Computational Fluid Dynamics
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Lecture No. # 13
Finite Volume Method: Some Conceptual Basics and Illustrations through 1-D Steady State Diffusion Problems

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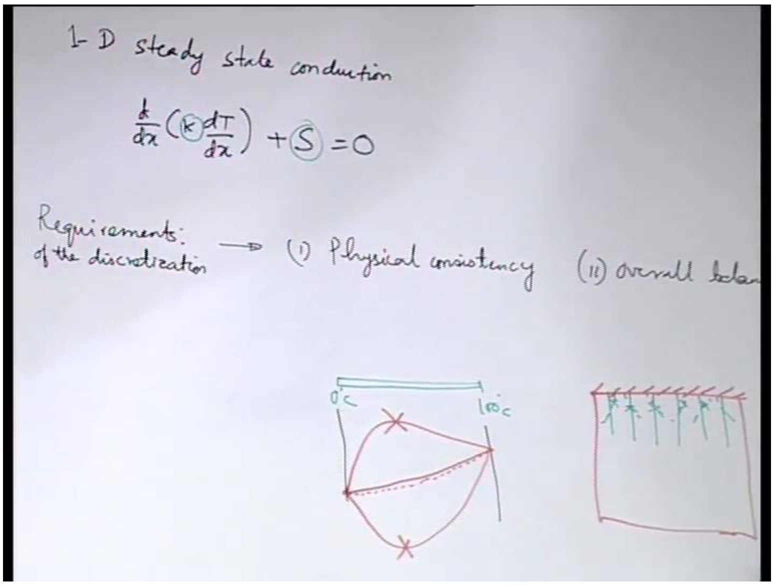

In our previous lecture, we were discussing about the finite volume discretization, and we illustrated it through the example of one-dimensional steady state heat conduction equation with some heat source.

Now, in the preliminary derivation that we had made, we made certain assumptions. One is, that the thermal conductivity is a constant, and there is S is a constant. Now, there can be interesting nonlinearities in the problem, if the thermal conductivity and S both are functions of temperature. And then this equation will become a non-linear equation, and its solution may be based on an iterative strategy. So, for example, what one can do one can start with an initial guess temperature calculate all the coefficients, we will see how the coefficients may be changed or altered if, for example, S is temperature depended. So, there will be some coefficients - these coefficients may be calculated at the particular temperature which is the guess value of the temperature, based on that new temperatures can be solved, and this iteration may be continued till the new temperature, and old temperature at each of the grid points, that difference becomes very very small.

So, that is standard iterative procedure that one might follow. So, we will look into these issues one by one. So, the first and foremost important thing for us to consider is that, like it is possible that S may be more complicated than what we have considered, it is possible that k is more complicated than what we have considered. So, definitely with this new considerations, we will be getting new discretization, but what are the basic requirements that all these discretizations should satisfy. So, important requirements of the discretization will be as follows.

Physical consistency and overall balance. So, physical consistency means that the solution, that is obtain out of the discretized equations should be physically consistent. Let us consider an example. Let us say that you have a rod with the two ends at temperatures of 0 degree centigrade and 100 degree centigrade. Now, let us say that all the properties are constant then there is no heat source or heat seen. So, we know that the temperature will linearly vary between 0 to100 degree centigrade. So, that is say the exact solution. Now, if you get some solution which is like this, that may be inaccurate, but that may be considered as an approximate solution, but if you considered a solution, if you get a solution like this or maybe get a solution like this, these are not physically consistent, because in this cases, you are getting temperature somewhere in the domain, beyond the bonds of 0 to 100 degree centigrade and that is physically inconsistent.

So, whatever approximate solution you get from the numerical simulation. Of course, it will be approximate, but it will be still alright physically, if its approximate nature does not violate physical consistency. There are several other things like for example, you have a two-Dimensional domain, and let us say that this boundary is insulated. So, if you draw constant temperature line sorry isothermal lines, say like this. Say these are some isothermal lines, I am not completing the isothermal lines, because we have not specified the boundary conditions at the other ends, but say these are the isothermal lines closed to the boundary.

This is something which is physically consistent, because the normal gradient of temperature closed to the boundary should be equal to 0, if it is insulated. That means, the isotherms must be perpendicular to the boundary - at the boundary, but if you have this as inclined somewhat like this or like this, then that is physically inconsistent. So, these will not be the case. So, based on the physical description of the problem, you have to figure out that weather your solution is physically acceptable first. Then the question of the accuracy will come.

And overall balance is something that we have already discussed, that each of this equation represents conservation of something. So, overall balance means, it is possible to use this equations to represent the balance of the particular variable over the entire domain, which is a summation of many control volumes. So, if you can ensure the conservation law imposed on each control volume, then you can ensure that the conservation law is imposed over the entire domain.

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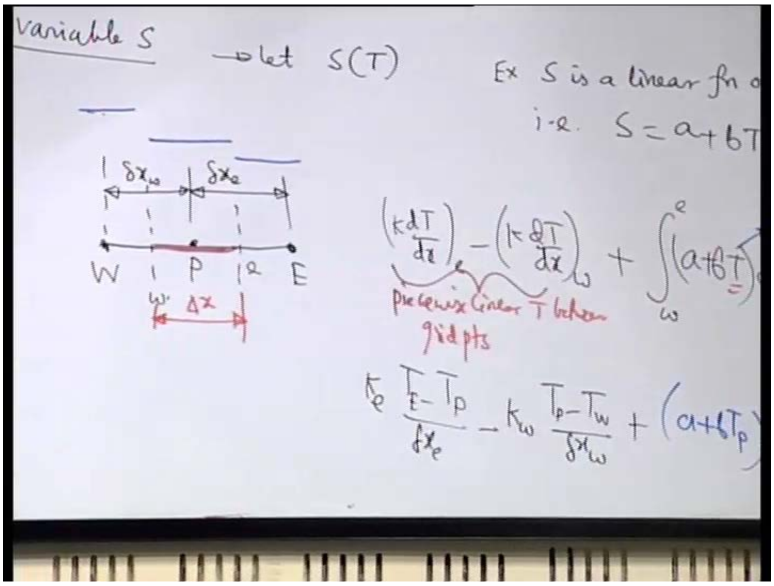

So with this requirements, we will now go into the illustration of variable S. Let us say that S is some function of temperature. So, S can be any arbitrary function of temperature, but since we are trying trying to restrain ourselves within a system of linear algebraic equations, we will consider an example where this is a linear function of temperature.

So, if you have domain like this with discretized grid points as shown, sub domain rather So, we integrate the governing equation over this control volume, and what we get k dT dx at E minus k dT dx. Now, what profile Assumption we have considered for these terms, piecewise, linear profile between the grid points.

So, that will give you… Now, the question of profile assumption for T in this equation, in this expression. See, we have already discussed that the finite volume method has one flexibility. What is that flexibility? You can use different profile assumptions in different terms, because eventually the profile assumption is required only for evaluating the necessary integrals. Once the integrals are evaluated, the history of the profile assumption is no more important, until and unless there is something which is physically inconsistent. So, keeping that in mind what is the simplest profile Assumption for T that you can choose for this term, constant right.

So, piecewise constant temperature within each control volume. So, let us illustrate it with a sketch, something like this. So, so if we do that, then you can approximate this T within the control volume as T at p. So, it is as good as a plus b T P , where T P is a constant. So, a plus b T P is a constant it comes out of the integral. So, that times delta x that is equal to 0. So, if you assemble this equation.

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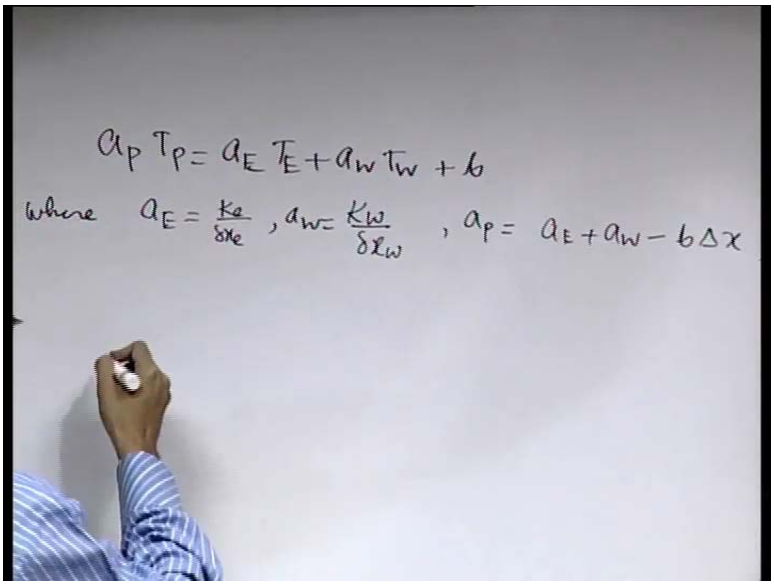

You can write it again in the same form, where…So the form remains the same, only the source term was treated by considering it to be within the integral. If you considered a piecewise linear temperature variation, that is the same profile as we considered for the conduction terms, then also it is possible, but then you have to write this T as a linear function of x, considering different parts that is if the profile was not this one.

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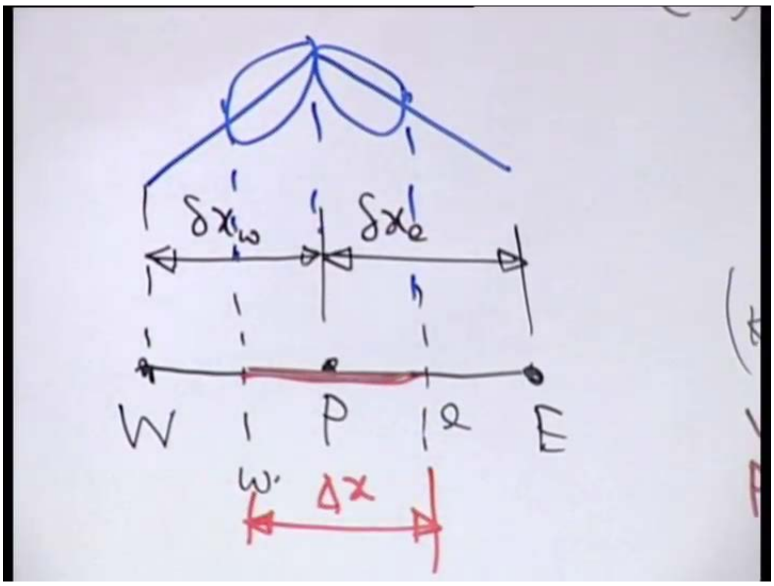

But say, say the profile was something like this one. Then within the control volume, you have to decomposed into two parts, because there are the equations are define piecewise between one small w to capital P, and then capital P to capital E Small e. And then integrate divide this integration into 2 different segments, and evaluate the necessary integral. So, the principal remains the same that you use the profile to evaluate the integral, depending on what profile you choose your integral will of course, be different.

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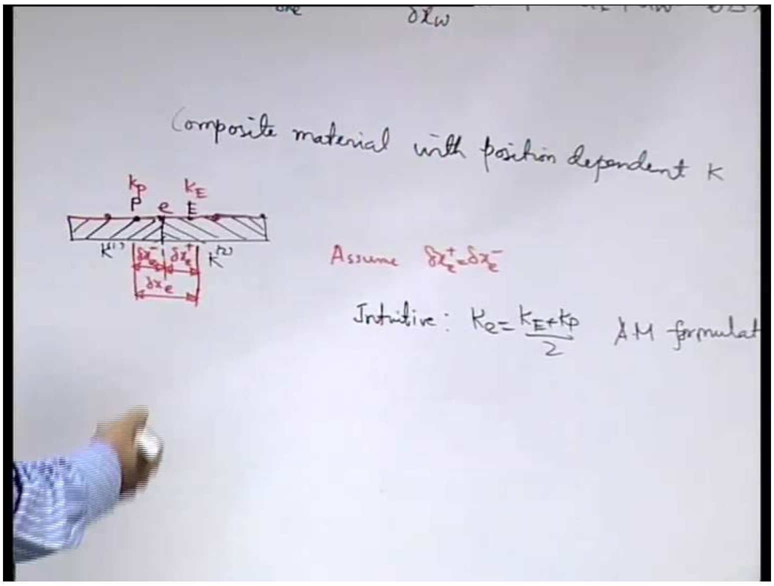

Now, next we will consider the case of the composite material with variable thermal conductivity with position depended k. So, let us say that the domain is sum of two different materials. The first material has a conductivity of a particular value say k 1, and the second part has the conductivity k 2. So, you can divide the domain into a number of sub domains or control volumes. Let us say we divided it into 4 control volumes. And let us consider the names of the grid points as p E, small e like that. So, you can see that where lies the ambiguity. You require to calculate the thermal conductivity at the interface small e, now the interface belongs to what to the left part of the domain or to the right part of the domain. It is it is shared by both. So, there must be some equivalent thermal conductivity that should be prescribed at the interface, because the interface has its own share of the left and also of the right.

If the thermal conductivity was necessary at the main grid points then it is fine, because then it is it has a unique value of the thermal conductivity, but here the interface which is shared by two different materials, its thermal conductivity needs to be described properly. So, how do we do that. Now, for simplicity let us first give some names of the dimensions, and then we will consider something for simplicity in algebra delta x e plus, and delta x e minus. At the two lengths, the total length is of course, delta x e. Assume that these two are the same. So that, the control volume face is located at midway between two adjacent grid points. This is just for algebraic simplicity nothing more than that.

So, what could be an intuitive way of defining the thermal conductivity at small e, if you know k at P and k at E. If small e is exactly at the midway average right. So, that is the mostly most intuitive interpolation. So, intuitive it is a linear interpolation actual, for equal length this linear interpolation becomes an average. So, this is an arithmetic average or arithmetic mean formulation. Now physically, we have to access whether this formulation is acceptable or not. Because this we have just done from a mathematical interpolation perspective, without looking into the physical issues.

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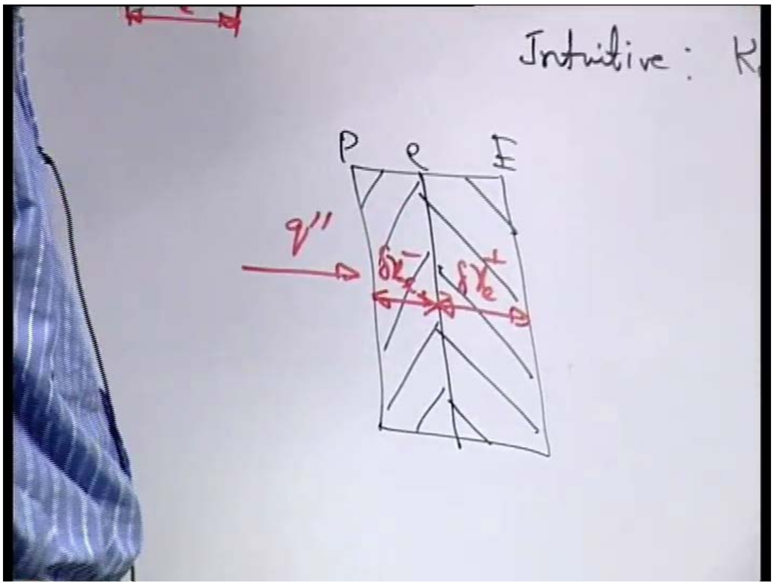

What could be the physical issues? Physically you can create a domain like this as a composite slab. So, in the composite slab you have 2 different slab lengths with 2 different materials. Let us say that q double prime is the heat flux, that is passing through the slab. At steady state whatever heat flux enters the left face, the same heat flux enters the middle face, and leaves it and the same heat flux leave the domain.

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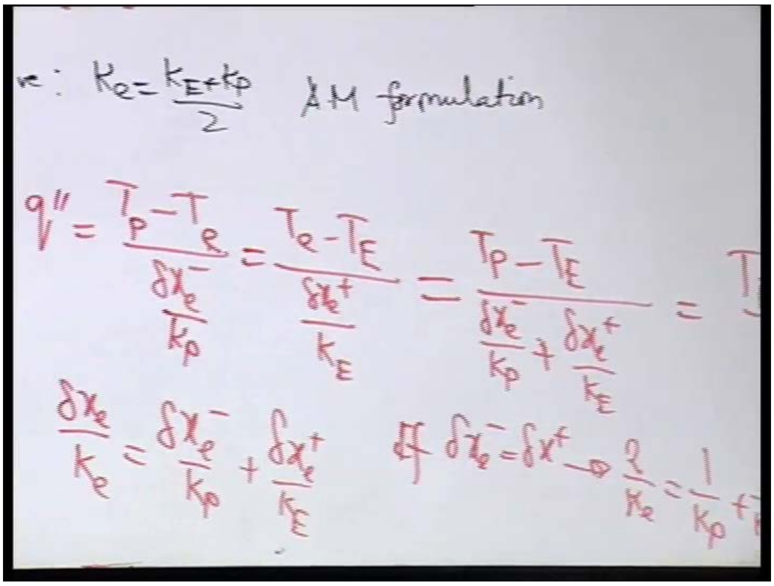

So, we can write this is for the left material that has to be multiplied with k of the material, that is we can just write it in a different way. We can write the denominator as delta x by k itself, that is same as the heat flux that flows through the right material sorry, T's small e minus T capital E

(( )) capital E minus (( )).

This will be T P minus T. Heat is being transformed from higher temperature to lower temperature. So, if you add this together both the numerator and denominator. So, this you can write as T P minus T E by delta x e by k e, where k e is the equivalent thermal conductivity. That means, if you replace these two slabs by a single slab, maintain the same heat flux and maintain the same temperature difference, then what would be the corresponding thermal resistance. So, where k e is the equivalent thermal conductivity. So, from this and if this two are equal that is delta x e minus equal to delta x e plus then you have 2 by k e is equal to 1 by k P. So, k E is 2 divided by which is the harmonic mean of k P and k E. This we call as harmonic mean formulation.

Now, which formulation is physically more appealing. Of course, the harmonic mean formulation we derived from the basic physical sense of the heat transport. So, it has some physical meaning associated associated with that. Let us see that, what is that physical meaning. So, let us consider some limiting cases.

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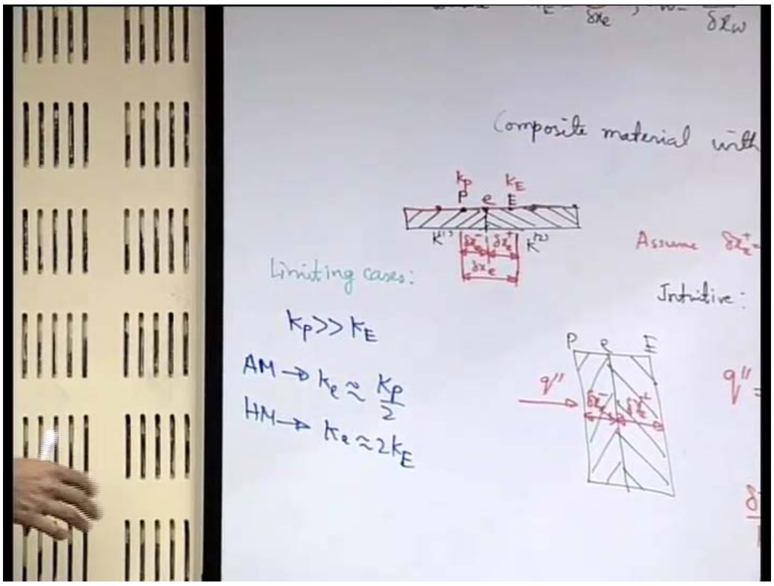

One of the limiting cases is let us say that, k P is much much greater than k E. That is the left material has much higher thermal conductivity than the right material. So, the arithmetic mean formulation will give k e is approximately k P by 2, because k capital E is much much small as compared to k capital P. Let us see what the harmonic mean formulation gives… In the denominator you have 1 by k P, and 1 by k e. k e is much much less than k P. So, 1 by k e is much much more than 1 by k P. So, k e will be 2 k E.

Now look at the situation. When k P is much much greater than k E, then that means, left part of the slab is highly conducting, and the conductivity at the interface will depend on what is the resistance provided mainly by the right part of the slab. But in the arithmetic mean formulation that is not reflected. Here, so even if it happens so that k e is

0. Let us say that it is highly insulating material still k of small e will show a value depended on k P, but not k at capital E. Whereas if k e is very small and tending to 0. Then there is no heat flux at the interface that this formulation will rightly show. So, from here we can conclude that the harmonic mean formulation is physically much more appealing than the arithmetic mean formulation for the interfacial conductivity variation.

Next, what we will discuss is something which are called as four basic rules or which are like golden rules for finite volume discretization of one-Dimensional steady state diffusion type of problem. What are these number one, physical consistency of fluxes at control volume faces. So, what is this? This we have already discussed, that if you have a control volume face. Let us say that you have, you are calculating the flux here based on a temperature profile.

Then the flux calculated from one side should be same as the flux calculated from the other side. So that, there is no discontinuity of flux across the control volume face. So, this means that profile should be chosen in such a way that there is no discontinuity of flux at control volume faces. Then the next rule which is perhaps the most important rule, all coefficients in the discretized equation must be of the same sign. So, look at this example which we have already written in terms of the discretization equation coefficients. So, this discretization equation coefficients when we have written. So, it has how how many coefficient it has a P, a E and a W this 3 coefficients.

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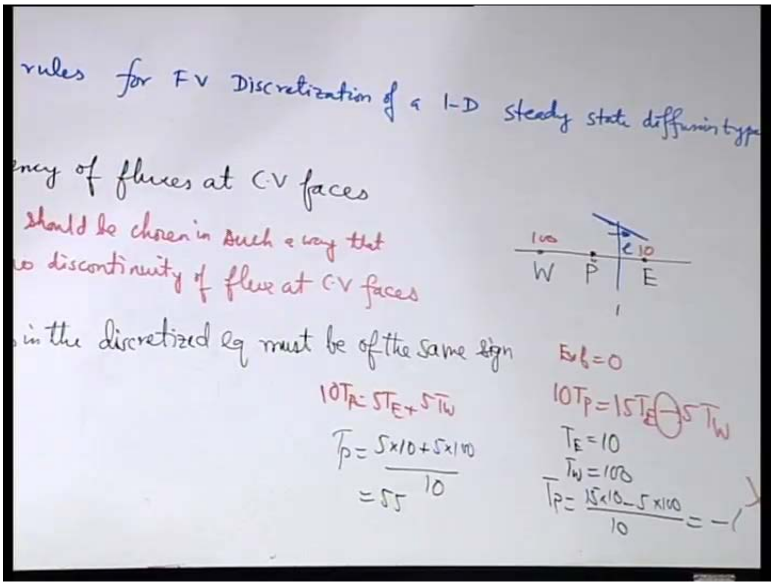

So, let us consider an example, where you have b equal to 0. And then you can see that in this example, you will have a P is equal to a E plus a W. So, let us considered some examples, say you have 10 T P is equal to 15 T E minus 5 T W. Let us say b is equal to 0, there is no source term. Let us say by some algebra, somebody has come up with this discretization equation where things are in appropriate units. So, now let us see what is the consequence. Let us say that T E equal to 10 units of temperature, and T w is 100. Then what is T P? 15 into 10 minus 5 into 100 by 10. what is this?

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Minus something. So, you have look it to physically, you have the temperature at W as 100, temperature at E at 10; there is no heat source in between that is why b is 0, and you are getting the temperature at P as something which is not bounded within this. So, it is physically inconsistent. Where from the inconsistency came, it came from the this negative sign in the discretized - negative sign of coefficient in the discretized equation. So, this could have been avoided, if all the coefficients are of the same sign. Then increase in the temperature of the neighbors will increase the temperature of the grid point in between, and decrease in the neighbors will result in decrease of the temperature of the grid point in between.

So, we can say that this problem could have been avoided, if we are ensured that all the coefficients are of the same sign. So, let us consider that as an example. So, if you consider 10 T P P is equal to 5 T E plus 5 T W. Then T P is equal to 5 into 10 plus 5 into 100 by 10. What is this? 55. So, this is acceptable between 10 to100. So, we must make sure that after discretization, all coefficients in the discretization equation should be of the same sign - the same sign could be positive or negative, but the sign convention that we will chose from now on words is that the same sign is a positive sign. So, by sign convention we will consider that sign to be positive.

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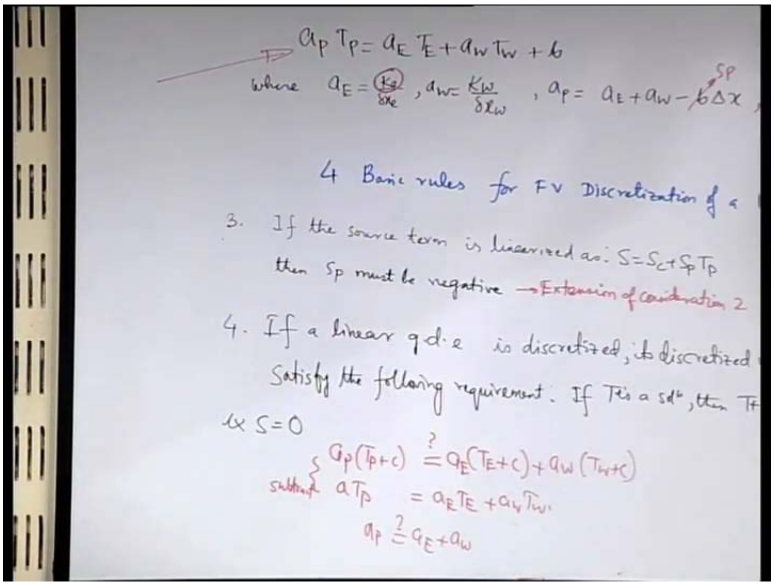

If the source term is linearzed as S is equal to S C plus S P into T P. So, remember we had S is equal a plus b T, as a linear form of the source term, and since we have use the constant temperature profile within each grid point, within each control volume for representing the source term that is why T is equal to T P . So, the form of the source term considering, the consideration that we had discussed just now is S equal to S C plus S P T P. If that is the case, then S P must be negative. So, in this nomenclature of S C and S P, this is S P and this is S C. So, you can clearly see, that why we would need to make S P negative. So that, we would make sure that irrespective of the values of a E and a W, and delta x, a P is always positive.

Because if we allow S P to be positive. In some cases a P will be positive, then we get rid of the problem, but in some cases a P may be negative. It all depends on a E, a W delta x. So, we do not want to take a chance, and we make S P itself negative. So, that a P will be positive, and there is no question of having different coefficients of different signs. So, the consideration number three is a extension of the consideration number two.

Then the 4th consideration. If a linear governing differential equation is discretized is discretized version should satisfy the following requirement. If T is a solution then T plus C is also solution is a property of a linear differential equation, that if the differential equation has temperature for example, as the dependent variable. If T is itself is a solution. Then T P plus C will also be a solution. So, let us see that whether, it is satisfied with a consideration that the source term is 0. So, example S equal to 0.

So let us see, let us add T with T P lus C, and see whether the equation gets satisfied. So, we are interested to see whether this is equal to source term is 0. So, there is no b. So, this equality, we are checking when we have already found out that a P, T P is equal to a E T E plus a W T W. So, if you subtract this, we need to check whether a P is equal to a E plus a W. If you subtract this two, C will get cancel. So, from here we can see, that this requirement is indeed satisfy a P is equal to a E plus a W, when there is no source term. So, this discretization is discrete form satisfies the linearity. That if the temperature is T and it is a solution that plus constant is also a solution, we have earlier seen that this constant is evaluated by imposing a Dirichlet boundary condition at one of the boundaries. So, this basic rules are very very important, and when we discretized even for more complex problems many times this discretization rules will help.

Now, next what we will discuss is that we have till now consider a source term, which is linear in form, but if the source term is non-linear then how we can treat it. So obviously, since we are preparing a linear algebraic framework of the system of equation that we are intending to solve, we will keep the source term in a linear form, although the actual source term may be non-linear. So, there is a method of conversation of a non-linear source term in to a linear form, and that is called as source term linearization.

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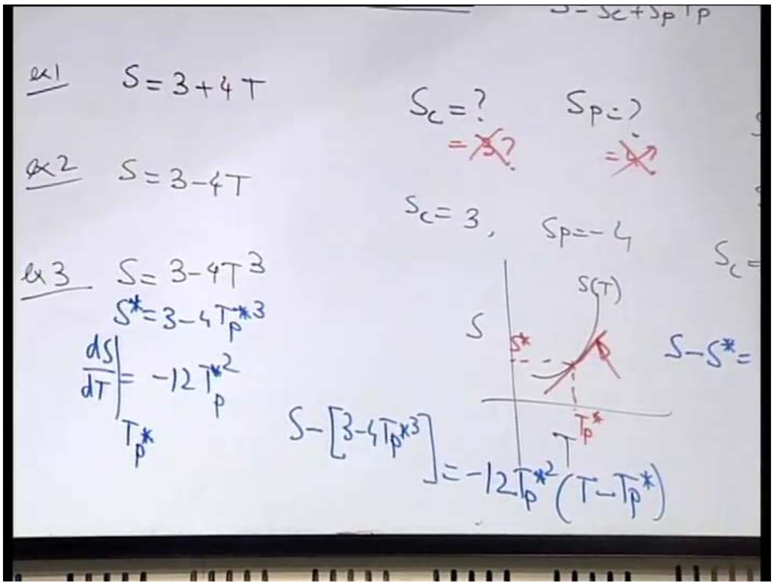

So, we will next see source term linearization. So, the best way to learn it is to through some examples. Let us say, you have a source term is equal to sum 3 plus 4 T. If you want to linearise, it our objective will be to say what is S C or what is S P? Considering S is equal S C plus S P T P. So, from the form it might appear that we could take S C equal to 3, and S P equal to 4. Can we do that. Just now we have seen that S P has to be positive S P has to be negative, but here S P is positive.

So, this will not work. So, what we can do? In an iterative framework, we can start with a guess for temperature as T star, and we can dump S c, damp dump the full value of the source term with S C. So, remember this is the guess value. So, this is this is a known value, this is no more a variable. So, we are dumping everything in S C and making S P equal to 0. Sometimes if you want to control convergence, what you can do is, you can put some effect on S P and some effect on S C.

For example, you can have S C as 3 plus 6 T P star and S P as minus 2. So, there could be many such choices possible. So, with this one you can sometimes slowdown the convergence a bit by considering this. So, if if if the iteration has a tendency to diverge first, then controlling the convergence may be necessary, and then such considerations may be taken. So, this comes out of experience that what kind of S C and S P that you can use. But obviously, there are certain kinds which you cannot use.

Let us consider a second example; say 3 minus 4 T. So, here you can easily take S C is equal to 3 and S P is equal to minus 4, and this is the best choice no doubt about it. If you slowdown want to slowdown the convergence, you could take for example, S C is equal to 3 plus 4 T P star S P is equal to minus 8 like that. So, you can see that there is no unique choice, but there are certain choices which are not acceptable for certain cases that we have to remember. But till now we have considered the forms where S is given as a linear function of a temperature, but what happens if it is a non-linear function of temperature. Let us say, say 3 minus 4 T cube.

So, forget about 3 minus 4 T cube. Let us say that you have some arbitrary S as a function of T. This is any arbitrary S as a function of T. We have a particular point, see this is a non-linear source term, so we have to go through iterations as we have discussed earlier. Let us say that during some iteration you have the value of T P as T P star. So, you want to represent this non-linear function as a linear function. What can be the best linear function? So…

Yes. So, it can be a tangent to the curve at that particular point. Why? Because a non-linear function has many higher order derivatives. If you want to replace it by a straight line you sacrifice the higher order derivatives, but at least the first order derivative you can represent correctly, and if you represent it by a tangent, the tangent has the same first order derivative as for the corresponding slope of the actual non-linear curve. So, that is why you can replace it by a tangent. Now, if you replace it by a tangent… So, what is the equation of this tangent? Let us write this one, let us say that the corresponding value is S star. So, we can write S minus S star; y minus y 1 is equal to M into x minus x 1 where x is like T and y is like S.

Let us illustrate this principle through the example S equal to 3 minus 4 T cube. So, S star is 3 minus 4 T P star cube. What is dS dT? minus 12 T square. So, dS dT at T P star is equal to minus 12 T P star square. So, S minus S star is S minus 3 minus 4 T P star cube is equal to minus 12 T P star square.

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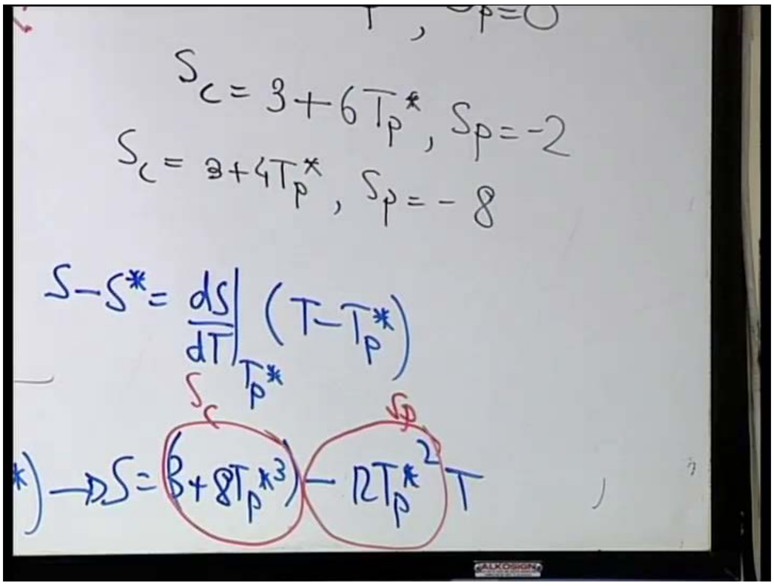

So, let us expand it and write S equal to… Now, what is the constant term on that side you will have 3 then minus 4 T P star cube plus 12 T P star cube. So, 3 plus 9 T P star cube sorry 8 right, there was 4 and 12. So, 8 minus 12 T P star square into T. So, what is S c? S C is 3 plus 8 T P star cube and S P is minus 12 T P square. So, you can see that S P is negative always, because T star square is positive, so this is negative, so this will work.

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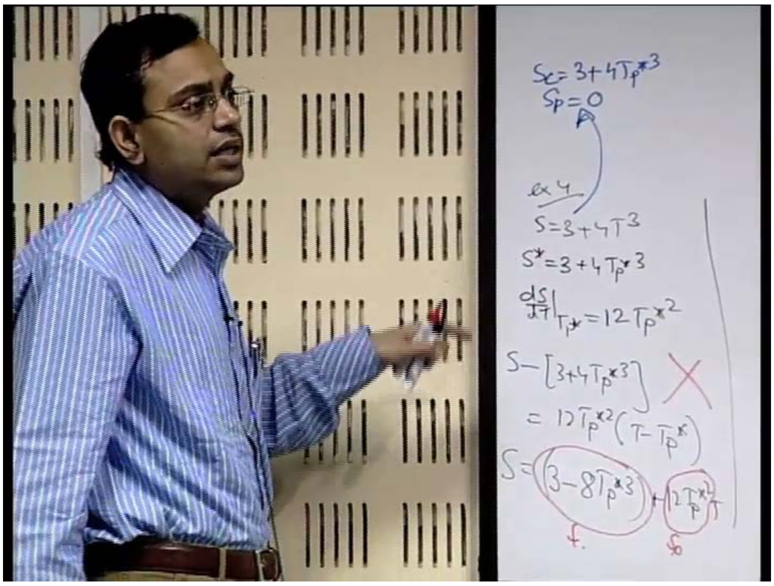

But let us consider a 4th example; say S is equal to 3 plus 4 T cube, then if you want to do the same linearization S star is 3 plus 4 T P star cube dS dT T P star just we replace the minus sign of the previous example with the plus sign. So, you have S minus 3 plus 4 T P star cube is equal to 12 T P star square into T minus T P star. So, what we get out of it? S is equal to 3, then here you have minus 12 T P star cube and on the other side will come plus 4 T P star cube. So, minus 8 T P star cube plus 12 T P star square T. So, this will be S C and this will be S P. See S C may be negative, positive, whatever, we do not have any restriction on the sign of S c. But we concentrate on S P and we see that here S P is positive. So, this will not work.

So, important thing is mathematically source term linearization we can always do, but that linear form of the source term may work or may not work. So, here when the linear form does not work then what we have to do? Then we can do several things, like we can has an alternative think in this way. We can dump the entire to S C and S P equal to 0 or we can dump something on S C with some negative on S P whatever, but we cannot do this linearization. So, this linearization is mathematically correct, but it will give you physical inconsistent solutions. So, this is what we have to remember, all the time we are stressing upon it. That the discretization is a mathematical procedure, no doubt about it. But the mathematics carries an important physics within it, and the discretization must not violate the essential physics that should come out of the discretization method.

So, we stop here today. In the next lecture, what we will do? We will we have now re-visited that we have now visited all the discretization intricacies, but we have not visited how to implement boundary conditions in the finite volume method. So that we will do and then we will consider one or two illustrative examples, and then we will move on to one-dimensional unsteady state problems. Thank you.