

**Foundation of Computational Fluid Dynamics**  
**Dr. S. Vengadesan**  
**Department of Applied Mechanics**  
**Indian Institute of Technology, Madras**

**Lecture – 15**

Greetings to all of you, today's class will be the last class for this week on this course CFD. So far, we have done information about different approximation methods, properties associated with the numerical scheme, then how to analyze a numerical scheme for consistency, convergence and stability. In today's class, we will get explanation of these with some more example equations. First, let us consider as shows in the past 1D unsteady diffusion equation  $\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2} = 0$ . We also learnt in the previous lecture, different scheme available for this model equation; one of thing is explicit scheme and forward in time central in space.

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### Some more info on FD scheme

Consider 1-D unsteady diffusion equation

$$\frac{\partial u}{\partial t} - \alpha \frac{\partial^2 u}{\partial x^2} = 0$$

Explicit Schemes: Forward in time and Central in space (FTCS)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{(u_{i-1}^n - 2u_i^n + u_{i+1}^n)}{\Delta x^2}$$

FTFS, FTBS, CTCS in any order is also possible.

Order of accuracy of this scheme is  $O(\Delta t, \Delta x^2)$  and scheme is stable if  $r \leq \frac{1}{2}$  where  $r = \frac{\alpha \Delta t}{(\Delta x)^2}$

Implicit Scheme:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{(u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1})}{\Delta x^2}$$

If you write down the difference equation, we get this form  $u_i^{n+1} - u_i^n$  by  $\Delta t$  equal to  $\alpha$   $(u_{i-1}^n - 2u_i^n + u_{i+1}^n)$  by  $\Delta x^2$ . We mentioned forward in time, so the superscript  $n$  is between  $n+1$  and  $n$ , central in space so the subscript  $i$  which is used for space and it is central, so we have node of interest  $i$ , and left node and right node  $i+1$  and  $i-1$ . It is also possible to write different other schemes, for example, forward in time forward in space, forward in

time backward in space, central in time and central in space. And it is also possible to write different order in any of these schemes and analyze appropriately. Order of this scheme order of accuracy of this particular scheme is  $\Delta t$  and  $\Delta x$  square. And we already learned this scheme is stable for  $r$  less than or equal to  $1/2$ , where  $r$  is defined as  $\alpha \Delta t / \Delta x$  that is  $\alpha$  is here, and  $\Delta t$  is moved from left hand side to the other side, and this is  $\alpha \Delta t / \Delta x$  this is what we learned through von-Neumann's stability analysis.

We can also write same forward in time central in space, but in explicit form. So we at that time we mentioned what is explicit and what is implicit, and here also we are going to reemphasize that point. So, this is forward in time on the left hand side for time derivative  $u$  of  $i$   $n$  plus  $1$  minus  $u$  of  $i$   $n$  by  $\Delta t$  this term is same as what is explained here. There is the small difference on the right hand side term for spatial differencing and here you can observe it is central in space because  $u$  of  $i$  minus  $1$   $u$  of  $i$   $n$   $u$   $i$  plus  $1$  we consider, but it is implicit which means it is evaluated or it is consider at the same time level, the time level here is  $n$  plus  $1$ . So, all this variables are considered at the same time level. So, you observe the superscript as  $n$  plus  $1$  in all the three terms, such a scheme is called implicit scheme.

And both these schemes you can understand by the sketch here. So, explicit scheme is what is shown here value at  $n$  plus  $1$  is evaluated based on values at  $n$  level, but using central differencing scheme  $i$  plus  $1$   $i$  and  $i$  minus  $1$  and this is for explicit scheme. And this figure demonstrate, how it is for implicit scheme, we consider again values at  $i$  plus  $1$  at  $i$  minus  $1$ , but at  $n$  plus  $1$  level.

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**Some more info on FD scheme**


- Various schemes of discretization:  
Explicit Schemes: (2) DuFort – Frankel Scheme (Central in Time and Space)

$$\frac{1}{2\Delta t} (u_i^{n+1} - u_i^{n-1}) = \frac{\alpha}{(\Delta x)^2} (u_{i-1}^n + \frac{1}{2}(u_i^{n+1} + u_i^{n-1}) + u_{i+1}^n)$$

The scheme is unconditionally stable and the order of accuracy is given by  $O(\Delta t^2, \Delta x^2, (\frac{\Delta t}{\Delta x})^2)$

Compare against FTCS  $\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{(u_{i-1}^n - 2u_i^n + u_{i+1}^n)}{\Delta x^2}$

Unconditionally stable and order of accuracy is  $O(\Delta t, \Delta x^2)$



Now we have try to understand, how to get different explicit scheme, there is a scheme called DuFort-Frankel scheme, which is central in time and space. So, if we look at time derivative discretization, we observe here  $u$  of  $i$   $n$  plus 1 minus  $u$  of  $i$   $n$  minus 1. So, it is actually evaluated as central scheme, but in time that is why you get superscript  $n$  plus 1 and  $n$  minus 1 corresponding denominator two is appearing. And for spatial derivative, it is central in space, but there is a small difference  $u$  of  $i$  minus 1  $n$ , so it is explicit; the last term  $u$  of  $i$  plus 1 at  $n$  th level, hence it is also explicit; the middle term is evaluated using central, so this is  $u$  of  $i$   $n$  plus 1 and  $u$  of  $i$   $n$  minus 1. This happens to be unconditionally stable.

If you remember or just recall we learned forward in time central in space is conditionally stable, whereas if you replace one particular term middle term by the central in time, so  $n$  plus 1 and  $n$  minus 1 stability condition changes from conditionally stable to unconditionally stable. And this scheme also happens to be of order of accuracy  $\Delta t$  square and  $\Delta x$  square and  $\Delta t$  by  $\Delta x$  square. So, if we compare against forward in time central in space, where it is conditionally stable and order of accuracy is  $\Delta t$  and  $\Delta x$  square. So, the middle term, which is shown here for the FTCS  $u$  of  $i$   $n$  which is completely explicit is replaced with  $u$  of  $i$   $n$  plus 1 and  $u$  of  $i$   $n$  minus 1. So, for changing this slightly, you are able to get a conditionally stable to unconditionally stable, and order of accuracy is also improved you can observe that.

There is also small note to be observed that is for the same scheme DuFort-Frankel scheme which is central in time and space, if you observe here  $u$  of  $i$   $n$  plus 1 and  $u$  of  $i$   $n$  minus 1, when you are starting the calculation that is the time equal to zero level for example, then this quantity that is  $u$  of  $i$   $n$  minus 1 is not available, because we have not done the calculation when you say  $n$  minus 1, it is before zero and that time it is not available. So, this particular scheme DuFort-Frankel scheme self-starting at time equal to zero level is not possible, as data at  $n$  minus one level is not available. So, at time is equal to zero alone, we do a calculation based on any other scheme once that quantity is available then you can switch to DuFort-Frankel scheme.

We move onto the next that is implicit scheme. So, general discretization for the same model equation, so this is time derivative which is forward in time  $u$  of  $i$   $n$  plus 1 minus  $u$  of  $i$   $n$  by  $\Delta t$ . There is small difference here on the right hand side for the spatial derivative, you get two components here, first bracket term  $u$  of  $i$  plus 1  $u$  of  $i$  and  $u$  of  $i$  minus 1, so it is central in space, but on the superscript, you see  $n$  plus 1 for all the quantity. So, it is central in space, but implicit. Now we move onto the next bracket term that is here, second central in space, but it evaluated as explicitly at  $n$ th level. So, we can see all the superscript for all the three terms as  $n$ .

This scheme is unconditionally stable for value of  $\theta$  greater than or equal to half. So, we have the factor called  $\theta$ , which is multiplying one part  $1 - \theta$  the factor multiplying another part. Now there are multiple variations for different values of  $\theta$ , if  $\theta$  equal to zero for that is if you look at the first term if  $\theta$  equal to zero, and implicit in time is not there, and you get one multiplying the second part of the equation, the second part of the equation happens to be fully explicit. So for  $\theta$  equal to zero, it will results in forward in time central in space explicit, this we have already seen. And for  $\theta$  is equal to half, 0.5 value, we get weightage actually, weightage of equal weightage equal weightage of implicit scheme and equal weightage explicit scheme such a scheme is called Crank Nicholson scheme, because it is proposed by both this people and it is neither explicit completely nor implicit completely. So, it is referred as semi explicit.

And for  $\theta$  equal to one, so if you substitute  $\theta$  equal to one in the second term  $1 - \theta$  cancels all. So, the explicit part goes to 0, only the implicit part remains, so becomes fully implicit scheme. So, you understand by writing this generalized

discretization equation, you are able to get three different scheme forward in time fully explicit, then crank Nicholson scheme semi implicit fully implicit also you are able to get. So, fully explicit, fully implicit and semi implicit all the three schemes are possible.

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**Some more info on FD scheme**

Consider the equation,

$$\frac{\partial u}{\partial t} = \alpha \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$


Explicit FTCS ,

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \alpha \left\{ \left( \frac{u_{i-1,j}^n - 2u_{i,j}^n + u_{i+1,j}^n}{\Delta x^2} \right) + \left( \frac{u_{i,j-1}^n - 2u_{i,j}^n + u_{i,j+1}^n}{\Delta y^2} \right) \right\}$$

$$u_{i,j}^{n+1} = u_{i,j}^n + d_x (u_{i-1,j}^n - 2u_{i,j}^n + u_{i+1,j}^n) + d_y (u_{i,j-1}^n - 2u_{i,j}^n + u_{i,j+1}^n)$$

$$u_{i,j}^{n+1} = (1 - 2d_x - 2d_y) u_{i,j}^n + d_x (u_{i-1,j}^n + u_{i+1,j}^n) + d_y (u_{i,j-1}^n + u_{i,j+1}^n) \quad \dots (1)$$

where  $d_x = \frac{\alpha \Delta t}{\Delta x^2}$  and  $d_y = \frac{\alpha \Delta t}{\Delta y^2}$



Next we take two-dimensional equation and try to get information about these quantities. Again we will take explicit forward in time and central in space. So, you write down the equation. Now the index for subscript, we have used i for x direction, now use i and j correspondingly x and y direction. So, forward in time, this we have already known and central in space, but we have two terms one for x, another one term for y. So, this term in the first bracket is for derivative in x, and second term is for derivative in y. We write accordingly central in space in x direction, so i minus 1 i and i plus 1 central in space in y direction, so it is i j minus 1 i j i j plus 1 and it is explicit. So, you observed all superscripts are n. So, all this quantities are evaluated at n time level.

You can rewrite this equation, by bringing all the known terms on one side and the quantity all variable that we determined on other side. So, in this case  $u_{i,j}^{n+1}$  is the quantity to be evaluated and that is retained on the left hand side as you can see here  $u_{i,j}^{n+1}$  and you bring all other quantity to the right hand side. So,  $u_{i,j}^n$  plus  $d_x$  on set of term plus  $d_y$  another set of term. It is also again you can rewrite, because you observed  $u_{i,j}^n$  appears two other places. So, you bring all  $u_{i,j}^n$  together, you will get a coefficient for  $u_{i,j}^n$  and then  $u_{i,j}^n$

minus 1 j and u of i plus 1 j and the remaining terms. So, this is the way you rearrange and write for coding purpose. And the dx is explained as alpha times delta t by del x square; similarly, dy is explained as alpha times delta t by del y square.

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### Some more info on FD scheme

Explicit FTCS  $u_{i,j}^{n+1} = (1 - 2d_x - 2d_y)u_{i,j}^n + d_x(u_{i-1,j}^n + u_{i+1,j}^n) + d_y(u_{i,j-1}^n + u_{i,j+1}^n)$

The order of accuracy is  $O(\Delta t, (\Delta x)^2, (\Delta y)^2)$ . The scheme is stable only if  $\alpha\left(\frac{\Delta t}{\Delta x^2} + \frac{\Delta t}{\Delta y^2}\right) \leq \frac{1}{2}$

Implicit FTCS  $\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \alpha \left\{ \left( \frac{u_{i-1,j}^{n+1} - 2u_{i,j}^{n+1} + u_{i+1,j}^{n+1}}{\Delta x^2} \right) + \left( \frac{u_{i,j-1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j+1}^{n+1}}{\Delta y^2} \right) \right\}$

$$d_x u_{i+1,j}^{n+1} + d_x u_{i-1,j}^{n+1} - (2d_x + 2d_y - 1)u_{i,j}^{n+1} + d_y u_{i,j+1}^{n+1} + d_y u_{i,j-1}^{n+1} = -u_{i,j}^n$$

Simultaneous equations need to be solved, because variables at different nodes are linked  
 Results in penta-diagonal matrix. Solution procedure is very time consuming.  
 Alternate is splitting method

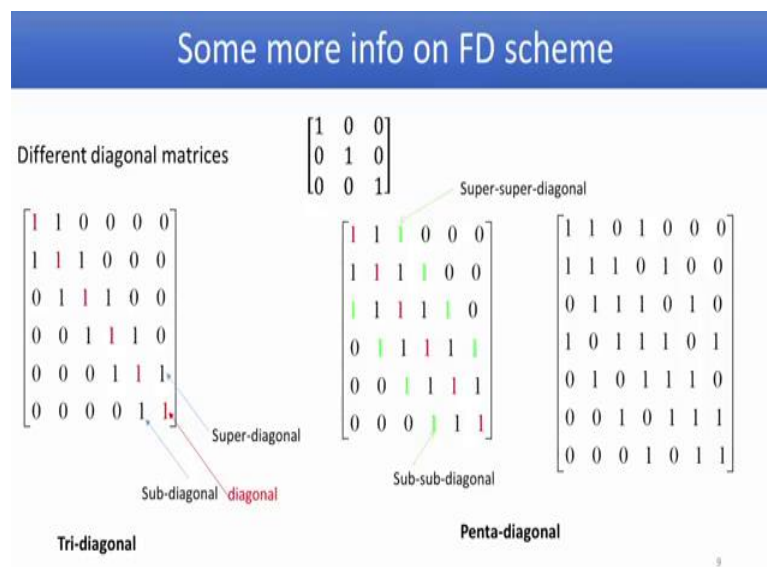
Now, let us look at this little more detail. Order of accuracy for this scheme is delta t in time and del x square and del y square for two different spatial direction we also learnt through last lecture that the scheme is stable only if delta t by del x square plus delta t by del y square multiplying alpha is less than or equal to half this is what is known as summed up condition and we also mentioned if you extend this for three d you get one more term here and it becomes restitute alpha is given in the equation delta t if you fix then you have the limited option on del x or del y. So, that you satisfy stability condition now we can rewrite the same in fully implicit form still following forward in time and central in space. So, you get superscript on all the right hand side term as n plus 1 which means you are actually evaluating at the current time level some of them are not evaluated some of them are part of the equation and if you rearrange as with it in the previous case rearrange all the term accordingly.

So, in this case the only term that is known is u of i comma j n. So, you move that to one side. So, that is what is taken here, than all other terms are brought other side which are not known because all are to be get to remain or to be evaluated at n plus 1 time level. So, you get rearrange and you get this step of equation. So, this particular equation is run

through entire computational domain are along a line nodes along a line then you get simultaneous equation for every node you will get one set of equation and you need to put them together and invert the matrix. So, you get simultaneous equation is to be solved because variables at different nodes are coupled with each other and this set of equation will result in what is known as the pentadiagonal matrix.

In the next slide, I am going to show what is pentadiagonal matrix usually either you adopt a separate procedure to invert a pentadiagonal matrix, it takes definitely time consuming. There is an alternate way of doing the same that is same equation we are using multiple methods of doing the same equation. The second have full dimensional diffusion equation; first we have seen explicit forward in time and central in space then we have seen implicit forward in time central in space we understand like order of accuracy as well as stability condition.

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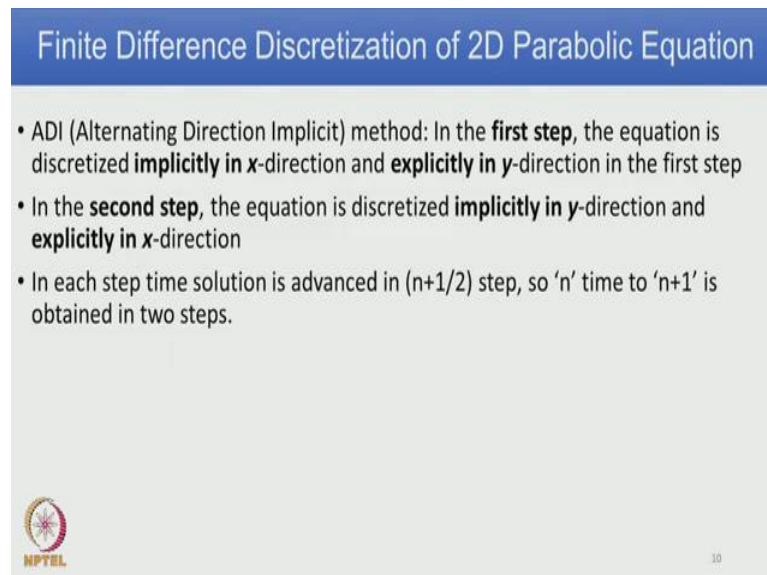


Now, let us look at different matrices what we shown here is just diagonal matrix, only one along the diagonal only one quantity is remaining, all other elements in the matrix are have 0 value then there is another matrix called tridiagonal matrix, this will extremely useful, we see later how it is used in CFD. In this the diagonal, main diagonal what is shown in the red, there is a value along the main diagonal then there is immediately there is one diagonal element one diagonal parallel to the which is called super diagonal and we have values along that. Similarly immediately below there is

diagonal called sub diagonal and we have values along that all other elements in this matrix is zero such a matrix is called tri diagonal matrix then we will see pentadiagonal matrix. So, this has the same structure as tri diagonal matrix, so that is we have one diagonal immediately below sub diagonal immediately above is a super diagonal, then the one more column or one more diagonal which is called super super diagonal which is following a super diagonal.


And we have values along the similarly on the lower side, one more diagonal, one more line following closely the main diagonal, but just below the sub diagonal were values are available. So, we have a pattern and this is what is called pentadiagonal that regular pattern. Now if you look at it is also possible to have pentadiagonal of different pattern. So, we can see main diagonal is there sub diagonal is also there super diagonal is also there the next sub sub diagonal or super super diagonal is not there, but it is after there. So, you get one more line with values another line with values. Now why I need to bring this, because you may get what is known as different lap structured matrix for different problem and solution procedures are different for each of this matrix structure.

(Refer Slide Time: 20:52)



Finite Difference Discretization of 2D Parabolic Equation

- ADI (Alternating Direction Implicit) method: In the **first step**, the equation is discretized **implicitly in x-direction** and **explicitly in y-direction** in the first step
- In the **second step**, the equation is discretized **implicitly in y-direction** and **explicitly in x-direction**
- In each step time solution is advanced in  $(n+1/2)$  step, so 'n' time to 'n+1' is obtained in two steps.

 NPTEL 10

Now, we will see little more detail about what we mentioned in the previous slide that is for two-dimensional diffusion equations. If we do completely implicit scheme then it results in pentadiagonal matrix inverting A, such a matrix is difficult. And there is alternative way of doing what is known as splitting and that is referred here as alternating



direction implicit method. So, you solve the same equation, but in two steps in the first step equation is discretized and implicitly solved in x direction and explicitly solved in y direction. In the second step, equation is discretized and implicitly solved in y-direction explicitly solved in x-direction.

So, each time step solution is advanced by n plus half level, which means to go from n time level to n plus 1 time level, it is obtained in two steps. Now such a matrix results in two tridiagonal matrices, and there is a standard easy procedure available to invert such a matrix. And this is easier compare to penta diagonal matrix. If it is a three dimensional equation, we extend the same logic that is to go from n time level to n plus 1 time level solution is advanced by one by three step. So, n, n plus 1 by 3, and n plus 2 by 3 and n plus 1, so that results in three tridiagonal matrices.

(Refer Slide Time: 22:49)

**Finite Difference Discretization of 2D Parabolic Equation**

- ADI (Alternating Direction Implicit) method: In the **first step**, the equation is discretized **implicitly in x-direction** and **explicitly in y-direction** in the first step

$$\frac{1}{\left(\frac{\Delta t}{2}\right)}(u_{ij}^{n+\frac{1}{2}} - u_{ij}^n) = \alpha \left[ \frac{1}{(\Delta x)^2} (u_{i+1,j}^{n+\frac{1}{2}} - 2u_{ij}^{n+\frac{1}{2}} + u_{i-1,j}^{n+\frac{1}{2}}) + \frac{1}{(\Delta y)^2} (u_{i,j+1}^n - 2u_{ij}^n + u_{i,j-1}^n) \right]$$

- In the **second step**, the equation is discretized **implicitly in y-direction** and **explicitly in x-direction**

$$\frac{1}{\left(\frac{\Delta t}{2}\right)}(u_{ij}^{n+1} - u_{ij}^{n+\frac{1}{2}}) = \alpha \left[ \frac{1}{(\Delta x)^2} (u_{i+1,j}^{n+\frac{1}{2}} - 2u_{ij}^{n+\frac{1}{2}} + u_{i-1,j}^{n+\frac{1}{2}}) + \frac{1}{(\Delta y)^2} (u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}) \right]$$

The order of accuracy is  $O(\Delta t, (\Delta x)^2, (\Delta y)^2)$  and unconditionally stable, whereas fully explicit FTCS is conditionally stable.

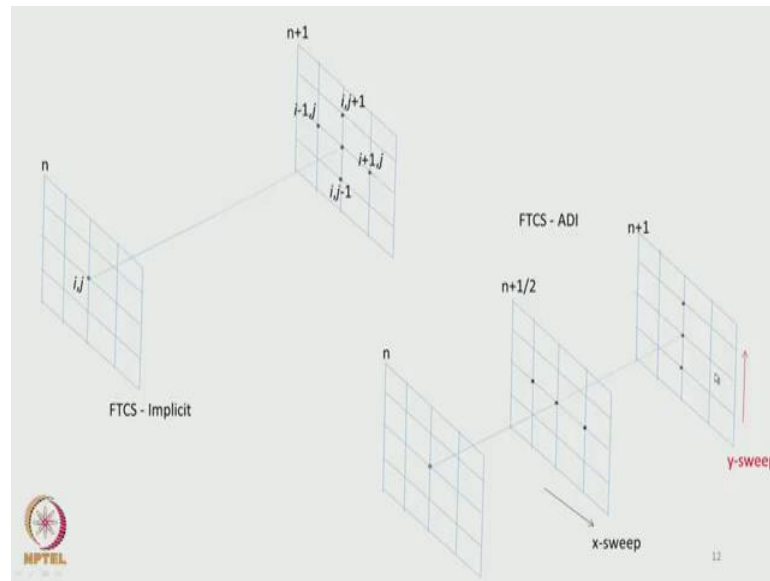
Now we look at the equation. So, first step equation discretized and implicitly solved in x direction, explicitly in y direction. If we look at the expression for the time derivative, we mention it advances by half. So, superscript is actually n plus half then it is implicit in x direction. So, all the quantities which are corresponding to derivative in x direction do square u by do x square the scheme is central in space. So, you get i plus 1 i and i minus 1 as a subscript, but it is implicit in time here evaluating at n plus half and that n plus half appears in spatial derivative term that is why becomes implicit in x direction. So, we have n plus half as a superscript on terms corresponding to second derivative do square

$u$  by  $\Delta x^2$  still central in space and it is explicit in  $y$  direction. So, term that corresponds to  $y$  direction that is  $\Delta y^2 \frac{\partial^2 u}{\partial y^2}$  you are evaluating central in space. So, we have  $j+1$  and  $j-1$ , but it is explicit in time. So, we have superscript appearing here.

Now once you solve this equation that quantity that is becoming to be known that is  $u_{i,j}^{n+1/2}$ . So, in the second step the equation discretized and it is implicit in  $y$  direction explicit in  $x$  direction. So, we switch implicit and explicit direction. Now we write down the equation as we mentioned when we solve the first equation, the quantity that is coming to be known is  $u_{i,j}^{n+1/2}$  and that is taken and we mention it is explicit in  $x$  direction. So, if we look at the derivative in the  $x$  direction term so that is  $\Delta x^2 \frac{\partial^2 u}{\partial x^2}$ . All the quantities are with the superscript  $n+1/2$  which means it is explicit in  $x$  direction and you have moved you actually come to correct time level  $n+1$  and we mention it is implicit in  $y$  direction.

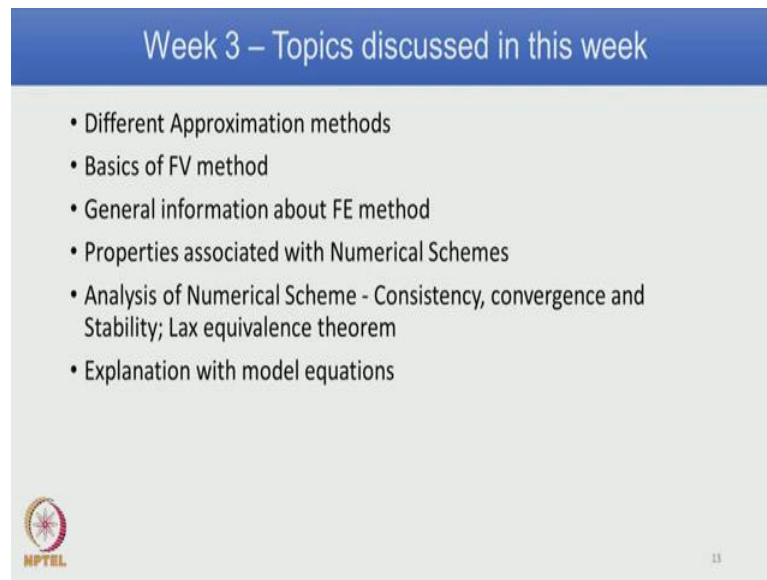
So, term that corresponds to  $y$  direction is here when we look at the superscript where all at  $n+1$  level. So, same equation is split in first step it is implicit in  $x$  direction explicit in  $y$  direction and the second step we switch the direction It becomes implicit in  $y$  direction and explicit in  $x$  direction. Now if you look at the order of accuracy, it is  $\Delta t \Delta x^2$  and  $\Delta y^2$  and it is unconditionally stable. Whereas, fully explicit forward in time central in space still is conditionally stable. So, we get advantage by doing this alternating direction implicit that is we get matrix simplified from pentadiagonal to tridiagonal matrix order of accuracy improved and it becomes unconditionally stable now let us understand this by graphical sketch.

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So, fully implicit forward in time central in space suppose these are the quantity grid and this are nodes and  $n$ th level. So,  $i$  and  $j$  is here  $i, j$  is here and to evaluate  $i, j$  at  $n$  plus 1 time level that is what displayed we moved we take all the quantities corresponding  $n$  plus 1 level for this same problem, but if we do forward in time central in space by Eddie method we introduce one more plane at  $n$  plus half level and plane at  $n$  plus half level we do  $x$  sweep and then at  $n$  plus 1 level we do  $y$  sweep. So, in today's class, we particularly looked at how to do different finite difference scheme or how to improve order of accuracy or how to get conditionally stable unconditionally stable and very important topic alternating direction implicit advantage associate with that.

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Week 3 – Topics discussed in this week

- Different Approximation methods
- Basics of FV method
- General information about FE method
- Properties associated with Numerical Schemes
- Analysis of Numerical Scheme - Consistency, convergence and Stability; Lax equivalence theorem
- Explanation with model equations

 NPTEL 13

With this class, we come to end of this week. And we have touched upon the initial aspects of CFD that is basic information about finite volume, finite difference, and finite element method, properties associated with the numerical scheme, conservativeness transportiveness boundedness, how to analyze numerical scheme, consistency, convergence and stability, and explanation with different model equations.

Thank you.