

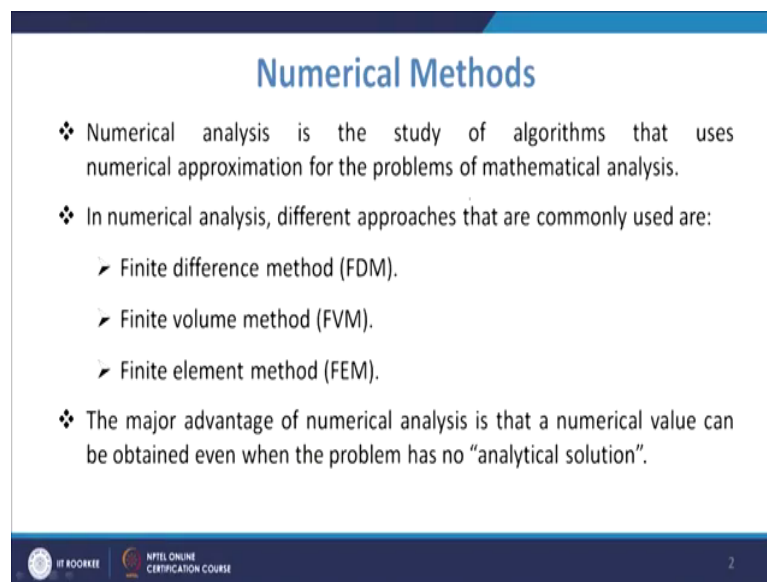
Modeling of Tundish Steelmaking Process in Continuous Casting
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Lecture - 27
Numerical Methods for Solving Governing Equations

Welcome to the lecture on Numerical Methods for Solving Governing Equations. So, in the last lectures, we talked about the different governing equations of fluid flow and heat transfer. And now we should go towards the modeling aspects, especially the numerical modeling which is normally carried out in the case of tundish modeling.



So, what are the typical numerical methods which are used for solving those governing equations, because we need to solve these governing equations to find the you know distribution of the variables like pressure, velocity, or temperature and many more at the different points in the domain. So, for that, there are different methods which are being adopted and among them. We will typically talk about one of the method that is finite volume method, but we will have certainly some idea about the other methods.

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Numerical Methods

- ❖ Numerical analysis is the study of algorithms that uses numerical approximation for the problems of mathematical analysis.
- ❖ In numerical analysis, different approaches that are commonly used are:
 - Finite difference method (FDM).
 - Finite volume method (FVM).
 - Finite element method (FEM).
- ❖ The major advantage of numerical analysis is that a numerical value can be obtained even when the problem has no “analytical solution”.

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So, let us talk about the numerical methods or numerical analysis when we talk. It is the study of algorithms that uses numerical approximation for the problems of mathematical analysis. So, as we know that we are normally getting the problems you know expressed

in the form of mathematical expressions. And now these expressions you know need to be solved, so you have to approximate it numerically.

And there are basically three types of different approaches which are most commonly used, and they are finite difference method, finite volume method and finite element method. Out of that normally we use for the fluid flow and heat transfer applications, we use the finite volume method especially in the domain of CFD that is computational fluid dynamics and even heat transfer.

So, the finite difference method which was first method which was you know devised that was you know that is still used, but then finite volume method has many advantages when we typically go for solving these fluid dynamics related problems. So, and then finite element is also used typically you know when you have this structural problems or related to deformations and all that.

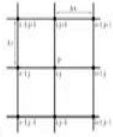
So, in those cases, in the case of metal forming or so typically they are used these finite element methods, but not necessarily you can say that always only finite element method should be used, only on those areas you can use even in the area of fluid mechanics and heat transfer also. So, the major advantage of the numerical analysis is that a numerical value can be obtained even when the problem has known analytical solution.

So, the thing is that in many cases, we are not likely to have the analytical solution, and in those cases we have to rely you know we have to go for the numerical you know approximation and that is why the numerical analysis is being carried out.

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Finite Difference Method

- ❖ **Finite-difference methods** are numerical methods for approximating the solutions to differential equations using finite difference equations to approximate derivatives *via* truncated Taylor series.
- ❖ These finite difference approximations are algebraic in form and the solutions are related to grid points.
- ❖ **The finite difference method involves three steps:**
 - Dividing the domain into set of grids of nodes.
 - Approximating the given differential equation by finite difference equivalence that relates the solutions to grid points.
 - Solving the difference equations subject to the prescribed boundary conditions and/or initial conditions.



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So, the finite difference methods these are the numerical methods for approximating the solutions to differential equations using finite difference equations to approximate derivatives via truncated Taylor series. So, basically what is required is that most of the these equations where you see these derivatives are there or there the differential equations, and we need to have the solution of these differential equations.

So, you have derivatives. And in the derivatives, you know we are approximating these derivatives via the truncated Taylor series. So, you have a Taylor series expansion, and in that we truncate it we try to ignore certain terms to find the expression for the derivative in terms of the neighboring you know points. And accordingly you know if you get the algebraic equation which is to be solved.

So, these finite difference approximations are algebraic in form and the solutions are related to grid points. So, what happens that suppose you want to go for this point, so, if you have to find you know the derivative. So, derivative at this point suppose if you have to find suit maybe this point minus value at this point minus this point divided by the whole distance or maybe you know if you want to have the derivative, so in this domain it will be at this value minus at this value divided by this domain.

So, like that if you go for the derivative with respect to the you know in this direction, so there you have the points at these two, you know the values are these two points and taken the distance between them as δy . So, accordingly you know you get you know these

differential equations in you are converting it into the algebraic equations, and then they are solved.

So, the finite difference method will be involving three steps first is that you divide the domain into a set of grids of nodes. So, you have a domain. So, you will be you know dividing it in the form of nodes. Then you are approximating the given differential equation by via finite difference equivalence that relates the solution to the grid point.

So, you will have you know the grid points in the in their form, you will be approximating those equations using the finite difference equivalence. And then you are solving these difference equations so that will be subjected to the prescribed boundary conditions or and or the initial condition.

So, once you have the equations at the different points you know, but not points basically for every node you will have the equation and then you will have also the conditions as the in the form of initial conditions or the boundary conditions which are there at the boundaries, so then they are solved. So, normally we go for we used to solve you might have done hopefully the solution of the steady state heat transfer in one-dimensional using the finite difference you can do it.

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Taylor Series

Taylor series is a expansion of a function $f(x)$ for some finite distance dx to $f(x \pm dx)$ as:

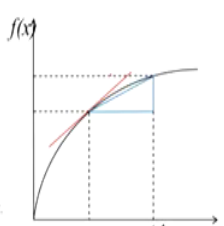
$$f(x \pm dx) = f(x) \pm dx f'(x) + \frac{dx^2}{2!} f''(x) \pm \frac{dx^3}{3!} f'''(x) + \frac{dx^4}{4!} f^{(4)}(x) \pm \dots$$



For getting $f'(x)$ from Taylor series

Forward difference:

$$f'(x) \approx \frac{f(x + dx) - f(x)}{dx} + O(dx)$$

* The error of the first derivative using the *forward* formulation is of order dx .





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So, as we are talking about, so that the minute from this Taylor series and that is truncated Taylor series. So, as you know that this is the Taylor series $f(x \pm dx) = f(x) \pm$

$dx f'(x) + \frac{dx^2}{2!} f''(x) \dots$, so like that it will go. So, you know if you have to find the $f'(x)$, and if you know remove these terms if you are trying to you know neglect these terms, so, dx will be divided, so dx will be divided for whole the terms.

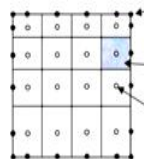
So, this will be of dx order, so that way it will be order dx . So, the error is or the order of dx . So, you are further you are neglecting, so that way you get the $f'(x)$ value, and that is being you know expressed in terms of with the function value at $x + dx$, and $f(x)$ and dx is the distance between the two points that is $x + dx$ and the x .

So, this is being used you know for that approximation and that you are getting one linear algebraic you know equation and that you will be getting at all the nodes and then you can solve it. Now, the important method which is normally used for the CFD calculations will be the you know finite volume method.

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Finite volume method



- ❖ Divide the domain into control volumes.
- ❖ Integrate the differential equation over the control volume
- ❖ Apply the divergence theorem.
- ❖ To evaluate derivative terms, values at the control volume faces are needed: have to make an assumption about how the value varies.
- ❖ Result is a set of linear algebraic equations: one for each control volume.
- ❖ Advantage of FVM is that the integral conservation is satisfied exactly over the control volume.
- ❖ Solve iteratively.



Boundary node

Control volume

Computational node

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Now in the finite volume method what is done is that this here the domain will be converted into the control volumes, and there will be integration over the you know control volume. So, integral conservation will be satisfied over the exact may be known over the all the exactly over the control volume. So, basically it is keeping that physics also into mind and so it will be and in this case you apply the divergence theorem because you will have, so you are integrating over the whole control volume.

So, you will have the divergence theorem applied, so that you are getting another equation for the further. And then you use the you know different type of discretization you know rules and these rules basically will help you to get the equations in the algebraic form which is solved. So, the to evaluate these derivatives, derivatives terms what is done is that values at the control volume phases are needed.

So, you have to make an assumption that how the value is varying. So, basically you know you have the control volume in that you have the node. At the center of the control volume, you have the you know control volume phases. So, you know when you need to have the values at the control volume phases, you will have to make the assumption that how the value is varying.

So, you will have the values at the nodes in their term you have to take the value at the nodes. So, for that you will have the different rules that we will discuss. And that this way, so that there may be you know there are discretion schemes are there. And then the result is that we try to you know have a set of linear algebraic equations and that is one for each control volume.

So, whatever be the of volumes you will have that number of linear algebraic equations and then you are solving these equations iteratively in most of the cases. And you get the values you know at the different you know points of interest. Now, the advantage of finite volume method is that the integral conservation is satisfied exactly over the control volume.

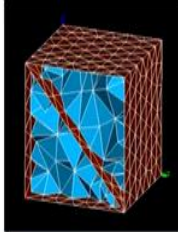
So, in those cases what you see that you are you know conservation is satisfied over the control volume. So, as you see this is a typical a control volume, these are the nodes - the computational nodes, and this is the you know as you see this is the boundary. So, you know and these are the you know, so you will once you find the control volumes then you will have, so this is typically a control volume, and this is the node at the boundaries this is boundary node.

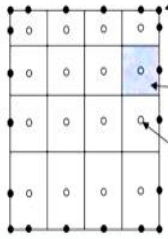
So, basically you use the boundary conditions, and then accordingly you will have the equations are at these points also. So, they will be helpful in solving the equation.

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Cells and nodes

- ❖ Solution domain is subdivided into a finite number of small control volumes (cells) by a grid.
- ❖ The grid defines the boundaries of the control volumes
- ❖ Computational node lies at the center of the control volume.
- ❖ The advantage of FVM is that the integral conservation is satisfied exactly over the control volume.







Boundary node

Control volume

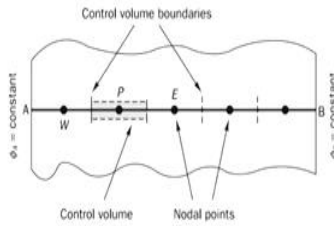
Computational node



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So, you will have this is your solution domain which is subdivided into number of you know small control volumes. Then the grid defines the boundaries of the control volume. Computational node will be lying at the centre of the control volume and all this that we have already seen.



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FVM for 1D steady state diffusion



Pure diffusion problem

$$\frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right) + S = 0$$



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Now, what we see that how we have to know that how this control volume method works. So, because when we are taking a domain in most of the cases, we will be solving the

problem in 2D or 3D, but just for understanding, we will start with one-dimensional problem and also the two-dimensional problem.

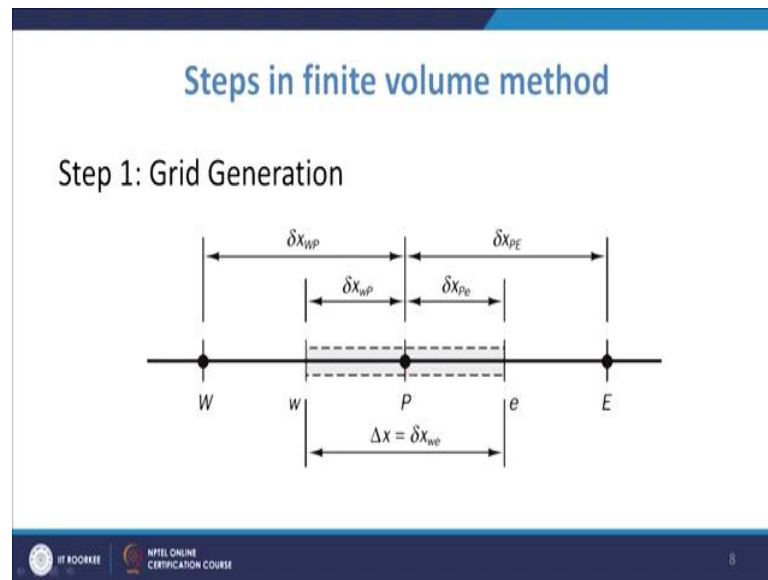
So, suppose we start with a simple problem of pure diffusion problem, so if you look at the pure diffusion problem, and if you do the 1-dimensional steady state diffusion, so in that case you know there is no you know the time derivative term, and you have the one-dimensional steady state diffusion equation can be divided $\frac{d}{dx}(\Gamma \frac{d\varphi}{dx}) + S = 0$.

So, that is the 1-dimensional steady state diffusion, you know if that is of 2-dimensional you will have x and y both will be coming into picture. Now, what we do you know in these cases as you see first of all you have the domain. So, you are having the formation of control volume. So, once you take these nodes, now surrounding these nodes you are finding the control volumes.

So, as you see you are you are having, so this way you will have the control volume at this point; similarly you will have one control volume at this point, so that way you can have these different you know control volumes. As you see the on this side and this side, so you will have certain you know conditions will be there.

Suppose φ is if you are do going for the heat conduction equation or so, φ will be nothing but the temperature. So, temperature values may be given at this point and this point. So, these are the boundary conditions, so that will be you know those conditions at boundaries they will be taken into account, and then accordingly you will have the equations formed.

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So, what we do is initially we go for the grid generation, and as you see that if you take any point P, so what happens on the, so on the this is the control volume. So, what you see this is the east phase of the control volume, this is a west phase of the control volume, and this is the grid node P.

And similarly you will have these distances; so they will be represented by δx_w is west to east surface, the small will be that surface denoting the surface. Similarly, this will be delta x P and this is δx_{wp} . So, these are the distances, and this will be again the distance between the nodes P and the east node, and similarly the between EP, and the west node it will be δx_{WP} .

So, you make these you know grids, and normally we practice is that we make these you know control volumes near the edge of the domain in such a manner that the physical boundaries should be matching with the control volume boundaries that is what you see that here also if you make these boundaries, so the control volume boundary will be making you know coming in you know here in the same line with this surface boundary. Now, after doing that what we do is, we do the discretization.

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Steps in finite volume method



Step 2: Discretization

After discretization of governing equation by finite volume method gives

$$\left(\frac{\Gamma_e}{\delta x_{PE}} A_e + \frac{\Gamma_w}{\delta x_{WP}} A_w - S_p \right) \phi_P = \left(\frac{\Gamma_w}{\delta x_{WP}} A_w \right) \phi_W + \left(\frac{\Gamma_e}{\delta x_{PE}} A_e \right) \phi_E + S_u$$

The above equation can be written as

$$a_P \phi_P = a_W \phi_W + a_E \phi_E + S_u$$



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And if you look at the x equation, so what we see that we get once you do the discretization, you get the equation in this form.

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For source term

$$S \Delta V = S_w + S_p \phi_P$$

$$\frac{d}{dx} \left(\tau \frac{d\phi}{dx} \right) + S = 0$$

$$\int_{\Delta V} \frac{d}{dx} \left(\tau \frac{d\phi}{dx} \right) dV + \int_{\Delta V} S dV = 0$$


$$\Rightarrow \left(\tau A \frac{d\phi}{dx} \right)_e - \left(\tau A \frac{d\phi}{dx} \right)_w + S_u \Delta V = 0$$



$$\tau_e = \frac{\tau_w + \tau_p}{2}$$

$$\tau_w = \frac{2\tau_w + \tau_p}{2}$$

$$\left(\tau A \frac{d\phi}{dx} \right)_e = \tau_e A_e \frac{\phi_P - \phi_E}{\delta x_{PE}}$$

$$\left(\tau A \frac{d\phi}{dx} \right)_w = \tau_w A_w \frac{\phi_P - \phi_W}{\delta x_{WP}}$$





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Now, how we get the equations in this form, so what we have seen we saw that you have $\frac{d}{dx} \left(\tau \frac{d\phi}{dx} \right) + S = 0$. So, this is your equation. Now, if you go for the integration of over the control volume, so what you do is you are doing the integrations, you do the integration

over the control volume that is ΔV , and it will be $\int_{\Delta V} \frac{d}{dx} (\Gamma \frac{d\phi}{dx}) dv + \int_{\Delta V} s dv$, so that will be also for the volume you are doing the volume integration.

Now, what happens that if you do that, so using that theorem you can write you know as, so this will may be written as $\Gamma A \frac{d\phi}{dx}$. And similarly you will have, so and then you this also you will have $s dv$. So, this will be for the area, and then you have $s dv$. So, this way you know that will be equal to 0. So, this will be 0 that seems to be you know accordingly you will have.

So, what happens you know now if you integrate, so first of all you will have the area term coming into picture. And then since it is integration, so you will have the value at the east phase and then value at the west phase, so you will have basically this as the Δv term will be coming later, and here you will have e minus again you will have the term $\Gamma A \frac{d\phi}{dx}$ and that will be at the west phase. And then you will have the term $s \Delta v$ will be equal to 0.

So, that way you are getting these values. So, you are converting them you know using the divergence theorem. Now, the thing is that you are getting these values at the nodes. And you need to have these values at the these phases or the phase of the control volume boundaries. So, you will have to basically do certain kind of differencing.

And if you use the central differencing for this tau term, so you will have to define the tau term at e if you look at the you know this, this point, so you will have the point e here. And if you have to have the you of tau at e, so you can have it you know as the average of using central differencing approach, you can have the average of at this point plus the plus this point.

So, you can have the you know this value that will be interpolating, linear interpolating we can have this value. So, tau e we can have the tau w plus you know $\Gamma_e = \frac{\Gamma_E + \Gamma_P}{2}$. And similarly $\Gamma_w = \frac{\Gamma_W + \Gamma_P}{2}$.

So, your diffusive fluxes what we have seen $\Gamma A \frac{d\phi}{dx}$. So, you know you are you know tau $\Gamma A \frac{d\phi}{dx_e}$, it will be you know you know tau so that is what it will be Γ_e . So, it will be $\frac{\Gamma_E + \Gamma_P}{2}$ that you can take it; otherwise you take these values at the phase itself.

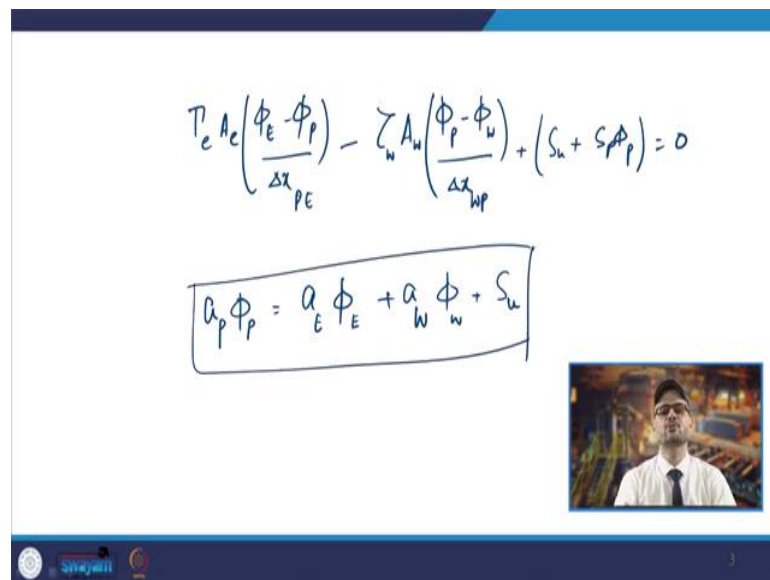
So, you can have the $\Gamma_e A_e \frac{[\phi_E - \phi_P]}{\Delta x_{PE}}$. Similarly, $\Gamma_w A_w \frac{d\phi}{dx_w} = \Gamma_w A_w \frac{[\phi_P - \phi_W]}{\Delta x_{WP}}$.

So, and also now what we do that for the source term what we do is we linearize it. So, once we linearize it, will be S will be, so what we do for the for source term, so it will be linearized and that we represent as this $S \Delta V$. So, if you take the $\bar{S} \Delta V$, if we take it as the you know one is $S_u + S_p \phi_p$.

So, we are linearizing this source term, so that the term which is you know when we are doing for the you know getting the equation in terms of ϕ_p at that time this will go on that side. So, what we see if you try to give these values in that particular equation, so in that case, you are getting you know this value.

So, what we get is that this will be $(\frac{\Gamma_e A_e}{\Delta x_{PE}} + \frac{\Gamma_w A_w}{\Delta x_{WP}} - S_p) \phi_p = (\frac{\Gamma_w A_w}{\Delta x_{WP}}) \phi_w + (\frac{\Gamma_e A_e}{\Delta x_{PE}}) \phi_E + S_u$. What you see, so that can be you know that you can get if you go further, so that will be you know once you do that. So, you will have, so that can be even understood by writing these equations.

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$$\tau_e A_e \left(\frac{\phi_E - \phi_P}{\Delta x_{PE}} \right) - \tau_w A_w \left(\frac{\phi_P - \phi_W}{\Delta x_{WP}} \right) + (S_u + S_p \phi_p) = 0$$

$$a_p \phi_p = a_E \phi_E + a_W \phi_W + S_u$$

So, what you got is $\Gamma_e A_e$, and you have the you know $\frac{d\phi}{dx_e}$, so it will be $\phi_E - \phi_P$. So, you will have $\frac{[\phi_E - \phi_P]}{\Delta x_{PE}}$. And similarly you will have $\tau_w A_w$ and then you have $d\phi$ by dx ,

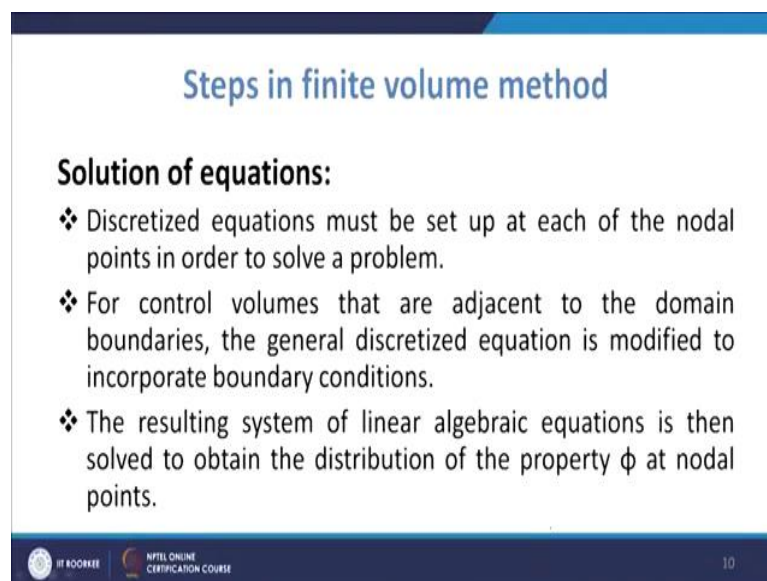
so that will be $\Gamma_w A_w \frac{[\phi_P - \phi_W]}{\Delta x_{PE}}$ or P W So, you can write. And then, so, that will be and then plus $S_u + S_p \phi_p$, so that will be equal to 0.

What do you see is that now this equation can be written you know what you see that you have ϕ_P , and you have a ϕ_E and ϕ_W , and there is one source term S_u . So, $a_p \phi_P = a_E \phi_E + a_W \phi_W + S_u$.

So, and then we write as a E, then a W and then you have the source terms that is what you are getting and a P will be. So, that is what you know this same equation you are getting. So, this will be $\phi_E / \Delta x_{PE}$, so that way you know now getting the ϕ_E , whether how should you get it you can have in general you can negate the that ϕ_E value as the average of the value at towards the at the east, and also at the p node, so that way you can get in simple terms, but you know that also may be taken differently and that we will study later on that how it is done.

So, what we see is that in this case you are getting just such kind of equation, and this equation you will be getting you know at for all the control volumes, and then they are solved, and you get the value at the nodes. So, this is how you know your equations are solved in this case.



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Steps in finite volume method

Solution of equations:

- ❖ Discretized equations must be set up at each of the nodal points in order to solve a problem.
- ❖ For control volumes that are adjacent to the domain boundaries, the general discretized equation is modified to incorporate boundary conditions.
- ❖ The resulting system of linear algebraic equations is then solved to obtain the distribution of the property ϕ at nodal points.

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Similarly, I mean we can go for the, so what we see normally in the finite volume method, you have the discretized equation which is must be set at each of the nodal points in order

to solve the problem. You know you we got the equations for the control volume and also we will have the equations for the you know at the boundaries.

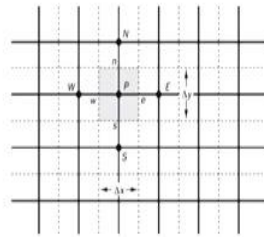
So, you will have certain boundary conditions will also lead to some set of equations, and accordingly you will be solving them. So, your discretized equations are set up at the nodal points and which are adjacent to the domain boundaries those volumes the discretized equation is modified to incorporate the boundary condition.

So, what happens that at the boundaries, you will have to modify now you know that equation because that condition needs to be satisfied. So, you will have the incorporation of the boundary conditions, and then the equation resulting system of equation is solved to obtain the distribution of property ϕ at all the nodal points.

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FVM for 2D diffusion problems

Step 1: Grid Generation



Two-dimensional steady state diffusion equation given by

$$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial \phi}{\partial y} \right) + S_{\phi} = 0$$

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Now, if you saw this that was done for the 1-dimensional and what we saw in the 1-dimensional flow, you have the control volume and you have one node towards the east and one node towards the west. And so they at this particular point you know you are getting the value at this point expressed in terms of the point at this end point at you know the value at this point as well as at this point neighboring two points, and then you are solving them, now that was a simple 1-dimensional case.

Similar can be extended for the 2-dimensional cases. So, when you have 2 dimensional diffusional problems, so it will be $\frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right) + \frac{d}{dy} \left(\Gamma \frac{d\phi}{dy} \right) + S = 0$. So, what happens here,

you will have the control volume and you will have the phases towards the north and also all towards the south.

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FVM for 2D diffusion problems

Step 2: Discretization

After discretization of governing equation by finite volume method gives



$$\left(\frac{\Gamma_w A_w}{\delta x_{wP}} + \frac{\Gamma_e A_e}{\delta x_{PE}} + \frac{\Gamma_s A_s}{\delta y_{SP}} + \frac{\Gamma_n A_n}{\delta y_{PN}} - S_p \right) \phi_P$$

$$= \left(\frac{\Gamma_w A_w}{\delta x_{wP}} \right) \phi_w + \left(\frac{\Gamma_e A_e}{\delta x_{PE}} \right) \phi_e + \left(\frac{\Gamma_s A_s}{\delta y_{SP}} \right) \phi_s + \left(\frac{\Gamma_n A_n}{\delta y_{PN}} \right) \phi_n + S_u$$

The above equation can be written as

$$a_P \phi_P = a_w \phi_w + a_e \phi_e + a_s \phi_s + a_n \phi_n + S_u$$

Step 3: Solution of equations

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So, what happens that in this case you get the value at the P point, it will be expressed in terms of west east plus south plus north and then plus the source term. So, same in the same way, you will have this equation coming in this form. And this equation will be you know, so you get these equations at all the nodes you will be getting those equations and these equations are solved and you are getting, so same thing applies for even the you know 3-dimensional problems where you have top and bottom also.

So, you will have the six terms plus the source term will be coming, and that needs to be solved using the proper algorithm. So, there are many algorithms for solving these set of linear equations in those cases. So, this is you know about the difference in finite volume method typically, there are methods like finite element also, but we will be talking more about the finite volume methods in our study in the coming lectures.

Thank you very much.