Introduction to CFD
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Module - 2
Lecture – 9
Methods for Approximate Solutions of PDEs Continued

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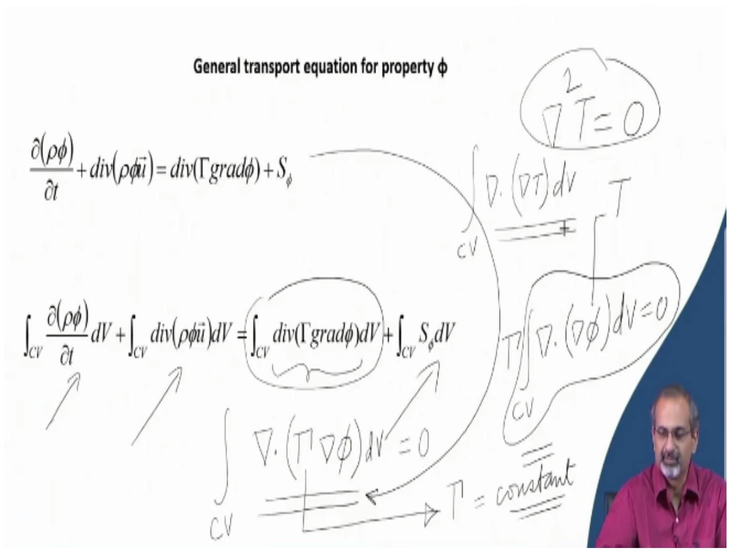

In this lecture, we will continue our discussion on the finite volume method. If you recall in the last lecture, we were talking about the general transport equation for property ϕ and we talked about both its differential as well as integral forms and we said that we are going to use the integral form for the finite volume method. Now, we will take an example problem from this general transport equation and try to understand the finite volume implementation of that problem.

If we ignore unsteady effects, advective effects and source terms in the equation, then we will be left with only a term which is coming from the diffusion and that term can be written like this

$$\int_{CV} \nabla.(\Gamma \nabla \phi) dV = 0$$

what you have inside the integral comes in the derivative form, that means in the finite difference form from the differential equation. Additionally, what you are doing is you are integrating that term here when you are discussing it in the context of finite volume technique.

So, in order to handle this kind of a term, we need to understand that what is the best way out, but before doing that we could have other simplifications possible. So, here if you imagine that gamma which is the transport coefficient is a constant, then it has no spatial variation or no dependence on phi. It can then be taken out of the integral. When gamma is a constant, you are left with this form of the equation.

$$\Gamma \int_{CV} \nabla . \left(\nabla \phi \right) dV = 0$$

And therefore it is sufficient to just set the integral to 0 without considering the gamma effect at all. So, that would reduce the complexity further and address the problem from a rather simple perspective. So, we are going to talk about a diffusion equation being solved in the finite volume framework. Additionally, what we are going to say is that here we set phi = T that means it is going to stand for temperature.

Therefore, we are essentially talking about steady state heat conduction. Additionally, the kind of simplifications we already imposed were that the thermal conductivity is constant, there are no heat sources, there are no unsteady effects and so on. In this situation, what you have in the differential form is the Laplace equation, but here when you are talking about the integral form of the equation, you are writing it slightly differently.

You are writing it as an integral of divergence grad T, so that is how you are putting it and you would like to retain it that way because one of the important vector calculus identities will help us take a very comfortable route using this form of the equation.

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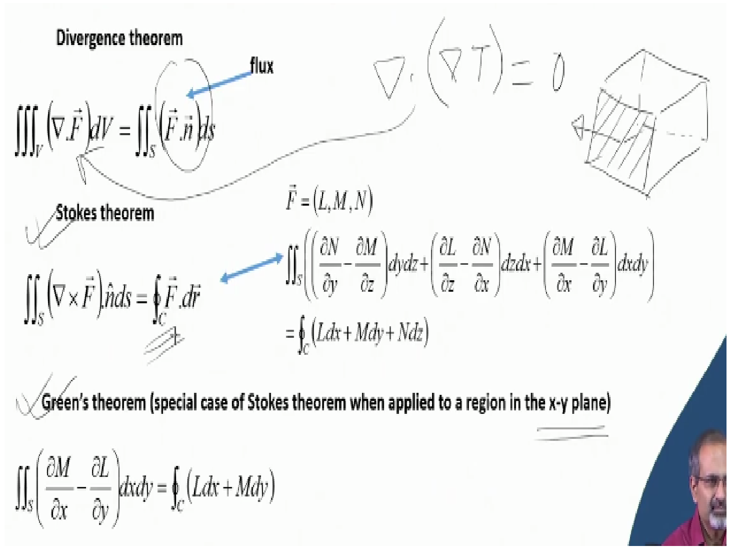

We do a quick recap of some of the important equations which might be required when we discuss about finite volume technique. The most important being the divergence theorem.

$$\iiint_V (\nabla.\vec{F}) dV = \iint_S (\vec{F}.\vec{n}) ds$$

So, you already saw that the governing equation for ϕ was written with terms which were expressed with divergence. So, that included the advective as well as the diffusive terms. So, here if we are solving this problem, then we have a clear convenience in expressing it in the divergence form.

So, it will be like divergence of grad T dv integrated over a control volume and then what the divergence theorem straightaway says is that the volume integral essentially reduces to a surface integral and what you have integrated in the surface integral is flux moving through different surfaces which form the control volume. So for example, if your control volume looks like this, then it has a certain volume included.

But you are not talking about the volume but rather you are talking about fluxes which move out or move in through the surfaces which define the volume, and therefore, you do not really need to work out the volume integral but rather the surface integral. So, this is the approach we will take to solve this problem. In finite volume technique for simplifying certain other kinds of terms in the governing equations, you may as well come across the use of Stokes theorem, which is in a general 3D framework.

$$\iint_S \left(\nabla \times \vec{F}\right).\hat{n}ds = \oint_C \vec{F}.d\vec{r}$$

$$\vec{F} = \left(L, M, N\right)$$
$$\iint_S \left(\left(\frac{\partial N}{\partial y} - \frac{\partial M}{\partial z} \right) dydz + \left(\frac{\partial L}{\partial z} - \frac{\partial N}{\partial x} \right) dzdx + \left(\frac{\partial M}{\partial x} - \frac{\partial L}{\partial y} \right) dxdy \right)$$
$$= \oint_C \left(Ldx + Mdy + Ndz\right)$$

Or if you are applying it in a plane, let us say in the x-y plane, then you would prefer to use a simpler form which is called as the Green's theorem.

$$\iint_S \left(\frac{\partial M}{\partial x} - \frac{\partial L}{\partial y} \right) dxdy = \oint_C \left(Ldx + Mdy\right)$$

So they both involve line integrals. They express the relationship between surface integrals and line integrals and are very convenient when you are working on planar control volumes.

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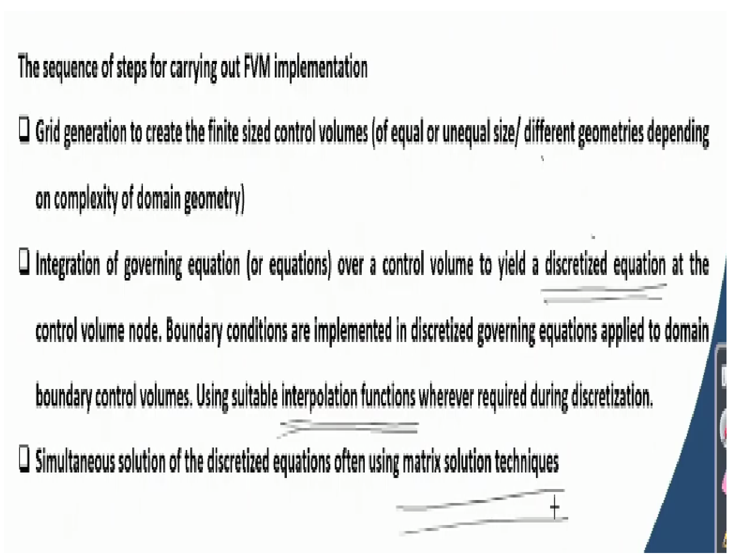

A quick recap of the sequence of steps which we will be using for the finite volume implementation. We have already discussed about the grid generation aspect, where we discretized the domain into finite sized control volumes of different shapes or sizes depending on the complexity of the problem. For very simple problems, we could have equal sized control volumes like the one we will use in our problem and then we follow the integral approach.

So, we would be integrating the governing equations on these control volumes and that is what will again yield discretized equations like you saw in the finite difference framework. And we are again going to see algebraic equations and most often linear algebraic equations which are easy to handle and solve. Boundary conditions need to be implemented and applied at the domain boundaries.

And this time you will see that instead of a grid point lying on the boundary, it will be a face of a control volume which will lie on the boundary and then at these control volume interfaces, that means common faces which are shared by two adjacent control volumes, you may also at times need certain interpolation functions in order to interpolate values of certain parameters, which will be discussed in due course in later lectures.

Then finally once you have a system of discretized equations, you will have to solve them simultaneously, and for that most often when you have a large number of control volumes to be handled, you would prefer to use matrix solution techniques, which again we will discuss in due course, but currently we are using a very few control volumes and therefore hand calculations can be done.

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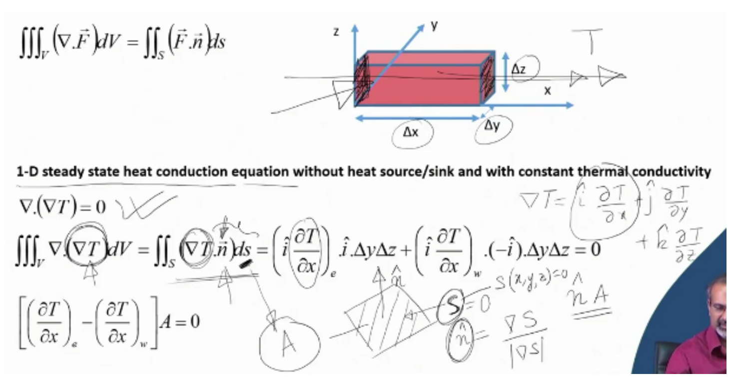

Here is a control volume which we have drawn having finite but small dimensions delta x, delta y, delta z along 3 directions and we are trying to figure out how the 1-D steady state heat conduction equation can be discretized on such a control volume using the finite volume technique. So, this is the governing equation in the derivative form or the differential form which is appropriate for finite difference approximation.

However, we are going to use its integral form now for the discussion of the finite volume technique. So, we end up using the divergence theorem to convert the volume integral into a surface integral. Note that what you have coming out of this is this function which in our case happens to be the gradient of T, it comes directly over here and now gets into a dot product with the unit surface normal vector.

That means, if you have a surface like this, you have a surface normal and the unit surface normal vector can be indicated as $\hat{n}$. If you have a functional description for this surface, let us say that the surface is represented by a function which looks like S = 0, then this unit normal can be defined as gradient of S by mod of gradient of S.

$$S(x,y,z)=0$$

$$\hat{n}=\frac{\nabla S}{|\nabla S|}$$

And then what you need to do is that once you have defined this unit normal vector, it has to be multiplied by the scalar value of the surface area.

So, if this surface area actually has a scalar value A, then you will be multiplying $\hat{n}$ by A to get the representation of the elemental surface area vector. So, $\hat{n}$ times A is what you have over here and mind that this small ds is actually standing for A, this small s and the functional representation of the surface given by the capital S are not the same thing.

This is essentially a function like f(x, y, z) = 0, alright, while this is only a scalar representation of the area. Now having said all these, you can now figure out that how this surface integral can be worked out for a control volume like this. So, this is a one-dimensional problem with variation of T along x direction only. So, T would change only along x. Now, that means T would have a gradient along x and what do you have over here?

It is the gradient of T that is what is represented here because grad of T in general would be represented like this.

$$\nabla T = \hat{i}\frac{\partial T}{\partial x} + \hat{j}\frac{\partial T}{\partial y} + \hat{k}\frac{\partial T}{\partial z}$$

However, you do not have any y or z dependence of T. So, the only term that contributes is this term $\hat{i}\frac{\partial T}{\partial x}$, and what we have done here is that we tried to figure out that which are the faces along which there would be a contribution to the surface flux.

So, what we understand is that there is a heat transfer going on in this direction and then the flux can take place only through this face and the face here. There are no fluxes moving through the other surfaces of the control volume, this is something that we have to understand.

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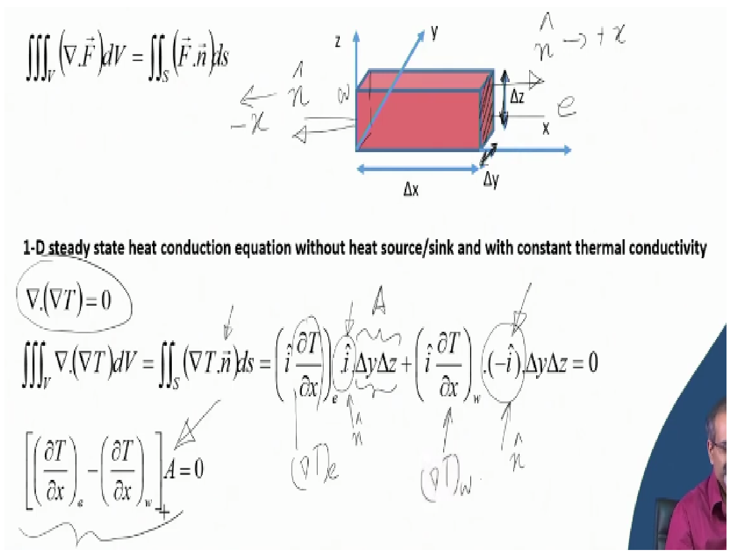

So if that is the case, you will have only the east and the west face of the control volume taking part in the flux transfer. So, this is your east face, this is your west face. So, this is west, this is east and the unit normal vector always points out of the surface. So, in one case it is pointing along the positive x direction, in the other case it is pointing towards the negative x direction. When it points towards the positive x direction, this $\hat{n}$ would be positive $\hat{i}$.

While in this case in the west face it will come out as a negative $\hat{i}$. So, you have grad T contributed from the east face here, you have grad T contributed from the west face here, this is the $\hat{n}$ for the east face, this is the $\hat{n}$ for the west face and the remaining terms are nothing but ds, that means this area in a scalar sense as I said earlier. So, you have delta y along this direction, delta z along this direction and therefore the product of that will give you the area.

So, now what do you have? You have basically an expression looking like this and that is the finite volume representation of this governing equation for an elemental control volume. Now, we need to think how we can attempt to numerically solve this discretized form of the governing equation.

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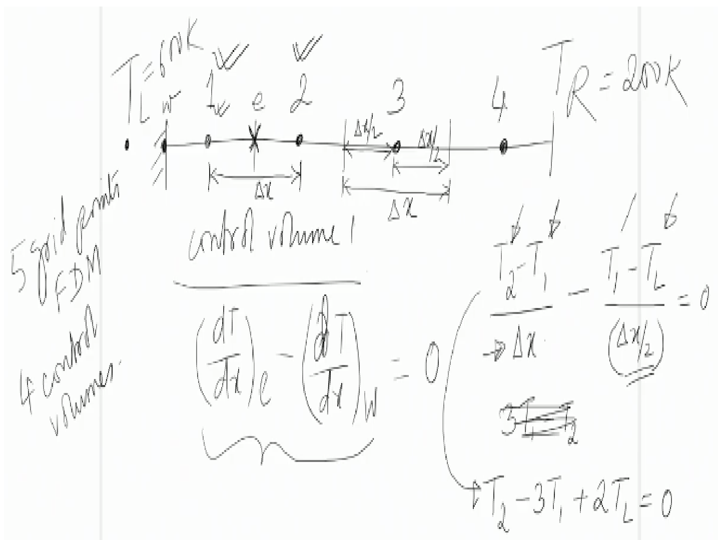

We will first try to draw a small grid where the control volumes are represented. So, like we did for the previous problem, we have a left end, we have a right end where the T_L and T_R are defined. We continue to use the same values so that we can easily figure out what the exact solution will be because we have the analytical solution available with us. This time, we will define the control volumes like this with the nodes indicated as 1, 2, 3, 4.

So remember that in the previous instance when we were doing the finite difference solution, we had 5 grid points. So instead of 5 grid points for the finite difference method, we now have 4 control volumes and what we need to do is we need to write the discretized form of the governing equation which we saw in the previous slide individually for these 4 control volumes.

Let us first look at how we write down the discretized equation for control volumes 1 and 4, which are lying with the boundaries sharing one of the faces with them. So, we will write down for control volume 1 to begin with. Let us see how we write it. For control volume 1, this is the east face, this is the west face and this is basically your definition because A is the common factor.

$$\left[\left(\frac{\partial T}{\partial x}\right)_e - \left(\frac{\partial T}{\partial x}\right)_w\right]A = 0$$

So, you are only left with this expression.

$$\left(\frac{\partial T}{\partial x}\right)_e - \left(\frac{\partial T}{\partial x}\right)_w = 0$$

How do we write it for control volume 1, let us try to do it. We have first derivatives to be approximated. So in order to approximate the first derivative here at this point e, we make use of the values at the neighboring nodes. Then what we have is $(T_2 – T_1)/\Delta x$. Now, we are assuming that all these control volumes are of the same size. If that is the case let us see what it means.

So, if I say that control volume 3 has a length delta x, then half of it would be delta x by 2 and this is comprised of two equal halves because the node is at the center. So, if I look at two adjacent nodes, then the distance between two adjacent nodes will come from two such delta x by 2 contributions and therefore the inter-nodal distances will also be equal to delta x. So, that is the basis on which we write delta x here, minus, we try to approximate the dt/dx at W which happens to be the boundary.

Now, unlike what we did here with two nodal points at a gap delta x, we do not have a node beyond the boundary, so that we have a delta x distance between 1 and a possible point beyond the boundary. So, the best bet would be to make use of the boundary condition with a slightly differing implementation of the derivative in this manner. So, what do we have? The derivative at the W face of the cell would then be approximated as $T_1 – T_L$, which comes from the boundary by half the length as compared to the previous case, so it is delta x by 2.

$$\frac{T_2 - T_1}{\Delta x} - \frac{T_1 - T_L}{\left(\Delta x / 2\right)} = 0$$

Now, having said that you can rewrite this by rearranging the terms and you will get an equation which looks like this $T_2 – 3T_1 + 2T_L = 0$. You can imagine something very similar to this would happen when you go to the control volume 4, let us do that.

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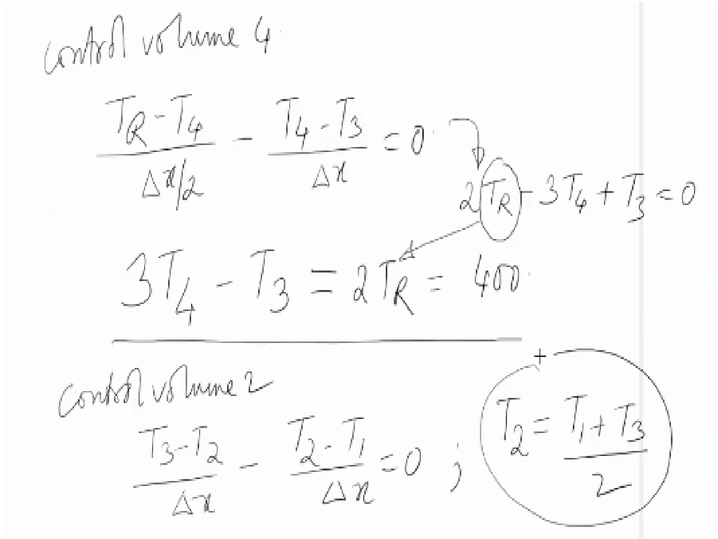

So for the control volume 4, the equation will be

$$\frac{T_R - T_4}{\Delta x/2} - \frac{T_4 - T_3}{\Delta x} = 0$$

and then once you rearrange you can write it like this 2TR – 3T4 + T3 = 0 and then you realize that you know T_R, so you can take it to the other side and you have a numerical value and therefore you get a condition like this.

$$3T_4 - T_3 = 2T_R = 400$$

So, you have two equations coming from control volume 1 and control volume 4.

Now you need to write the equations for control volume 2 and 3, which are not going to depend on boundary values because they are not sharing the boundary faces. So, if you look at control volume 2 for example, the governing equation will look like

$$\frac{T_3 - T_2}{\Delta x} - \frac{T_2 - T_1}{\Delta x} = 0$$

and on simplification this boils down to

$$T_2 = \frac{T_1 + T_3}{2}$$

and this form is somewhat familiar to you because you saw such equations in the finite difference formulation also. So, we are done with 1, 2, and 4.

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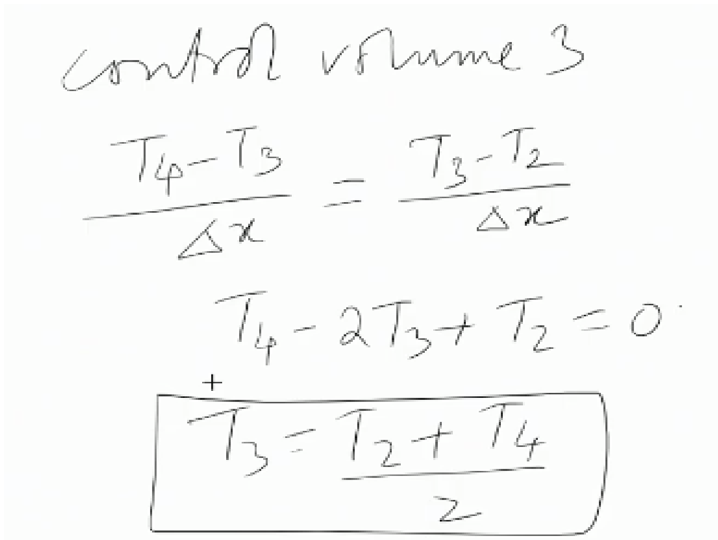

So, we will write one for control volume 3 now. So for control volume 3, the equation looks like.

$$\frac{T_4 - T_3}{\Delta x} = \frac{T_3 - T_2}{\Delta x}$$

$$T_3 = \frac{T_2 + T_4}{2}$$

So this also has a very similar outcome as control volume 2. Now, with a little more time spending, we can solve the problem, let us go ahead and do that. So for solving the problem, let us try to substitute the boundary conditions from the linear equations and try solving them through the elimination technique like we use for the finite difference method.

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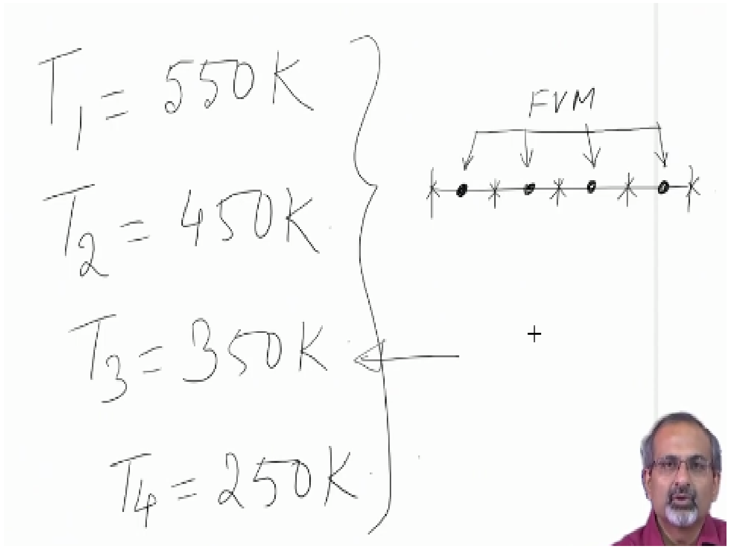

So, if you do that, then these 4 equations need to be solved and then you will be able to come up with the final solution which looks like.

$$T_1 = 550K$$
$$T_2 = 450K$$
$$T_3 = 350K$$
$$T_4 = 250K$$

So these would be the four temperatures that we will be able to solve once those four equations are solved manually and because we have a small number of equations, we can actually attempt a manual calculation. As you can understand that if we had a very large number of control volumes, then manual calculations would become prohibitively time consuming and chances of error would be enormous.

So, that is where we definitely need computer simulations. However, here our control volumes were chosen in such numbers that we could attempt manual calculations. One thing that you need to notice here is that you have now got values at different points compared to what you got for the finite difference method because if you remember for finite difference method, your grid points were at these cross locations.

While for the finite volume technique, the nodes are at the dots. So, naturally, the solutions would differ. However, if you again go back and look at the exact solution of the governing equation, you will find that what you have got at these dot locations using the finite volume method is exact. Why we are able to get exact solutions even with approximations of the kind we have used here?

We have discussed earlier in the context of finite difference method that the functional variation that we have here does not have content of higher order derivatives, therefore with the kind of approximations we have used, we are getting a solution which exactly matches with the analytical solution. When we have more complex variation of the function, these approximations will show differences.

And then the order of accuracy that you have used whether it is for the finite difference method or for finite volume method would make an impact. So, in general using higher order accuracy is always recommendable.

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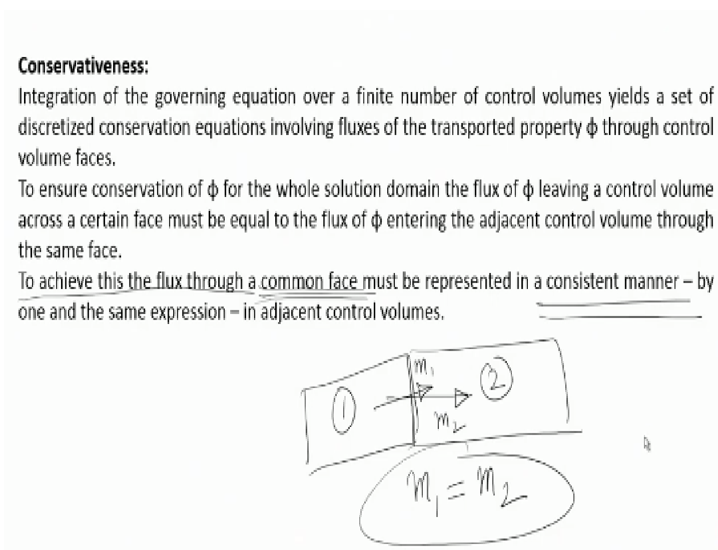

Before we finish this lecture, let us quickly glance at some of the desirable properties which the different approximations that we have attempted till now should be delivering us, so that when we approximate the governing equations, we are able to satisfy some of these very important properties. The first one being conservativeness. So, in the context of finite volume technique, we compute fluxes which are being transferred through common faces.

And only if we represent these fluxes in a consistent manner at each of the common faces, we would ensure that there is an overall flux conservation. What it essentially means is that if you have two adjacent control volumes like this, we always ensure that whatever mass leaves this face from control volume 1 should be exactly equal to the mass which enters the next control volume through the same face.

It may appear to be quite trivial, but in course of calculations when large computer programs are used for solving large number of discrete equations, if we have not accounted for proper balancing of these fluxes, then there will be lack of overall conservation and then the solution may finally diverge which means you will not get a solution at all or it may lead to certain erroneous solutions and it would not be possible for you to reduce the error significantly.

So therefore, what we are talking about is a consistent description of fluxes when we define them at these faces, which are shared by adjacent control volumes. So only when we use consistent flux descriptions, such conservations are ensured. This is an essential property of finite volume techniques and in finite difference techniques, we need to ensure overall conservativeness by applying certain techniques they may not be satisfied by default.

So, there should be certain measures through which we try to ensure reasonable level of conservativeness.

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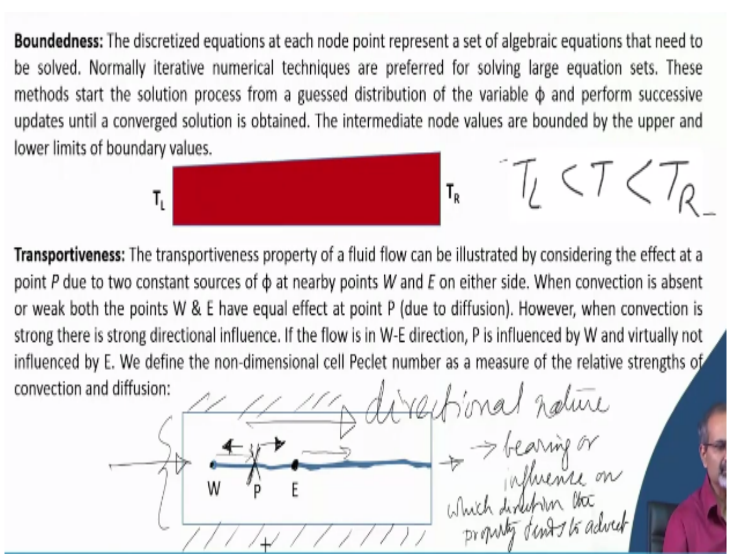

There are 2 other properties which are also of significant. One property happens to be boundedness. We were talking about the one-dimensional steady state heat conduction problem without any source or sinks. In such a situation, we saw that the solution is essentially defined by the boundary values. If you have imposed Dirichlet conditions at the ends of the boundaries, then you have a clear-cut definition of the temperature at the ends of the boundaries.

And you know that there would be a diffusion going on, which means the gradient which lies due to the temperature difference at the two boundaries will drive the heat transfer. So, the hotter end will transfer heat from that end to the colder end and so on. This is expected to give us a smooth variation through the domain and therefore, we need to have this condition that temperature everywhere in this domain will lie between the highest and the lowest values that are defined at the boundaries.

So, this is essentially the boundedness property. Another very important property is transportiveness, which is of course closely connected with fluid flow. When you are talking about a flow advecting a certain property, in that case there is a directional nature of the flow which is impacting the transport of the property.

So, the direction of the fluid flow will have an influence on direction of advection of the property. For example, if you have a flow channel through which you have movement of water from the left towards the right and you have injected some dye at a certain location W, you will see that a streak is formed downstream because the flow carries along with it the dye and takes it towards the right.

If you inject dye from another point E, similar thing will happen and the two dye filaments will tend to merge with each other if the point W and E are almost aligned with the flow direction. Now, if you are at a point P and then you look towards your left you see the dye coming towards you from the point W. However, before the dye reaches you, if you look towards the right, you would not see any dye.

That means, there is a very important directionality to this problem and therefore, you need to understand in which direction the properties are going to be transferred (advected) by the flow.

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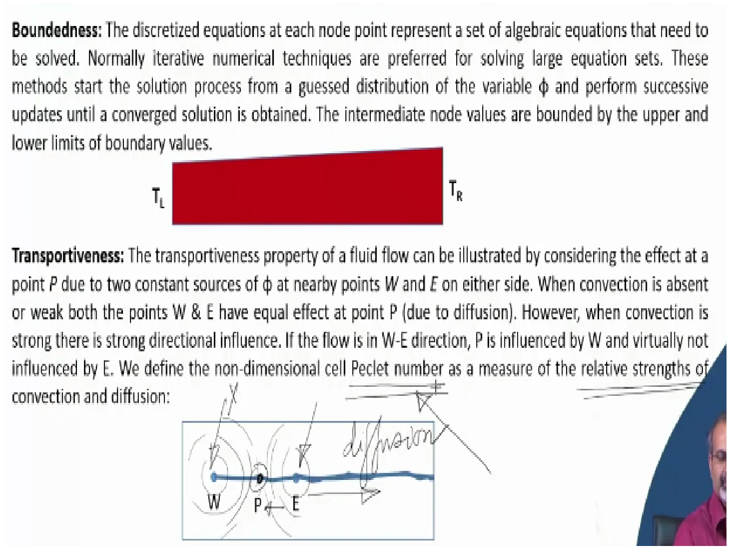

If the flow stops altogether for example, the dyes would not spread this way at all. What you expect is, through molecular diffusion, you may get a situation like this that gradually it spreads this way and then both the dyes at W and E start influencing the point P, after a long duration purely driven by diffusion and then both points W and E seem to be affecting the point P. In the earlier instance, it was not like this.

For example, if there was no injection here, then no dye would reach the point P at all because the dye injected at point P would move downstream only. It would not manage to go upstream at all because the flow drives it in that direction in a very strong manner. In CFD, we often talk about a comparison between the strength of convection and diffusion. So, when we try to compare their strengths in a relative manner, we define something which we call as the Peclet number. We will discuss more on this in later lectures. Thank you.