Computational Fluid Dynamics

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Lecture No. #11

Fundamentals of Discretization: Finite Difference and Finite Volume Method

In the previous few lectures, we were discussing about the weighted residual method, and several forms of that including its discretized discretized form in terms of the Finite elements method. We will proceed further with that one, but before that let me give you some homework exercises, which you can solve by considering the discussions that we had in our previous couple of lectures.

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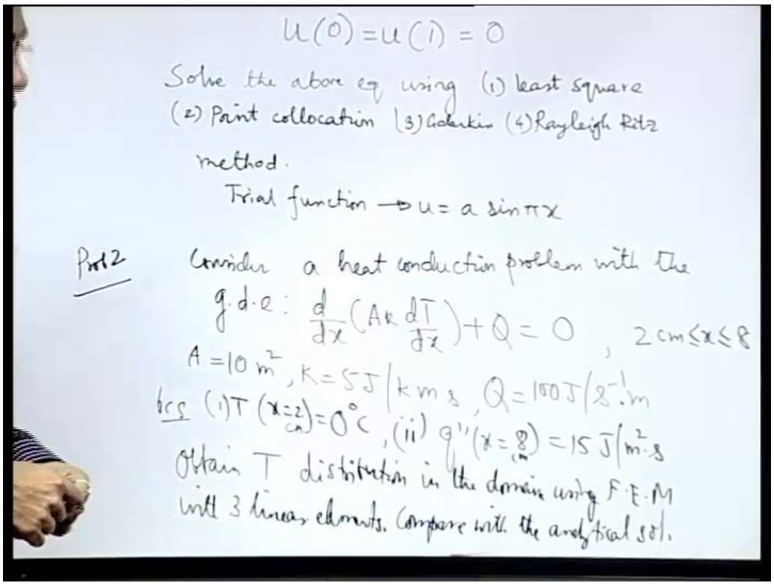

So, the first problem consider the differential equation with the boundary conditions solve the above equation; using say least square, Point collocation, Galarkin, and Rayleigh Ritz method for the methods where you require to choose a Trial function. You can choose a Trial function u equal to a sine pi x, where a is the undetermined parameter. So, we have worked out similar examples in the in the class. So, you can use that concept to solve this problem.

Second problem, consider a heat conduction problem with the following governing differential equation d dx of A k dT dx plus Q equal to 0, where A is equal to 10 meter square, k is equal to 5 joule per Kelvin meter second, Q equal to 100 joule per second meter. This problem is valid within the domain x lies between 2 centimeter to 8 centimeter. The boundary conditions are T at x equal to 2 equal to 0 degree centigrade and the heat flux at x equal to 8 both are centimeter, 2 centimeter and 8 centimeter is equal to 15 joule per meter square second obtain temperature distribution in the domain using finite element method with three linear elements and compare with the analytical solution.

So, these are the two problems that you can try and the second problem you can try by hand because there are three linear elements, but I would prefer that you first get familiar with it by trying it by hand and then write a computer program to regenerate the same solution and check whether your program is working fine.

Now, we will move on to our subsequent discussions and when we say subsequent discussions we have to keep in mind that our agenda broad agenda for all these discussions were to introduce was to introduce the fundamental concepts of discretization. We have introduced one concept of discretization by going through the roots of variational formulation, but that is not all that is not all because variational formulation is one way of arriving at the discretized equations one could have other possibilities.

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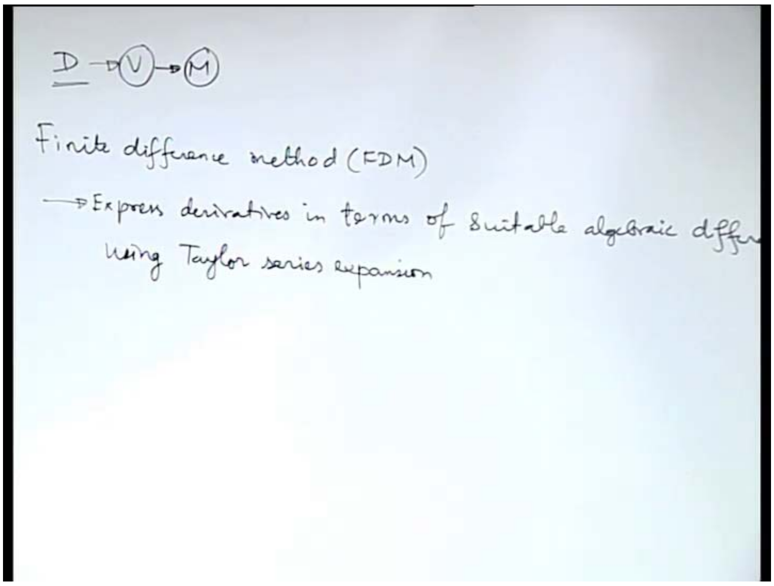

Because one has the differential equation in its D form, variational form is a variant of that and one could have M formed from that one. So, we have till now focused our attention on V form and similar concepts could also be valid for M form because, like we have seen that under certain special circumstances these forms are inter changeable.

So, you could derive for example, finite element finite element equations starting from the M form provided the M form exists and it is it is physically a very meaningful way of deriving some of the finite elements equations because M form sometimes has a very important physical meaning like, if you are solving a structural mechanics problem then M form M form essentially is the statement of minimization of potential energy of a system which governs the stability of a system in equilibrium.

So, if you minimize the potential energy of the system then that will give you the equilibrium configuration. So, the numerical method turns out to be consistent with the physical requirements as well. So, M form also happens to be physically appealing, but it is possible to derive discretized equations without going through these roots, but directly through the D form and one such method which does that is known as the Finite Difference Method.

So, what is the basic philosophy of the finite difference method what we do is in the governing differential equation. We manipulate with the governing differential equation directly rather than through its V form or M form. So, we use the D form, in the D form there are expressions for derivatives and we express the derivatives in terms of suitable algebraic differences by using the Taylor series expansion, that is what is the basic philosophy of the finite difference method. So, Express derivatives in terms of suitable algebraic differences by using Taylor series expansion .

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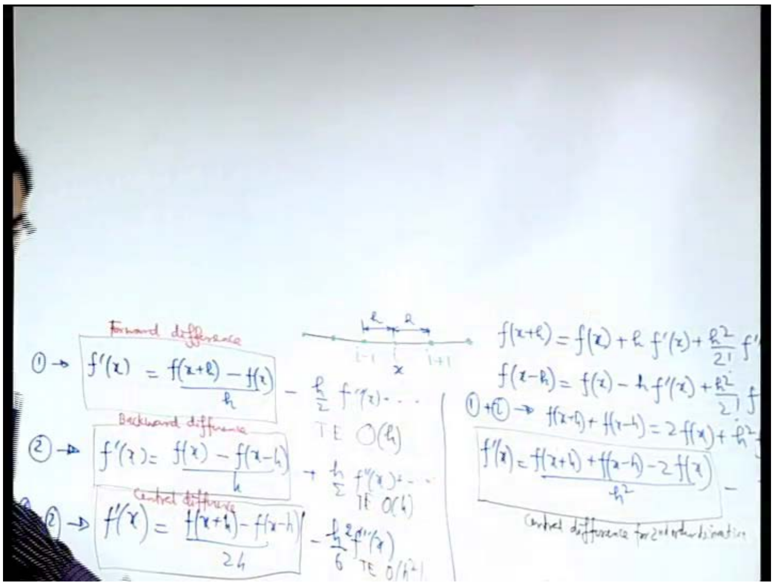

Let us, see a simple illustration of how we do it, if you have a domain like this say one Dimensional domain, we divide the domain into or we identify a few numbers of grid points. So, we actually do not divide the domain into a number of sub domains in the meaning of an element what we do for Finite elements, but what we do is essentially, we do a very similar thing because essentially we represent domain by a collection of discrete grid points. So, these grid points are similar to the nodes of a finite element method, but there are conceptual differences because you here, you do not have logical elements which are connected by the nodes.

Here, you have just discrete grid points now, how they are logically connected or how they are laid out is a matter of choice of the geometry rather than or it is a matter of choice of the coordinate system. So, to say rather than having some particular shapes corresponding to each element. So, there is a no concept of element as such, but you have just discrete grid points. So, let us say that you have some grid points say i, you could have i plus 1, i minus 1. In a two dimensional frame work, you could have the other direction. So, here then you would have got (i j), i plus (1 j) like that and so on.

Now, we are just considering a one dimensional example to begin with of course, we will go into more details in our subsequent lectures, but the objective of this part of the lecture is to introduce the method; rather than going into more details of the method. So, what we will do we will try to write a function let us say, i represents the point x and, this distance is h and, this distance is h.

So, we are interested in expressing f x plus h while f is any function let us the temperature for a heat transfer problem in terms of f at x. That is, we are interested to express the value of the variable at i plus 1 grid point in terms of the variable at i grid point. So, f x plus h is equal to f x plus h f dash x plus h square by factorial 2 f double dash x and so on. This is the Taylor series expansion. Let us say this is equation number 1. Similarly, you could also write f x minus h is equal to f x replace h with minus h. So, this is by keeping the point i minus 1 in mind.

Now, let us say that we are interested about an algebraic expression for f dash x. So, there could be different ways in which you could derive that. For example, you could write f dash x from equation one as f x plus h minus f x divided by h minus h by 2 f double dash x and so on and so forth. So, if you truncate the Tailor series up to this and try to use this is the formula. So, you can see that you are replacing the continuous derivative as a discrete difference quantity and since it is not exactly the same.

It has it is inaccurate and the inaccuracy is attributed to several things later on we will study that what are the sources of errors in this discretization methods, but at least we can intuitively guess one particular type of error that is we have truncated the Taylor series up to a finite number of terms and that is the one of the sources of the error. So, that is called as a truncation error and the truncation error is here of the order of h because this is the leading order term. So, we expect that h is small for this implementation to be accurate and if h is small the subsequent terms like h square h cube they are expected to be smaller than h and hence the truncation error is dictated by the leading order term that is of the order of h.

Similarly, from equation two, you could write f dash x is equal to f x minus f x minus h divided by h plus h by 2 f double dash x the terms which are remaining are which are not considered whether it is plus or minus is not important only the order is important because any way we are interested about the truncation error. So, if we truncate this expression up to this then the truncation error is of the order of h. We can also find out f dash x by subtracting two from one. So, that will give you f dash x is equal to f x plus h minus f x minus h by 2 h then.

So, when you subtract h square by factorial 2 term gets cancelled out. So, h cube by factorial 3 into f triple prime x that remains. So, that into 2. So, h cube by 3. So, h cube by 3 f triple dash x by. So, it is h square by. So, it was 3 factorial and that multiplied by 2. So, that it becomes 3 and divided by 2 yes. Now, whether it is plus or minus sign let us just check. So, it will be f dash x, if you keep on one side then it will be minus, but at the end it is not important again whether it is plus or minus only the order is important. So, the truncation error is of the order of h square.

So, the these are known as different ordered difference formulas. So, this is Forward difference, this is Backward difference and the third one is central difference corresponding to the first order derivative. So, these names are quite clear I mean why such names do appear because Forward difference as if you are going Forward from x to x plus h, backward as if you are going backward from x to x minus h and central means x is central to x plus h and x minus h it is the mid way. So, the names are quite matching with the corresponding implications. Now, this is about the first order derivative you can do similar things with the second order derivative.

So, let us try to do that let us say we are interested about f double dash x. So, to get f double dash x what we can do we can add one and two. So, if you add one and two you get f x plus h plus f x minus h is equal to 2 f x plus h square f double dash x then h cube by factorial 3 term gets cancelled out. So, you have h 4 by factorial 4 into 2 that means, h 4 by 12. So, from here you can write f dash x is equal to f x plus h plus f x minus h minus 2 f x divided by h square minus h square by 12 .

So, this formula where you can truncate it up to this term. This is known as central difference for the second order derivative and truncation error of the order of h square. You can also express the second order derivative in terms of differences in the first order derivative.

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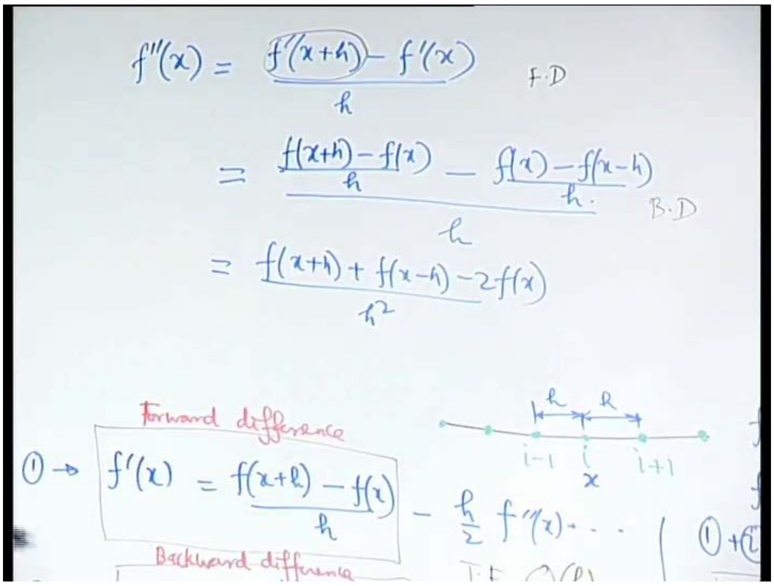

For example, you can write f double dash x as f dash x plus h minus f dash x divided by h. What formula is this one, which difference - forward difference, backward difference or central difference, this is forward difference right. Now, you can write individual f dash terms in terms of f by considering the first order difference formula. So, you can write this as f(x plus h) minus f(x) divided by h for f dash x plus h. So, which formula is this one backward difference. Similarly, for f dash x f(x) minus f(x minus h) divided by h the whole thing divided by h.

So, f x plus h plus f x minus h minus 2 f x by h square. So, the central difference formula may be perceived as two successive steps of one Forward difference and another Backward difference formula for first order derivatives. If the matter it is the manner in which you perceive it is the ultimate interpretation, but eventually whatever may be the formula it may be generated by the Taylor series expansion that is the simple way of looking into it. Next is, how do we make use of this formula to understand that let us, consider an example let us take the same same one dimensional steady state heat conduction problem this is example.

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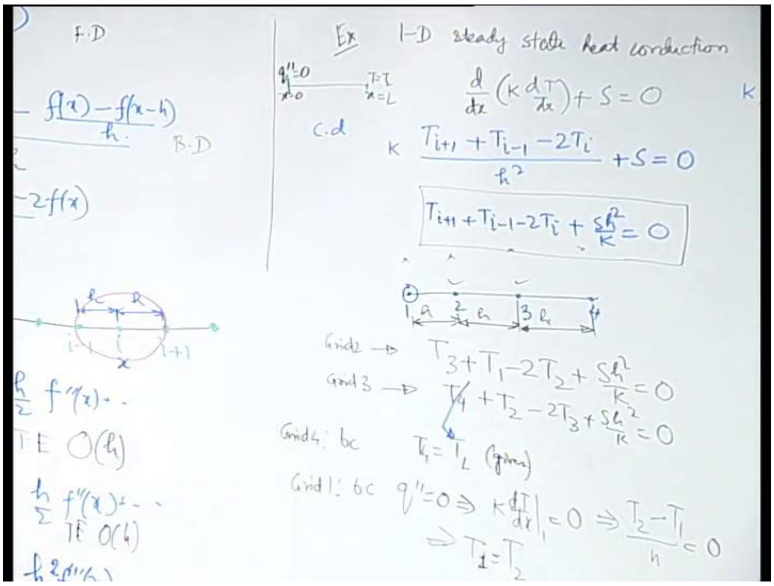

So, we take the same problem which we considered for illustrating the finite elements method that is d dx of k dT dx plus S equal to 0 and we consider k to be constant for the particular example that we choose the boundary conditions. So, we considered a rod from x equal to 0 to x equal to L at x equal to 0 it is insulated and, at x equal to L it is giving temperature. So, now, let us write the corresponding derivative in terms of a difference quantity and see that how the corresponding finite difference looks like.

So, if you write express it in terms of a difference quantity you you of course, are free to choose Forward difference, Backward difference, central difference whatever formula that you are interested in the central difference is a good one because its error is of the order of h square. Now, if you use the central difference formula our assumption is k and s both are constants. So, you have f x plus h that is T i plus 1 plus f x minus h plus T i minus 1 minus 2 f x minus 2 T i divided by h square what is h, h is that distance between the grid points.

Now, if it is the non uniform distance between the grid points then; obviously, h for one particular term and h for another term they will be different. So, you when you are writing f x plus h in terms of f x then there is 1 h when you are writing f x minus h then that h may be h 1 another different h. So, this h may be h 1 accordingly the algebra will change, but basic philosophy will remain the same for illustration we consider the same h. Although, it is not necessary that one has to use same h why is it not necessary that we have to use the same h what will dictate that what whether we should use a large h or a small h.

In a domain, there may be locations where the temperature gradient is very large to capture that you require grid points which are spaced in a very fine manner. So, they are very closely spaced or densely placed. On the other hand, there are may be parts of the domain where the temperature gradient is not that steep. So, you can use a courser grid at those locations. So, obviously, depending on the physics of the problem you can economize it by choosing finer grids and courser grids. It is not necessary that everywhere you use fine grids that will unnecessary increase the computational cost.

So, wherever there is a less steep gradient you use courser grids. So, you it is possible and it is very much practical that in a particular problem you have non uniform grids. So, this example is an illustration with uniform grids, but similar algebra can be arrived with non uniform grids the expression will be different, then plus s equal to 0. So, what we have basically done is since k is a constant we have taken it out of the derivative. So, k d square T dx square in place case of d square T dx square we have written that difference expression.

So, from here you can write T i or T i plus 1 plus T i minus 1 minus 2 T i plus s h square by k is equal to 0. So, you have an algebraic equation involving T i T i plus 1 and T i minus 1. So, if you have let us let us consider three elements and see that how we can assemble it. Again when we say three elements in finite difference there is nothing called an element; it is just for our own perception. So, we consider basically that there are four grid points, but that does not mean that it has three elements because concept of element is not there. So, it is just some isolated points 1 2 3 4.

So, the domain is now of just a collection of 1 2 3 4 four points disregarding how they are connected and all that that information is not a part of the finite difference method. So, you can write this remember that these equations are valid this equation is valid for the internal grid points not the boundary because when you consider the boundary say one you require basically three grid points at a time, one to the right and another to the left there is nothing at the left of the boundary.

So, it is not valid at the boundary it is valid only at points two and three. So, for point two you have T 3 plus T 1 minus 2 T 2 plus s h square by k is equal to 0 this is for the grid point two, for the grid point three you have T 4 plus T 2 minus 2 T 3 plus s h square by k equal to 0 then you have a boundary condition say T 4 is equal to T L that is given. So, that is given, but still you have T 1, T 2, T 3 as three unknowns. So, you require another equation obviously, grid point one will give you another equation. So, for grid point one what is your corresponding governing equation that you have to derive from the boundary condition.

So, this was grid point four for grid point one boundary condition is the heat flux is 0; that means, k d T dx at 1 is equal to 0. So, you can write it in terms of a difference formula T 2 minus T 1 by h equal to 0 as a Forward difference formula, where h is the distance between each of the grid points. So, which implies T 2 or rather T 1 is equal to T 2. Remember, when you write a computer program there is a difference in the statement T 1 equal to T 2, and T 2 equal to T 1. Always when you are writing a statement for a boundary; that means, you are writing the expression for the boundary condition.

So, express the boundary as a function of the interior; that means, there is some value T2 which is assigned to T 1 which is the value at the boundary. So, it is not T 2 equal to T 1 of course, when you do it by hand it does not matter, but when you do it through computer programming it is the boundary assigned in terms of interior once that is how you have to organize the boundary condition. We will come to the more details on the boundary condition subsequently.

But here, the objective is to illustrate that at the end what you have achieved at the end you have these three equations, three linear algebraic equations with three unknowns. So, you can solve for T 1, T 2, T 3. So, and in between how it varies it depends on your interpolation, but it has no sense of an element. So, it does not care how you interpolate it it is up to you and then. So, it will give you just the values of temperature at discrete points and then you can may maybe you can smoothly join them or join them by piecewise straight lines it is up to you.

So, this is the basic implementation philosophy of a Finite Difference Method, of course, we have to remember that is it sufficient to know this implementation strategy it is not because, many times we may use the same implementation strategy, but the method may fail the method may become. So, called unstable, the method may become inconsistent.

So, these are certain important terms and we will see that eventually, if these are the cases then there is the high chance that the method does not converse to the exact solution or even an approximate form of exact solution that you are looking for.

So, mere implementation of the Taylor series expansion is not all. We have to see that at the end whether it satisfies certain requirements which are called as consistency and stability requirements. So, later on when when we will be considering error analysis. We will revisit the finite difference method and see that for study as well as unstudy problems whether any type of discretisation will work or not, but again as I am repeating that the objective of this part of discussion is not to go into the details of the method, but to introduce the method and that is why we are just restricted to such a simple example we will take up more involved examples on finite difference method in subsequent part of our course.

Now, we have seen one example of a method through the D form and one example of the discretization method through the V form. We will make their relative assessments, but before that we will try to make a few remarks on the nature of the problem through which you are intending to get the discretized solution. That is, how well the problem is posed that is one of the important natures of the problem that we need to discuss on not only that how does it relate to the boundary conditions.

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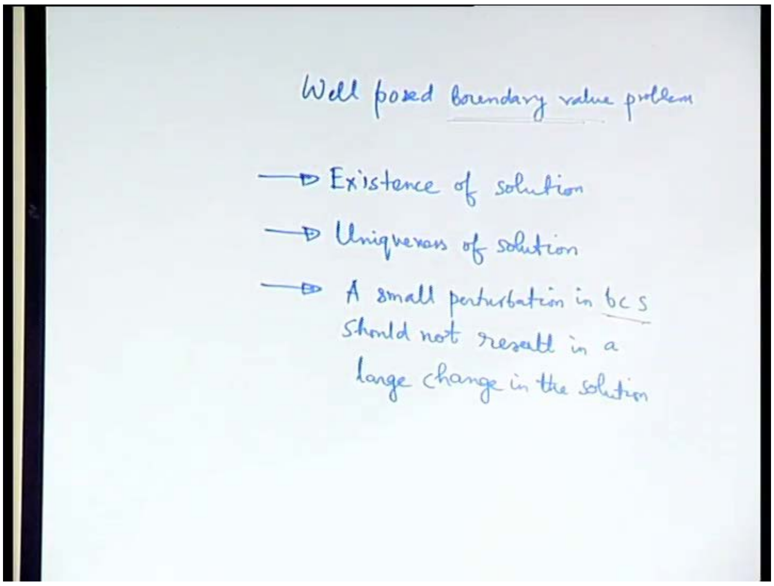

So, we will look into certain terminologies the first terminology that we will consider is what we call as a Well posed boundary value problem. Sometimes, we in a loose sense say that the problem is ill posed or the problem is well posed. So, we have to understand that what we mathematically mean by these terminologies at least in a in a qualitative sense if not by very rigorous mathematical definitions. So, when we say that a problem boundary value problem is well posed. We have already discussed what is the boundary value problem were you require boundary conditions throughout the domain of the problem just like an elliptic problem elliptic partial differential equation.

Now, what are the requirements first of all, the requirement is Existence of the solution. That is, the boundary value problem should be posed in such a way that the solution exists. It should not be posed in a way that the solution does not exist not only that, the solution should be unique and there is a third requirement that a small perturbation in the boundary conditions should not result in a large change in the solution. So, these are very obvious things for obtaining a numerical solution. Remember these we are these terminologies we are introducing in a context of getting a numerical solution.

So, Existence of a solution is important; obviously, otherwise there is no need or there is no good in going through the definition of the problem if the definition does not give you a solution. The solution has to be unique. So, that you get a solution without ambiguities and a small perturbation in the boundary conditions should not result in a large large change in the solution; that means, it should not be over sensitive to a small change in the boundary conditions.

This is very very important because, a perturbation in the boundary condition may be unwillingly implemented through round of errors and then it may be possible that because of that slight round of error you could have a large change in the solution; and that means, the problem is over sensitively dependent on changes in the boundary condition. So, if such situations occur we do not call it a Well posed boundary value problem.

The other important characteristic of course, it if it is a boundary value problem it is boundary conditions are to be well posed. So, then the question comes that small perturbation in the boundary conditions value first, boundary conditions have to be posed then of course, you you test for perturbations and so on. So, what are the possible types of boundary conditions. So, that we will look into more carefully.

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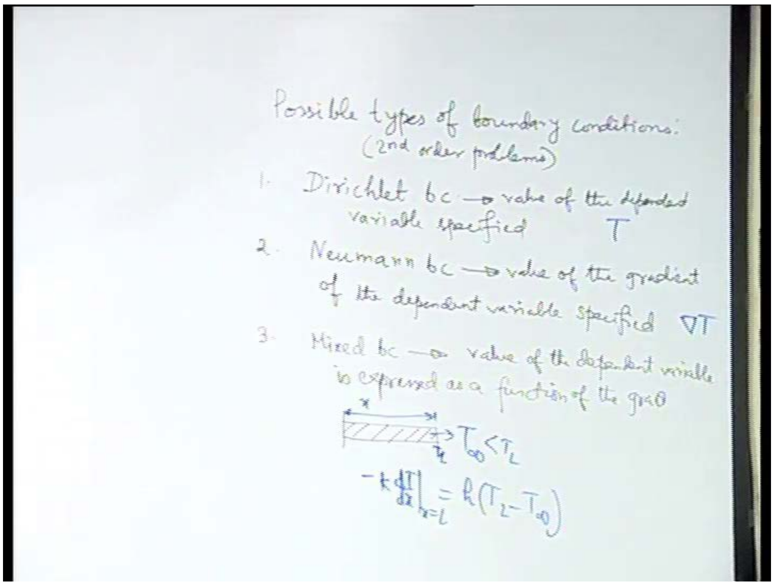

Possible types of boundary conditions through the variational formulation we have come across two types of boundary conditions, but those are not the only two types, but let us first note down the two types, the first one is the boundary condition, where value of the dependent variable is specified. So, that in the variational formulation terminology we called as essential boundary condition and in general, we call it Dirichlet boundary condition which is equivalent to the essential boundary condition this means value of the dependent variable is specified.

The other one is that, the gradient of the value of the dependent variable is specified which for a second order problem remember, when we are considering possible types of boundary conditions. We are restricting our self to second order problems why because second order problem, we have seen that those are more common in the numerical heat transfer and fluid flow that we are going to discuss. We have looked into the equations we have found that the equations are maximum up to the second order derivatives.

So, for a second order problem the value of the dependent variable specified is the Dirichlet boundary condition, then the natural boundary condition is termed as the Neumann boundary condition, of course, these are to honour the names of the mathematicians who contributed a lot towards understanding these concepts. Neumann boundary condition means value of the gradient of the variable gradient of that dependent variable is specified. So, for example, for a heat transfer problem if the temperature is specified it is Dirichlet boundary condition, if the temperature gradient is specified it is a Neumann boundary condition that is if the heat flux is specified.

The third type of boundary condition is called as Mixed boundary condition where value of the dependent variable is expressed as a function of the gradient. So, it is mixed because it is neither the value is specified nor the gradient is specified, but one is specified as the function of the other. Classical example is the convective heat transfer boundary condition.

So, let us say that you have a rod like this at the tip, the temperature is T L which is not known this is exchanging heat with the ambient which has a temperature T infinity and there is a heat transfer coefficient because of heat transfer from the rod to the ambient T infinity is less than T L as an example. So, the boundary condition here is whatever heat flux comes at the tip because of by virtue of conduction the same heat flux is dissipated to the outside because of convection. So, minus k d T dx at x equal to L is equal to h into T l Minus T infinity where h is called as convective heat transfer coefficient.

So, it is basically the conduction flux equal to convection flux at the interface. Can you use the same boundary condition, if the heat transfer is unsteady yes or no why why do you if you are saying no, then why do you think that you cannot use the same boundary condition if it is unsteady, of course, T if it is if it is unsteady T is function of both x and time. So, you can replace this by the partial derivative with respect to x.

If you replace that, that is if you replace d T dx with del T dx then can we use the same boundary condition you can definitely use because this is what, this is an expression that at the interface whatever is the heat flux coming by conduction the same is the heat flux that is leaving because of convection and that remains true even if it is unsteady because interface is not a volume it cannot store any thermal energy. So, no matter whether it is steady or unsteady at any instant whatever energy comes to the interface by virtue of conduction the same has to be dissipated by it to the surroundings .

So, you can use the same with the ordinary derivative replaced by the partial derivative for an unsteady problem. So, here you can see that the temperature is expressed in terms of the gradient of temperature at the boundary. So, it is a Mixed type of boundary condition. There is an another type of boundary condition which we commonly come across in numerical solution of equations . That is called as periodic boundary condition .

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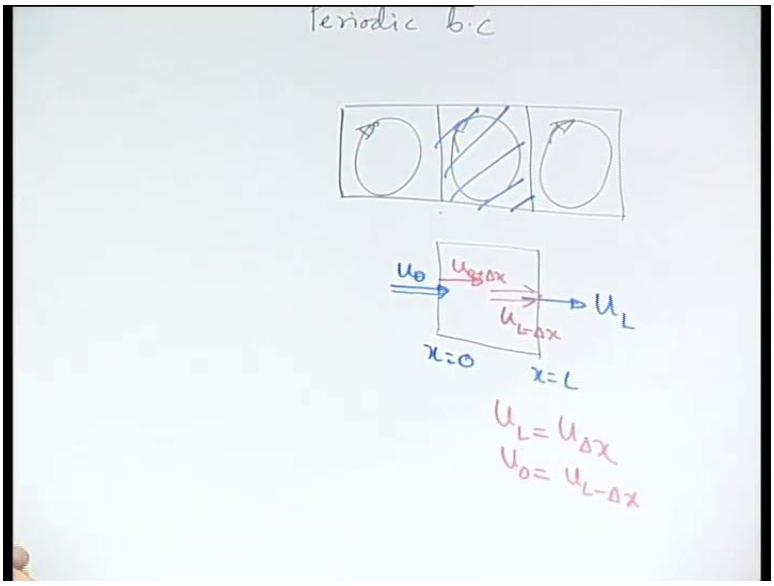

So, if you have a domain where the physics of the problem is such that the solution is periodically repeated. So, let us say that you have some vertices like this, again the same vertex like this, again the same vertex like this and it is a periodic structure in the flow that is repeated. So, that means, that if you can solve one periodic or repeating part of the domain sub which is the sub domain and then extrapolate or extend in all directions then it will give you the complete solution of the domain. So, then what kind of boundary condition you put here.

So, let us let us let us isolate this particular cell let us let us say this is x equal to 0 this is x equal to l. So, we say that let us say this is velocity at x equal to L say u L and this is velocity at x equal to 0 say u 0 we do not know these one, but what are the things that we know we know that they are repeating; that means, what we can say is that, whatever is the value of u 0 numerically we can say that the same is repeating at let us say x at L minus delta x. So, u at L minus delta x and similarly whatever was u at 0 plus delta x the same u is repeated at l. So, so we can say that u L is equal to u delta x and u 0 is equal to u L minus delta x. So, the periodicity is actually not equal to l, but equal to L minus delta x.

So, in this way one can implement the periodic boundary condition again you can see that we have put the boundary as a function of the interior and not the interior as a function of the boundary this is how to write it technically. Now, the other important issue is we have discussed about the boundary conditions and we will keep in mind that in the second order boundary value problems either of these boundary conditions will appear and one can specify the boundary conditions, but there is a more important (( )) issue the (( )) issue is any condition specified at the boundary a boundary condition. Boundary condition of course, is a collection of two English words. So, boundary condition sometimes it is misnomer because you feel that any condition you specify at the boundary could be a boundary condition.

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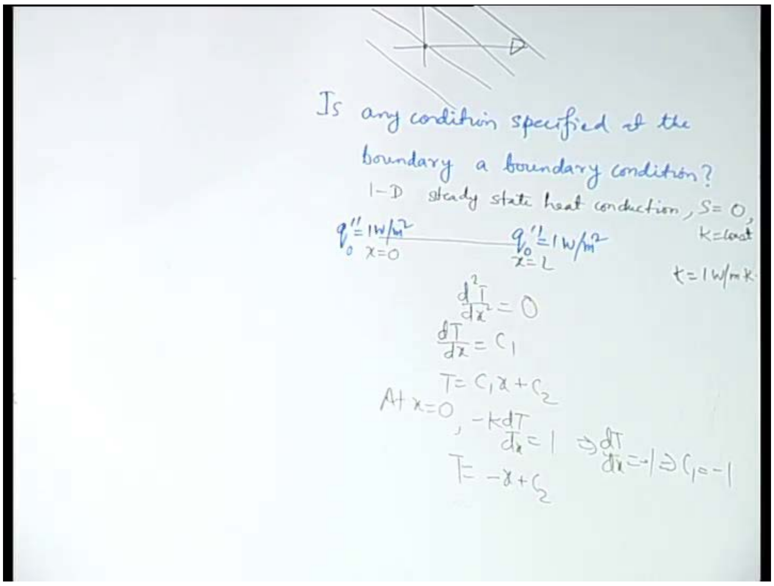

So, let us try to answer this question is any condition specified at the boundary a boundary condition.

It is important to discuss about this through a very simple example because then it is easy for us to appreciate. Let us say that we have a simple one dimensional steady state heat conduction problem with s equal to 0 and k equal to constant. Let us say this is x equal to 0 let us say this is x equal to L we give a boundary condition that at x equal to 0 the heat flux is say 1 watt per meter square and at x equal to L the heat flux is 1 watt per meter square this of course, we have to give right because it is a steady state problem.

So, let us say that what is the solution of this problem we have given boundary conditions to the two boundaries and it is physically a consistent one because whatever is the rate at which heat flux enters, the same rate at which the heat flux leaves at steady state. So, it is consistent with the steady state energy balance. This is what type of boundary condition this is Neumann boundary condition at both the boundaries. Now, let us try to solve this problem it is it may appear to be very simple, but let us try to solve it and see how simple it is. So, you have d 2 T dx 2 is equal to 0 that is the governing differential equation. So, dT dx is equal to C 1 T is equal to C 1 x plus C 2 .C 1 and C 2 are 2 independent constants of integration which you can find out from the boundary conditions if you can find out then its fine.

Let us say that the thermal conductivity of the material is 1 watt per meter Kelvin just for simplicity in numbers. So, at x equal to 0 you have minus k dT dx equal to 1 so; that means, d T dx equal to 1 minus 1; that means, C 1 equal to minus 1 similarly at x equal to L also it is the same thing. So, at x equal to L also you will get if you use the boundary condition you will get C 1 you will not get C 2. So, you get basically T is equal to minus x plus C 2 you cannot determine C 2. So, it violates the requirement of uniqueness of the solution. So, it does not mean that the solution does not exist it only means that infinite number of possible solutions will exists depend on depending on C 2. So, all these solutions are parallel straight lines in the T x plane.

So, if you plot all the solutions these all these could be possible solutions question is when all these could be possible solutions which one will do you accept as a solution because for a physical problem you you expect a unique solution these boundary conditions are not able to answer to that question because these boundary conditions are simply telling that you get a family of solutions with this one where there is an undetermined constant, this undetermined constant may be determined provided. You are given the value of temperature at one of the boundaries so; that means, if you have a steady state heat conduction problem one dimensional heat conduction problem then at least at one of the boundaries you have to specify the temperature; that means, at least at one of the boundaries you must have a Dirichlet boundary condition otherwise you cannot solve the problem as a unique solution you can solve it, but you will get infinite number of possible solutions.

So, we can understand from this example, that we have given some condition at the boundary, but that is not a legitimate boundary condition. So, whenever whenever you are interested to pose a well posed boundary value problem you must keep in mind that the boundary conditions should be such that it should be a well posed boundary value problem otherwise you can arbitrarily specify the boundary condition that may be physically consistent, but that does not give you a guarantee that it will give you a unique solution.

So, till now we have studied the finite difference method to some extent, the finite element method to some extent. Next the logical objective will be to look into a comparison of these methods, and see that how these methods are relatively performing with respect to one another. What are there possible merits, and demerits in comparison to one another, and we will bring the finite volume method in perspective of that we will see that what are the possible consequences of this methods, and how does the finite volume method evolve as a consequence as a natural consequence in terms of overcoming some of the limits, some of the limitations of these methods.

So, it will it will of course be established as a method which tries to consider or borrow the good points of both the finite elements method, and the finite difference method becomes inherently suitable for problems in fluid flow, and heat transfer and we will illustrate that in more details in a next class. Thank you.