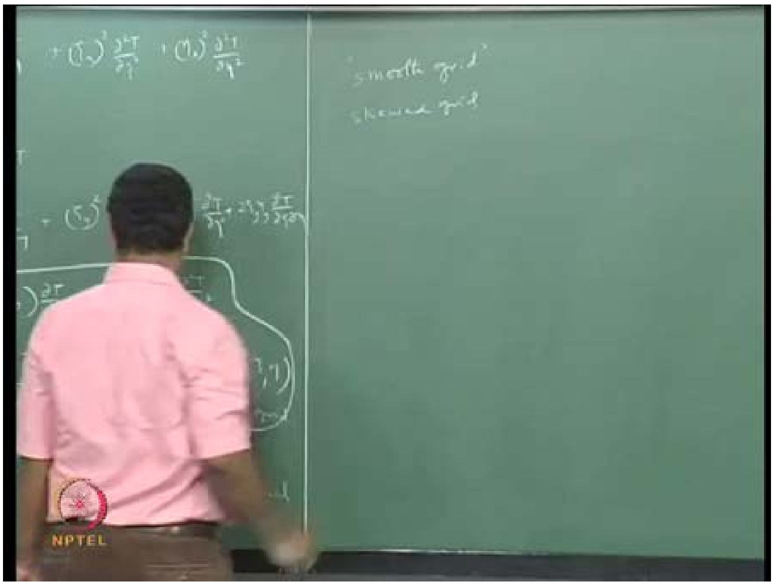

If we have a skewed grid, which is not orthogonal, then this term may dominate and that may reduce the overall rate of convergence of an iterative solution of this in a deferred correction mode. So, these are some of the things that we will have to take into consideration when we are trying to solve the transformed equations in the computational plane.

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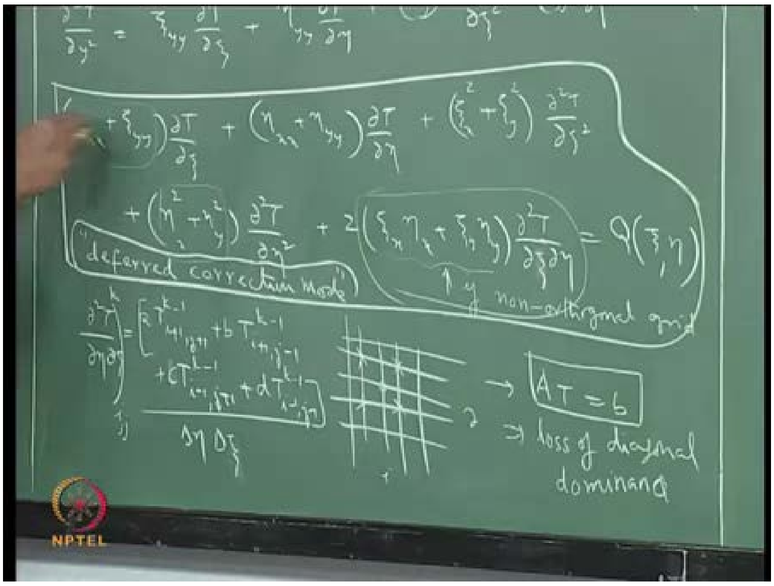

Now, this particular form of the equation, where it is like this, where we have psi xx and eta xx and psi x like this, these are not very useful, because we are trying to write approximations for these things.

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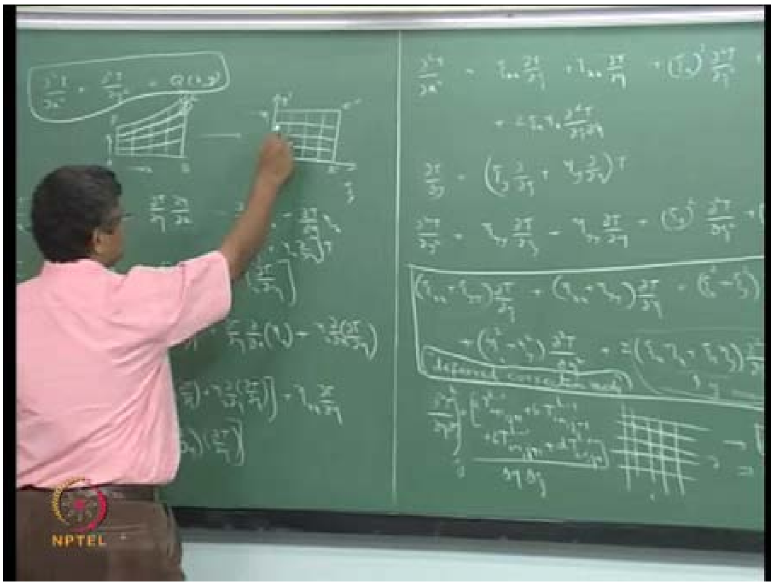

And typically, our computational grid is very simple like this by design. And, it is very easy to discretize this into equal spacing here and equal spacing here.

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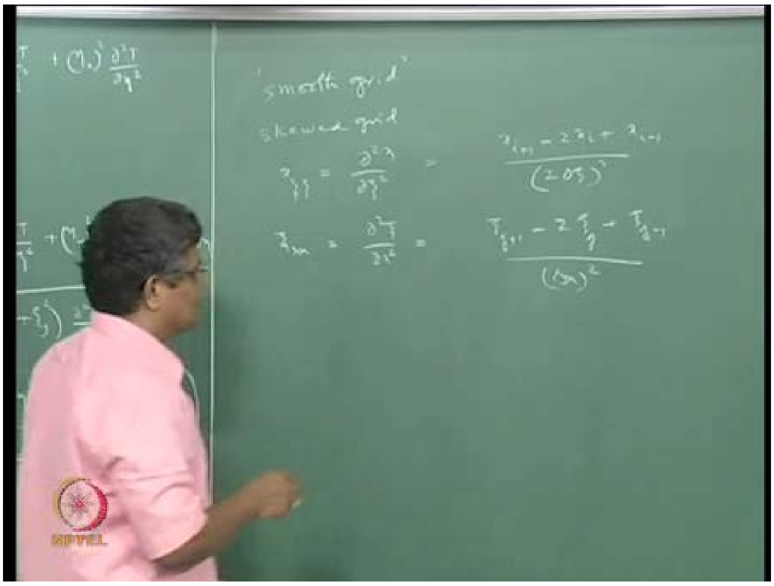

So, if you were to rewrite this not in terms of psi xx, but in terms of x psi psi like (Refer Slide Time: 24:57) this, then x psi psi, that is, dou square x by dou psi square can be written for example, as xi plus 1 minus 2 x i plus x i minus 1 by 2 delta psi whole square; whereas, psi xx, which is dou square psi by dou x square will have to be written as psi j plus 1 minus 2 psi j plus psi j minus 1 by delta x square.

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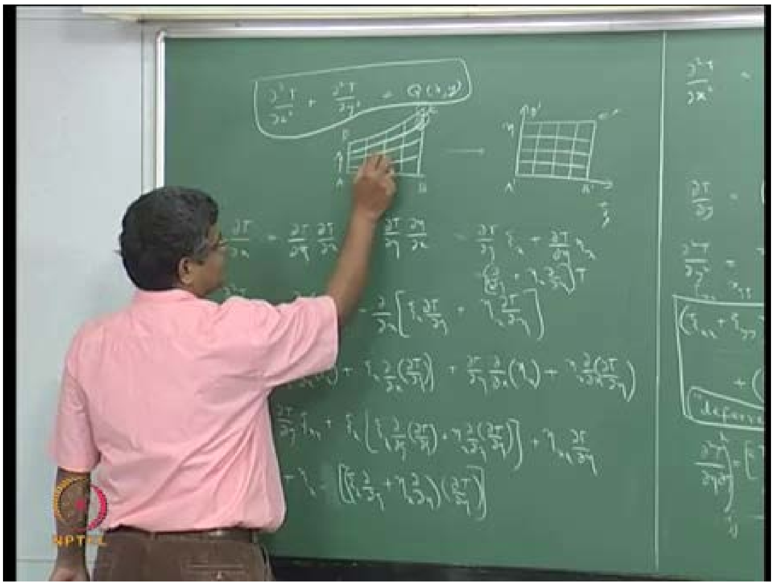

In the computational plane, in the physical plane here, the delta x's and delta y's are changing all the time. But, in the computational plane, it is easy to take this rectangular and divide this into constant delta x and constant delta eta.

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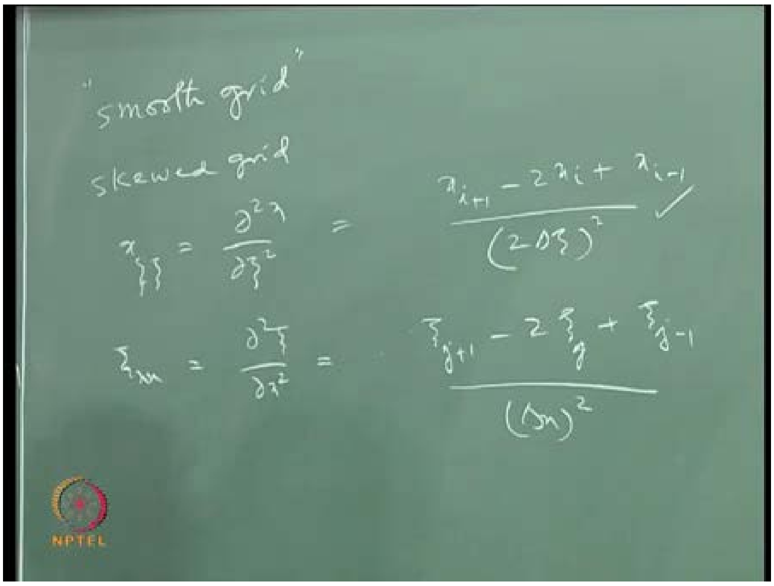

The evaluation of this is much more simple than evaluation of this. And, here you have uniform grids and here you have non uniform grids. So, the accuracies of the evaluation of this is also compromised.

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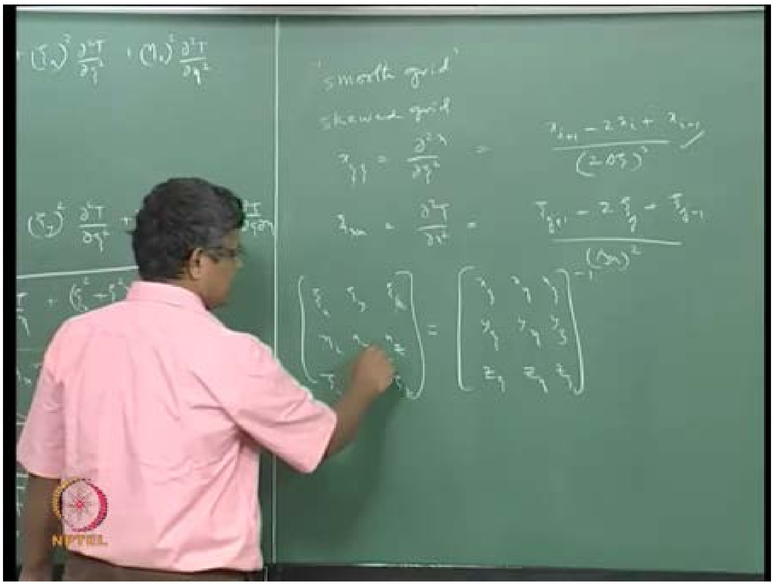

So, making use of the relation between (Refer Slide Time: 26:20) metrics expressed in terms of psi x and x psi, which we have derived earlier, we have shown that psi x psi y psi z; eta x eta y eta z; zeta x zeta y zeta z can be expressed as x psi x eta x zeta; y eta y psi y zeta; z psi z eta z zeta, which we expressed in terms of the Jacobian. Now, we can go from here to here or from here to here. And, we are saying that it is easier to deal with dou x square by dou psi square rather than dou square psi by dou x square. So, we make use of this relation.

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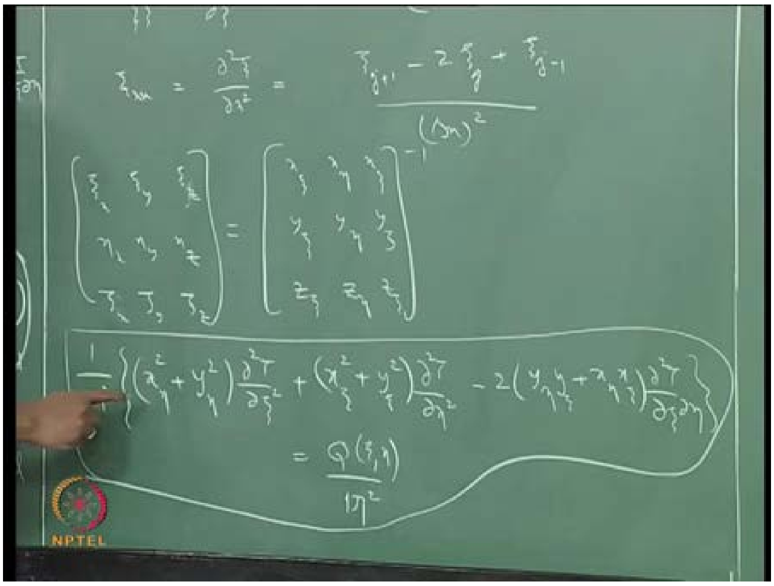

To rewrite this in terms of psi like this, (( )) x eta square plus y eta square dou square T by dou psi square plus x psi square plus y psi square dou square T by dou eta square minus 2 y eta y psi plus x eta x psi dou square T by dou psi dou eta equal to Q psi comma eta by (( )). In this form, we see that the metrics of transformation in terms of dou x by dou psi and dou x by dou eta and dou y by dou psi, these are appearing especially when we have a smooth grid, so that these first derivative terms will go to 0.

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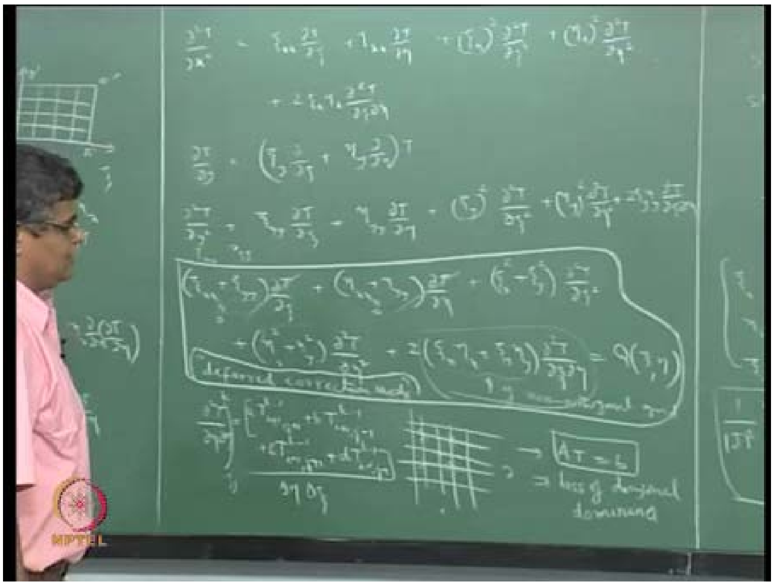

I think here we have made the assumption that we have a smooth grid. And, for a smooth grid, this is equal to 0 and this is equal to 0, so that we can cancel out these terms and we have a simpler form of this.

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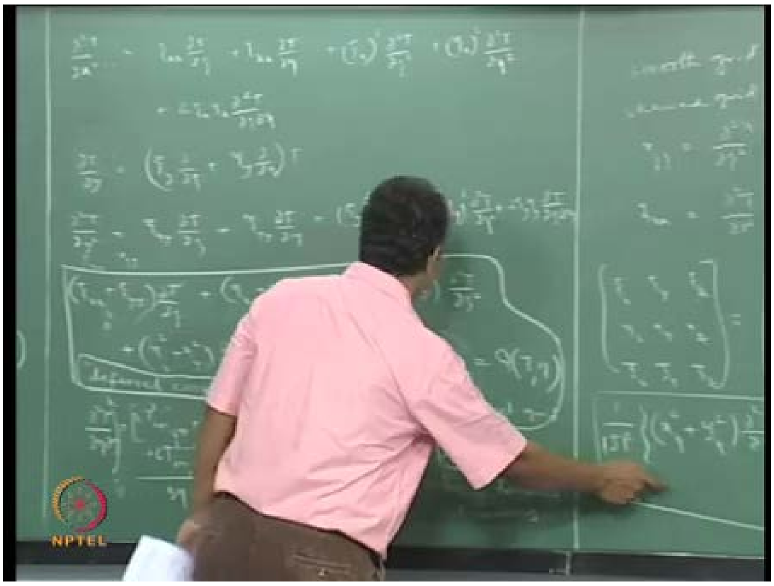

So, the idea of the computational plane approach now is to solve this equation for a given relation between these lines (Refer Slide Time: 30:47) and these lines. So, we are trying to map the physical domain like this into this. So, this is…

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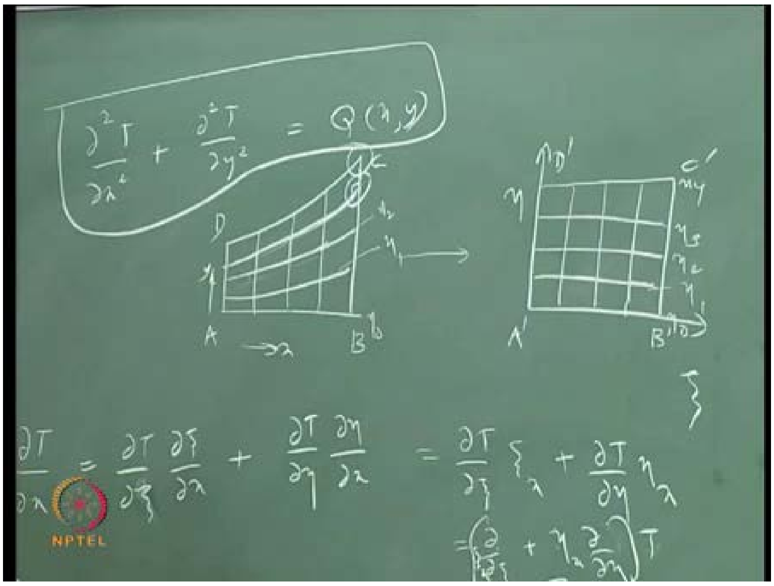

For example, if you say that this is eta 1, eta 2, eta 3, eta 4 and eta 0… So, this corresponds to eta 0. On this line here, this is eta 1, is constant; this is eta 2, is constant; and, eta 3 is constant like this. And, these lines here corresponds to psi 1, psi 2, psi naught like this.

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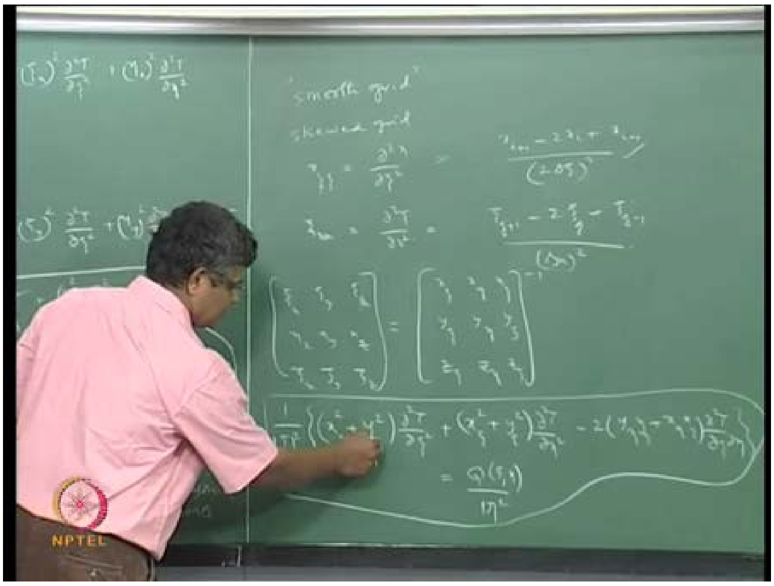

If you want to discretize this, we need to evaluate dou psi by dou eta, dou y by dou eta and dou x by dou psi like this. And, that comes from the transformation. And, how do we get the information?

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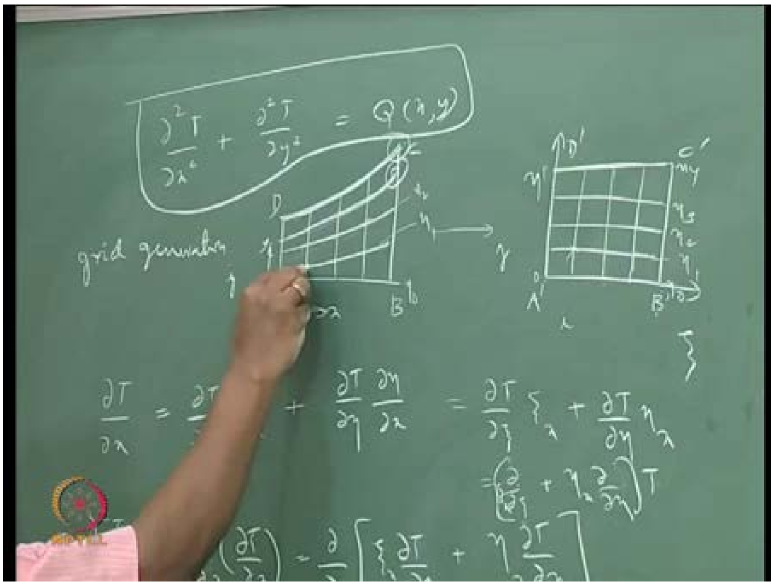

We can say that we know this boundary; and, one can say that this boundary and this boundary are mapped. And, we know that this varies from say 0 to 1 and 0 to 1 like this. So, we know what this line is. That is a horizontal line at eta equal to 1. And, we know that eta equal to 1 corresponds to this line. And, since this is part of the boundary, we can potentially evaluate the metrics corresponding to this. But, we do not know these lines. That is part of the grid generation. So, the objective of the grid generation is to find out all the interior points in the physical plane given that the external boundaries here is A B C D, correspond to the computational plane of A prime B prime C prime D prime and subject to the condition that in the computational plane, we have uniform grid spacing. So, this point here is topologically the same as this point here.

Topologically means that we have i equal to 0 let us say 1 2 3 4 5 and j equal to 1 2 3 4 5. So, this is i equal to 2, j equal to 2; and, this is also i equal to 2 and j equal to 2. So, if you were to write this in terms of i and j and similarly, i and j (Refer Slide Time: 33:29) here, this point is 2 comma 2 and this point is 2 comma 2. So, the objective of the grid generation is to identify all the interior points in the physical plane given the interior points in the computational plane and given the boundaries of the physical plane to map with the boundaries of the computational plane. So, that is… And, we have a number grid generation methods by which we calculation find all the interior points. And, one can even use the condition of smoothness in order to derive these interior points, so that we can cross out these terms here.

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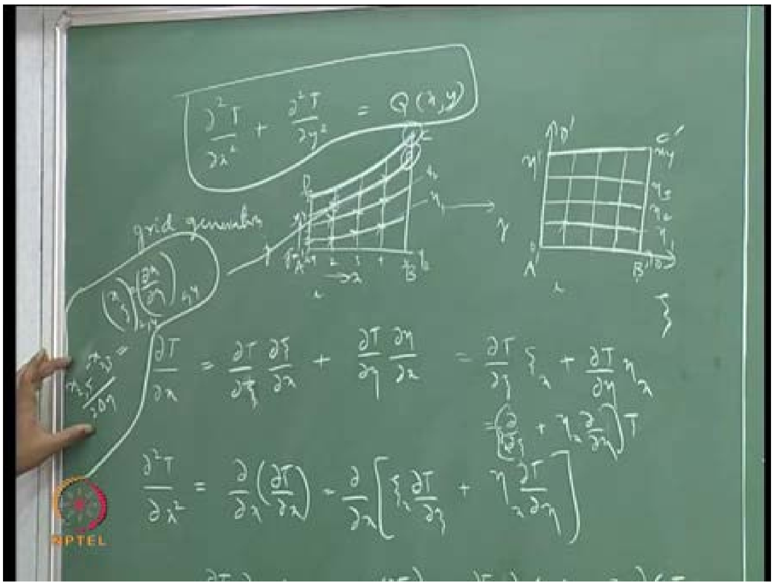

And, based on that, we will be able to find all the interior points. So, once we know the interior points, we can evaluate this x eta. For example, x eta for this point here is dou x by dou eta. So, it means that this is x of this point minus x of this point divided by this distance. So, that is, we can write this as at constant i here, this is i equal to 1, 2, 3, 4, 5. And, this is j equal to 1, 2, 3, 4, 5. So, we are writing x eta at 2, 4. So, this is 2, 4. And, we can write this as x 2 comma 5 minus x 2 comma 3 divided by 2 delta eta. And, delta eta is what we are getting from computational plane. And, x 2 5 and x 3 5 are known from the grid generation. So, from that… because we know all the x y of the interior points. So, once we know the interior points, we can evaluate the derivatives in this way. And, we put those things here.

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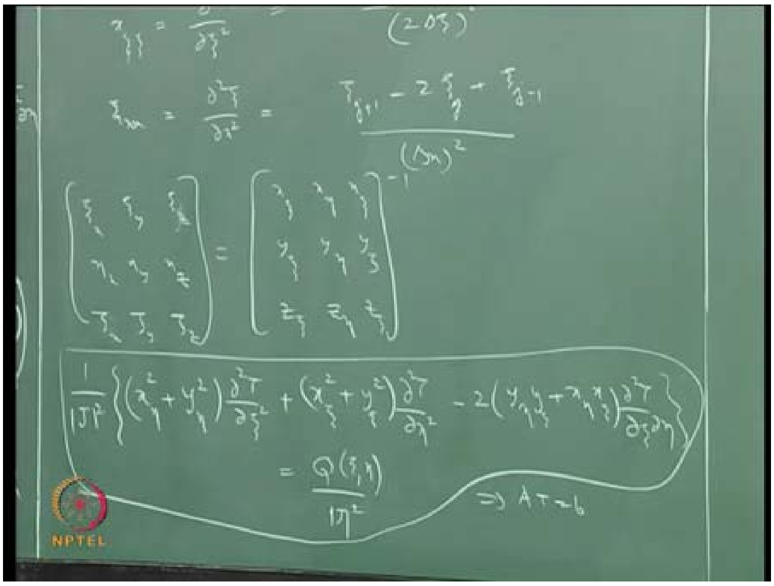

So, after the grid generation stage once we have found all the interior points and once we have numerically evaluated all these derivatives for the general case, then we will have an equation with coefficients based on the grid generation and all that. So, these coefficients will be constants. And, we have a second order equation with constant coefficients, which we can then discretize as per the usual second order accuracy or fourth order accuracy as we wish. And then, we can convert this into an equation like A T equal to b. And, this A T equal to b can then be solved for T at psi and eta. And, using those values, we can then come back to T at this point. So, the approach in the computational plane is to first identify the mapping between the physical plane and the computational plane. The computational plane is such that it is rectangular in case of two-dimensions. And, in the case of third dimension, the zeta dimension will also vary between… It is like a cube going from 0 to 1 and 0 to 1 and 0 to 1 in the three directions.

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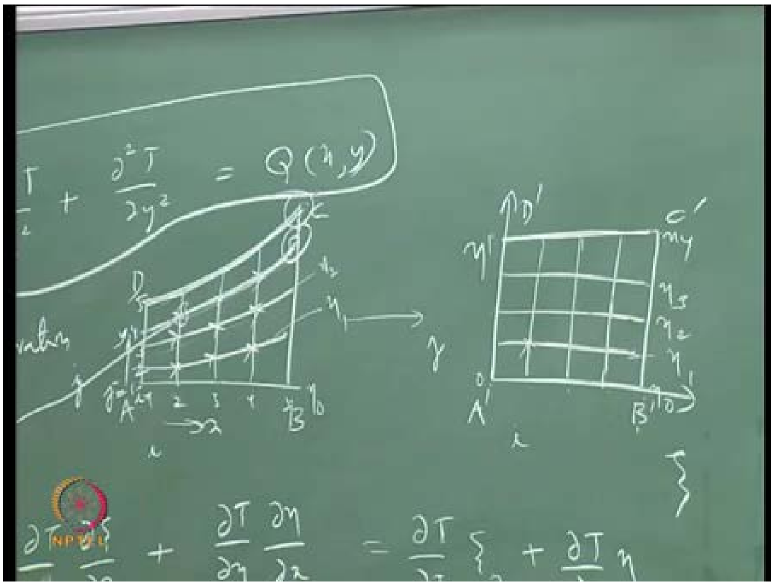

And, within this, we can have uniform spacing of coordinates of lines of constant psi, constant eta, constant zeta, so that you have small cubes of delta psi and delta eta and delta zeta depending on the number of grid points we have in this direction, in this direction. And, what we then say is that this line A prime B prime maps onto the physical plane – in the physical plane, the line or the curve AB. And, we have as many number of points here as number of points here. Then, we try to identify where we want to have these 5 points here and then we fix the points on this side and this side. This is already fixed. And, based on our consideration of where we want to have the grid points, we can fix these points here. Similarly, the points on these things are fixed and points on these are fixed, points on these are fixed.

Now, once we identify the boundary points, then we have to get the interior points such that we have a smooth grid. And then, these lines here (Refer Slide Time: 38:45) map on to the constant psi and constant eta lines here. Based on that, we derive all the interior points; that is, we find at every i j, what is psi i eta j and what is x i y j, so that for a given point i j in the computational plane and the physical plane, we get psi i eta j in the computational plane and x i y j in the physical plane.

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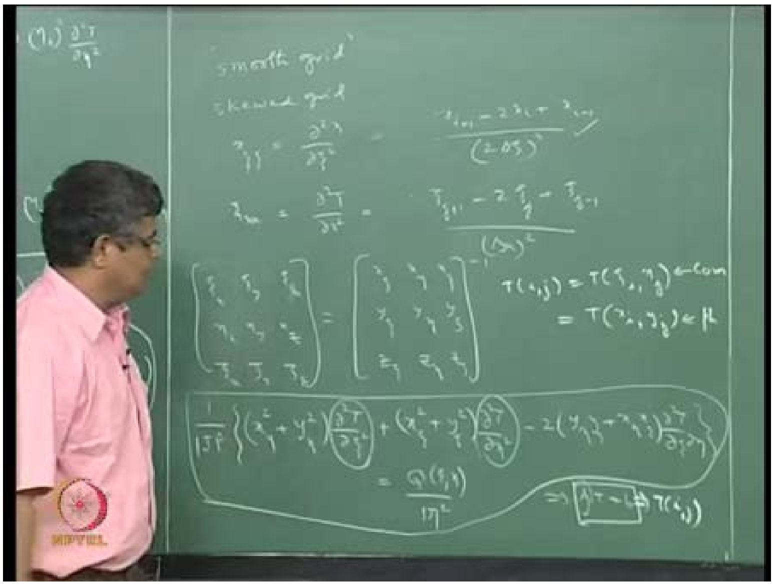

Based on that, we can derive the metrics either like this or in this way. And, once the metrics are derived, we can substitute them into the transformed governing equations to come up with governing equations with coefficients, which depend on the metrics of the transformation, these kind of transformations. So, at that point, we have an equation of this kind and j, the determinant of the transformation is also evaluated as we have already seen in terms of the metrics, so that we now have an equation, which has derivatives of the variable in terms of psi and eta and zeta. And, for each of these derivatives, we make finite difference approximations and then this equation is converted into a discretized form.

And, for good measure, because we are getting extra terms in this, we will have to do a stability analysis to see that their discretization scheme that we have got is reasonable. And, we also have to derive the stability conditions for this particular scheme with these coefficients that are coming here for a given transformation. And then, based on that, we finally select the suitable discretization scheme. And then, using the discretization scheme, we convert the transformed equations into A T equal to b. And, depending on the structure of this A metrics, we may choose to use either a Gauss-Seidel method. If for example, the diagonal dominance is preserved, if it is not there, then we have to choose something else, some other method or we have to treat this term as a deferred correction.

We finally use a particular method and then we solve this to get (Refer Slide Time: 41:29) T as a function of at i, j. And, T at an i, j is also T at psi i, eta j; and, it is also equal to T at x i, y j. So, this is the computational plane and this is the physical plane. So, this is how we can get a solution in this approach, which calls for a fairly complicated approach for a complicated geometry. So, that means that we have to first generate the grid knowing only the boundary transformation. And, from the generated grid points, the internal point and the boundary points, we evaluate the metrics of the transformation. And, we substitute the values of the metrics of the transformation corresponding to each grid point and then get a transformed equation in the computational plane. And then, we choose a discretization and then come up with A T equal to b and then we solve this and then finally get the solution. This kind of solution can be applied to any arbitrarily complicated geometry.

If it is completely a two-dimensional problem, then it may be possible to generate a grid, which is orthogonal. For example, if one uses a conformable map techniques, then one can come up with an orthogonal transformation, which will mean that the cross derivatives will not appear if the cross derivatives are not there in the original equation. But, for a general three-dimensional case, it is not possible to ensure an orthogonal transformation. And so, in such a case, the cross derivative terms will appear and we have to deal with them. And, it would be the grid generation and transformation would be very easy if we had an (Refer Slide Time: 44:00) analytical expression for the transformation; that is, analytical expression for psi in terms of x, y, z or x in terms of psi, eta, zeta like that. In the general case, it is not possible.

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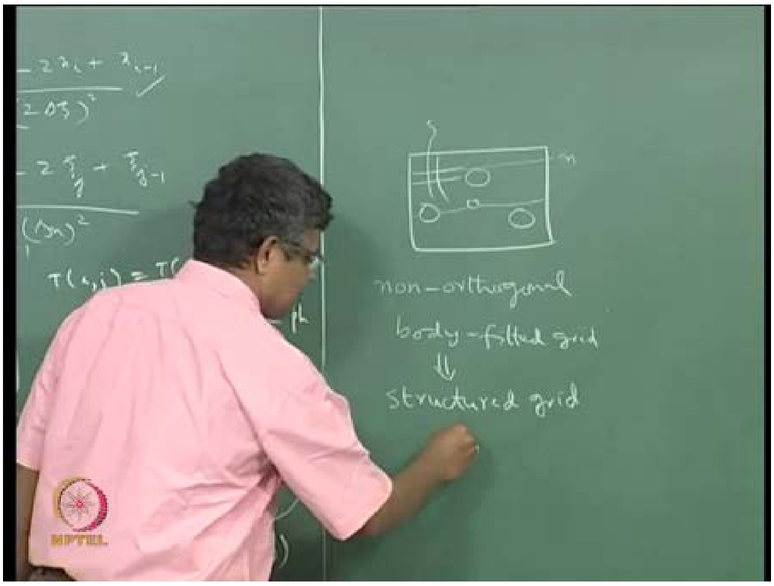

For example, if you are considering a case where even a rectangular domain with three tubes and you have flow going in the outer things like this and if you have another thing, which is smaller. So, in the general case like this, may not possible to have an orthogonal thing, but it is still possible to come up with a corresponding non-orthogonal body-fitted grid. And, this non-orthogonal body-fitted grid is such that this is also a structured grid. A structured grid in the sense that the structured grid has the grid points here or at intersections of constant coordinate lines. For example, this may be a constant eta line, this may be a constant psi line like this. So, all the grid points are located along intersections of constant psi and eta lines. That is what is known as structured grid.

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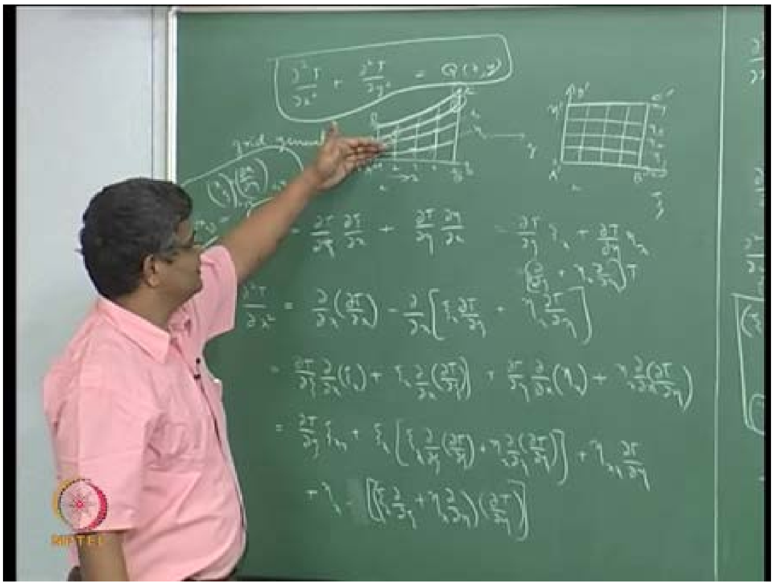

And for example, every point here is at an intersection of constant psi line and constant eta line. This is also constant… So, we are looking at this transformed line here. So, the corresponding point between this and this is along this constant eta line and this constant psi line. So, the grid points here are intersections of the family of lines of constant coordinate directions. And, in such a case, a cell here will have four phases in two dimensions. And, in the case of three dimensions, it will have six phases. And, not only that, if you know that this is i comma j, you know that immediate left neighbor, that is, i minus 1 j and right neighbor – i plus 1 j and also the top one, which is i j plus 1 and the bottom, which is i j minus 1 and also the front and back. So, in this particular case in a structured grid, you know where you are with respect to the neighboring points. And, that kind of structure is inherent in this. And, this structured grid will preserve, for example, the diagonal structure of the A metrics in that we get for elliptic equations and so on. So, the resulting A T equal to b based on the transformed equation will still remain diagonal although we have expected terms coming here.

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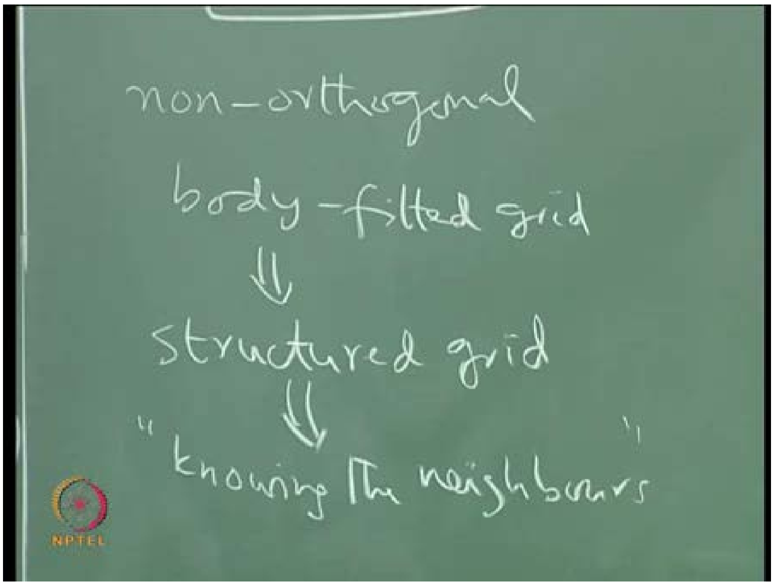

So, structured grid is useful from the point of view of knowing the neighbors, which is important when we want to deal with higher order accurate approximations for the derivatives. If you want to have a third order accurate one sided difference, you need to have four neighboring points. So, that means that you must have i minus 1, i minus 2, i minus 3. And, that kind of information is readily available in the case of structured grid. But, in unstructured grid, that information is not available, because these points are not at the intersection of these coordinate lines. So, in terms of knowing the neighbors, that is an important aspect.

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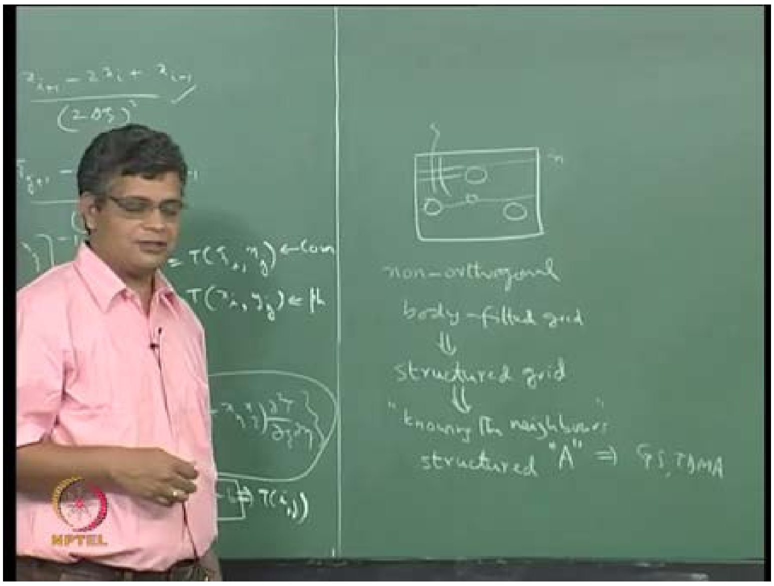

And, this also has possibility of structured coefficient metrics A. And, we know that if we have a structured coefficient metrics, then the application of the specialized methods like Gauss-Seidel method or the TDMA and the strong LPC procedure. These kind of methods are much easier with a structured coefficient metrics and there is an advantage with this. And, there are also modeling advantages in the case of a structured grid.

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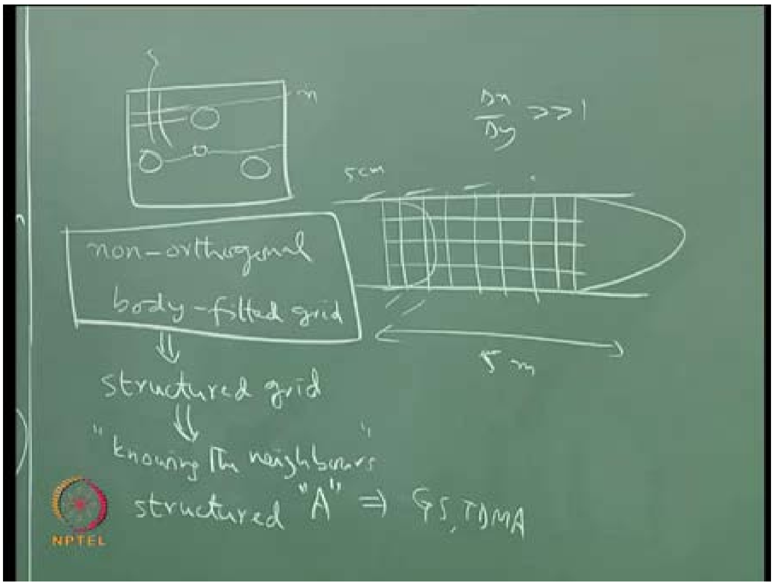

For example, if you are looking at a flow domain like this and the flow is developing, then the velocity profile may be like this here and then it may be finally going towards this. And, this dimension may be typically some 5 centimeters and this dimension may be something like 5 meters. So, you have a very long and thin pipe. In a structured metrics, it is possible to make it into grids such that the aspect ratio – it is delta x by delta y can be large without affecting the overall accuracy of the solution too much. But, if you have an unstructured grid and if you have a large aspect ratio, then the accuracy of the solution is going to be compromised. So, there are certain advantages for a structured grid.

And, that structured grid is actually carried forward, is used in this case of non-orthogonal body-fitted grid approach to the solution of the governing equations in which all the computations are done in the computational plane and then the information is sent back to the physical plane. But, this approach requires us to have a smooth grid; and then, the fairly complicated transformations of the equations happens; and then, addition of new terms of the cross derivatives is a possibility. So, there are certain things – advantages and disadvantages. But, this approach is a generic three-dimensional approach, which has proved to be very successful in dealing with fairly complicated geometries. So, in the next lecture, we will look at an alternative view point, alternative approach to the solution of equations again on a physically complicated geometry.