Introduction to CFD
Prof. Arnab Roy
Department of Aerospace Engineering
Indian Institute of Technology – Kharagpur

Module - 2
Lecture – 7
Finite Difference Method

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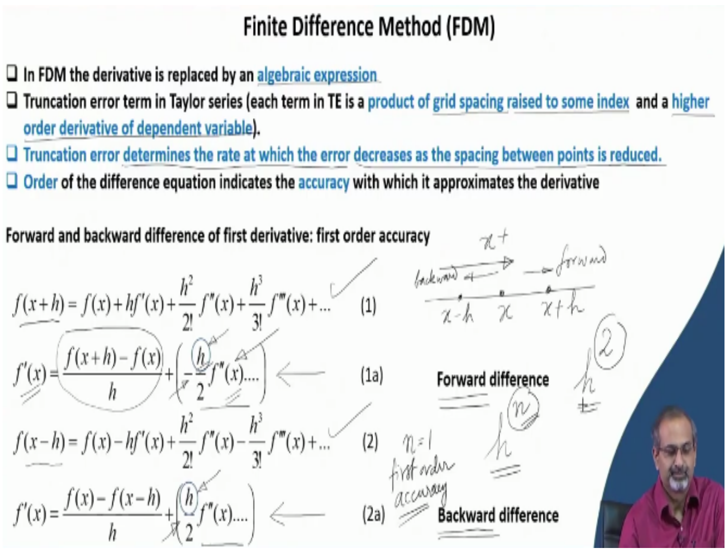

In this lecture we will continue our discussion on finite difference method. In the previous lecture, we had looked at the Taylor series expansion. We realized that Taylor series can be written for both directions. If you are expanding it about a point x, it could be x + h and it could also be x – h where h is a small distance. So, we derived both these expressions last time for f(x + h) and f(x – h).

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \left(-\frac{h}{2} f''(x).... \right)$$

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \left(\frac{h}{2} f''(x).... \right)$$

And by rearranging the first equation,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + ...$$

we can see that we derived an expression for $f'(x)$ and by rearranging the second equation,

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + ...$$

we got the expression for $f'(x)$ for two different cases, what we call as the forward and the backward difference. If you have a point x (x>0), a nearby point (x + h) to the right and another nearby point (x – h) to the left; the direction towards the right is the positive x direction; then if you move towards the positive x direction, it is the forward direction.

If you move towards the origin (x=0), this is the backward direction and accordingly we name the difference expressions as forward or backward differences. Interestingly, we noticed that the leading truncation error terms for the forward as well as the backward difference cases had terms containing 'h'. In one case it had a negative sign, in another case it had a positive sign, and in both cases it contained a second derivative of 'f'.

So, we go back to the points noted above, the bullet points, to realize that finite difference method produces algebraic expressions to approximate the derivatives. So, expressions like this are algebraic in nature. The truncation error term of the Taylor series, which we drop out in course of the approximation, contains terms which comprise of grid spacing raised to some index that is the 'h' term and a higher order derivative of the dependent variable.

So, we are finding an approximate expression for the first derivative of 'f' and we are left with a second derivative of 'f' with respect to x in the truncation error part. In general, we look at the index of the 'h' term 'n' in order to decide on the order of accuracy. So, we realize that both forward as well as backward difference here have first order accuracy. Of course, we do not know what exactly would be the contribution of the second derivative of 'f' in the leading error term of truncation error.

But we at least know that the index 'n' over here is equal to 1 and that gives it the first order accuracy. We also discussed that in general we would like to have larger values of 'n' in order to have higher order of accuracy. Importantly, truncation error determines the rate at which error decreases as the spacing between points is reduced. So, for example, if you were to make the grid twice as fine in this case, then the error would reduce by a factor of 2.

However, if you had a scheme whose truncation error leading term had an index of 2, that means you had a h^2 term as the first term in the truncation error, then if you refine the mesh and make it twice as fine, then the error will go down by 4 times and that is one of the major advantages of going for higher order accurate schemes.

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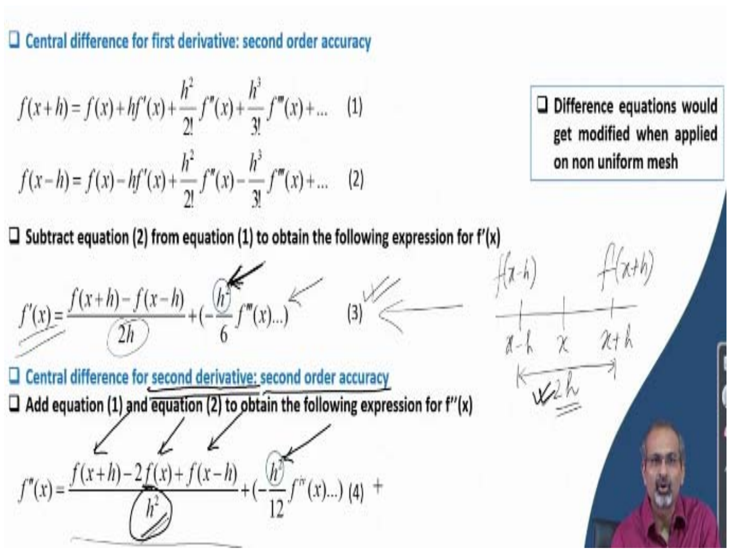

Let us now look at how we use the equations 1 and 2 in order to derive expression for the first order derivative, but now going for higher accuracy. So, the forward and backward differencing that we have used earlier given by equations 1a and 2a respectively in the previous slide gave us only first order accuracy. This time, we are going to manipulate the equations 1 and 2 in such a manner that we get an expression for first order derivative, but with second order accuracy.

So, it is a very simple manipulation that we need to do to achieve that result. So, if you subtract equation 2 from equation 1, you would obtain that result. You would now have an expression for $f'(x)$, which looks like this.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + (-\frac{h^2}{6} f'''(x)...)$$

You have [f(x+ h)– f(x – h)]/2h. Now you have a ‘2h’ in the denominator instead of ‘h’, the reason is that you now have a gap of ‘2h’ connecting the two points which forms the formula.

So, you are looking at f(x – h) here, f(x + h) here, and the gap between them is ‘2h’ and that is what you essentially see in the denominator. What are you left with in the truncation error? That is very important. You now have an h^2 term and that is what is going to give you second order accuracy. This is going to make a big difference because as you understand that with this kind of a formula for the first derivative, you are going to have a reduction of truncation error by an order 4 if you refine the grid and make it twice as fine

So, this would certainly be a more appropriate equation to use for the first order derivative when we are going for higher order accuracy. Now, let us look at a possible equation for obtaining the second derivative. So till now we were looking at the first derivative. Now we will have a look at the second derivative and straight away we approach with second order accuracy in mind.

Again, we use a simple combination of the equations 1 and 2 in the previous slide to obtain the second order derivative with second order accuracy in mind. If you add the 2 equations and transpose the terms, you reach the result. So this is the equation for second order derivative with second order accuracy.

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + (-\frac{h^2}{12} f^{iv}(x)...)$$

Now, you have 3 points in the stencil. You need the functional value at x, at (x–h) and at (x+h) and also note what you have in the denominator.

In the earlier expressions for first derivative, the denominator contained ‘h’ terms, while now it contains h^2 terms. What do you have in the truncation error? The leading error term in the truncation error has h^2 term, and therefore you have the desired second order accuracy.

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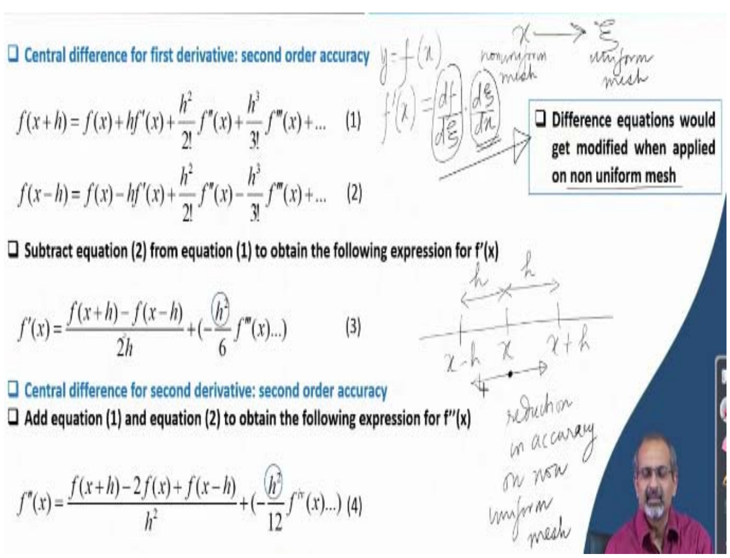

All this analysis is applicable when we are looking at grid points disposed at constant intervals. We have x, we have (x+h) or (x–h) and so on. So, the gap between 2 adjacent grid points always remains constant. However, this may not always be the case. You may like to take difference equations on nonuniform mesh. In that case, the equations will get a little more involved in the sense that you will then have to expand in Taylor series with varying gaps between adjacent grid points.

In general that may also affect your accuracy to some extent. If you have nonuniform mesh and Taylor series expansion is done in that manner with different grid intervals, you will generally have a reduction in accuracy. So, this is indicated here saying that we can have different equations for nonuniform grid or mesh applications, but then we have to suitably modify our approach.

Another interesting thing which you may think about is that if you are defining a function 'f' and you are now trying to obtain a derivative with respect to x and you do not have a uniform mesh in the x direction, you may think about transforming the mesh to some other plane from x plane to a ξ (zi) plane, x has a nonuniform mesh while ξ has a uniform mesh and then you could think about doing a calculation like this.

$$f'(x) = \left(\frac{df}{d\xi}\right) . \frac{d\xi}{dx}$$

So, in that case, the advantage would be that you can calculate this derivative on a uniform mesh,

$$\left(\frac{df}{d\xi}\right)$$

but then you have another factor here which needs to be evaluated.

$$\frac{d\xi}{dx}$$

This factor would have to be correctly evaluated. This does the scaling between the uniform and nonuniform mesh. We will discuss about this aspect later, when we discuss about grid generation.

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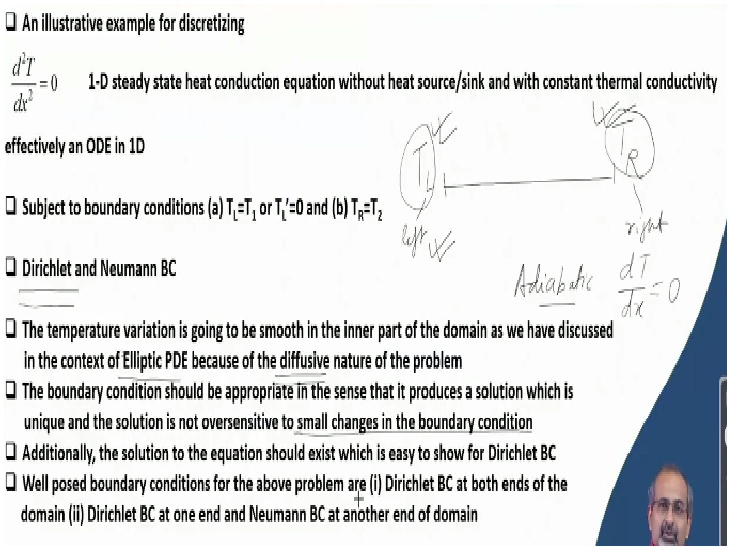

We will now try to do an illustrative example. We are going to discretize the one-dimensional steady state heat conduction equation without any heat sources or sinks and with constant thermal conductivity. We have come across this equation earlier when we talked about the Laplace equation and Laplace equation in general could be in multi-dimensions, but here we have reduced it to one dimension.

$$\frac{d^2T}{dx^2}=0$$

And that is what makes the partial differential equation essentially an ordinary differential equation and now let us try to solve this equation by using some suitable boundary conditions. Now, if you want to solve this problem, you need to know what kind of boundary conditions or combinations of boundary conditions could actually work out to give you a unique solution.

Such kind of boundary conditions will be stated as well posed boundary conditions. Incidentally, in order to solve this problem, you could either go about imposing the value of the temperature at the two ends of the domain. So, this is a one-dimensional problem as we said and we can try to solve the problem by defining a domain like this and then imposing the temperatures at the ends of the domain.

Let us say this is the left end and this is the right end of the domain and since it is a one-dimensional problem, we can just draw a straight line of a certain length and impose the boundary conditions at the ends of the straight line. So those are essentially the temperatures.

Now, when we set the temperature directly at the ends of the domain, that is what is called as a Dirichlet boundary condition.

This is not the only possible way of defining the boundary condition. We could also set the gradient to a certain value at ends of the domain, but then we have to be a bit careful here. We can do something like this that we keep the left end temperature intact and we try setting the temperature gradient to 0 on the right hand side, which makes it an adiabatic boundary because that would not enable any heat transfer.

Another way of imposing boundary condition could be that you keep the right boundary temperature intact and try to set the temperature gradient equal to 0 on the left boundary. However, we do not impose the 0 temperature gradient condition simultaneously at the two ends of the domain because that would fail to give us a unique solution. There are some other issues as well depending on the kind of equation that we are handling.

We expect a certain variation of the dependent variable which happens to be temperature in this case. So, this being governed by an Elliptic partial differential equation, which is essentially modeling a diffusion phenomenon, we expect that since there are no sources and sinks in the intermediate domain, the temperature should linearly vary between the end conditions that you have imposed if it is a purely Dirichlet boundary condition based problem.

Also remember that if you make some small changes in the boundary condition that should not significantly change the solution. So, these are some of the important issues of the solution, which we have to keep in mind. Again, for any problem that we try solving using CFD, we need to ensure that a solution to that problem actually exists.

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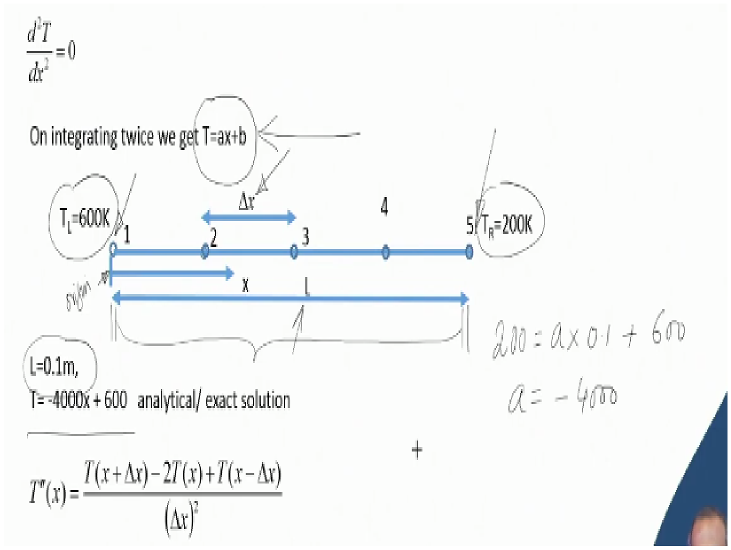


Let us look at the domain that we have set for ourselves. So, here is a one-dimensional domain of length L which we have set equal to 0.1 meter and we have a left end temperature equal to 600 K (Kelvin) and the right end temperature of 200 K and we want to find out by using a finite difference approximation that how temperature could vary in the intermediate domain, that means this region, just leaving apart the boundary conditions.

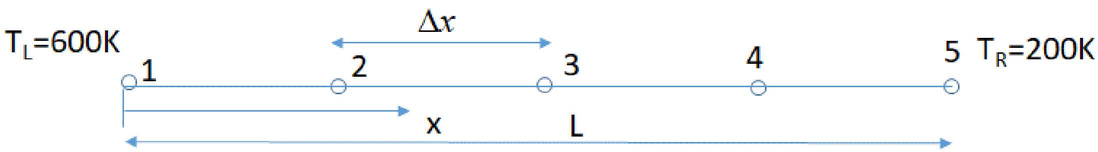
For doing that, here is a convenient situation we have in hand. We have an exact solution to the problem. If you integrate it twice, you get the temperature expressed in terms of two arbitrary constants and then if you impose the boundary conditions in that expression, so T = 600 K at x = 0 because we are setting the left end of the domain, x=0, as the origin. So, T = 600 K when x = 0.

Which means b takes up the value of 600 and then you impose the condition that at x = 0.1 meter you have a temperature of 200 K. So, you already have b, therefore on the right hand side you will have 200 = 0.1a + b which you have already found to be 600. So, you can solve for a, which will come out to be –4000 and therefore you have the analytical or exact solution available.

T= -4000x + 600

Now, this would be a good situation because you will know how good or how bad your finite difference solution is doing when you try to apply it to this problem. For doing FDM, we put two grid points at the ends of the domain corresponding to where you are imposing the boundary conditions and we put as many intermediate points as we want.

In this case, we have decided to create 4 equal intervals spanning the total length L and therefore we had to put 3 internal grid points. So, now, once we put the 3 internal grid points in such a manner that we get a constant delta x between adjacent grid points, we can say that the grid points vary from 1 to 5.



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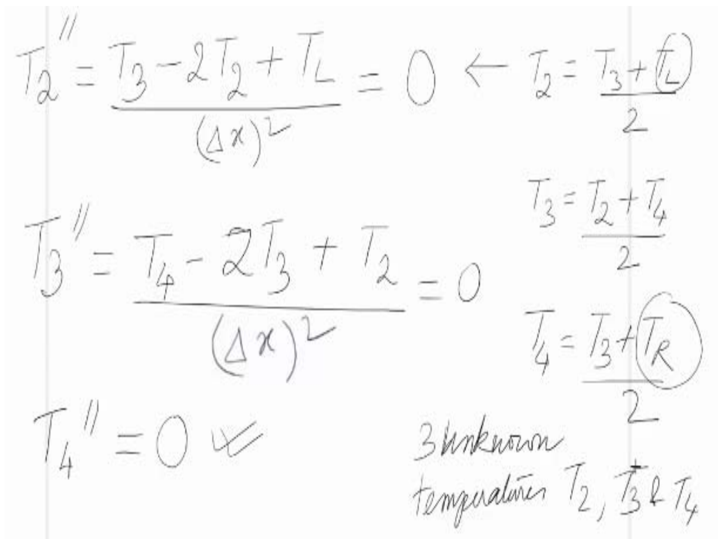

Now, let us try to write down the equations at each of those grid points. Let us see how they would work out. So, using the finite difference expressions that we wrote earlier, we take the grid point 2 and I am putting double dashes to indicate that we are expressing the second derivative of T at that grid point. You know by this second order accurate central difference scheme that this would be the description for the second derivative at that grid point and by the governing equation this should be equal to 0.

$$T_2^{//} = \frac{T_3 - 2T_2 + T_L}{(\Delta x)^2} = 0$$

$$T_2 = \frac{T_3 + (T_L)}{2}$$

Similarly, you can go about writing the governing equations at the different grid points, adjacent to point 2. So as we move further into the domain, you go to the point 3 and point 4. So, you can write the detailed expression for point 4 on your own, but finally you need to set it to 0. I am not writing the complete expression here, you should be doing it on your own.

Now, if you look at this equation, if you slightly rearrange it, what do you have from that equation?

You have a result which looks like $T_2 = (T_3 + T_L)/2$. When you look at the next equation, what do you have? You have $T_3 = (T_2 + T_4)/2$ and then once you write down the equation for $T_4^{''}$, you will have this equation coming up.

$$T_4^{//} = 0$$

So, what do you have now? You have 2 known temperatures T_L and T_R and 3 unknown temperatures; namely T_2, T_3 and T_4 respectively.

So, since you have only a few linear algebraic equations here, you could try solving these equations yourself in order to generate the solution. So, we will take a few minutes, try solving it.

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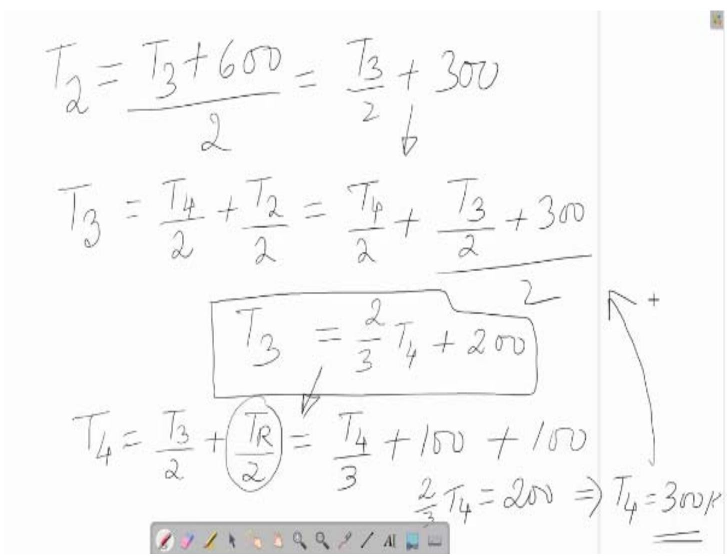

So let us try to put in the values and try writing the equations. For example, you can write $T_2 = (T_3 + 600)/2$, which is nothing but $T_3/2 + 300$ followed by an equation for T_3 which I will be now writing as $T_4/2 + T_2/2$ and from this equation, I can write it as $T_4/2 + (T_3/2 + 300)/2$, and therefore T_3 will finally come out to be $2T_4/3 + 200$. So, this is an equation for T_3 expressed in terms of T_4.

And now what we are going to do is we are going to go to the T_4 equation and we will write it as $T_3/2 + T_R/2$ and substitute this equation here to give you $T_4/3 + 100 + T_R/2$ (which gives you another 100). So, finally this equation can be slightly rearranged to give you $2T_4/3 = 200$ which implies that $T_4 = 300$ and mind it that it is 300 K.

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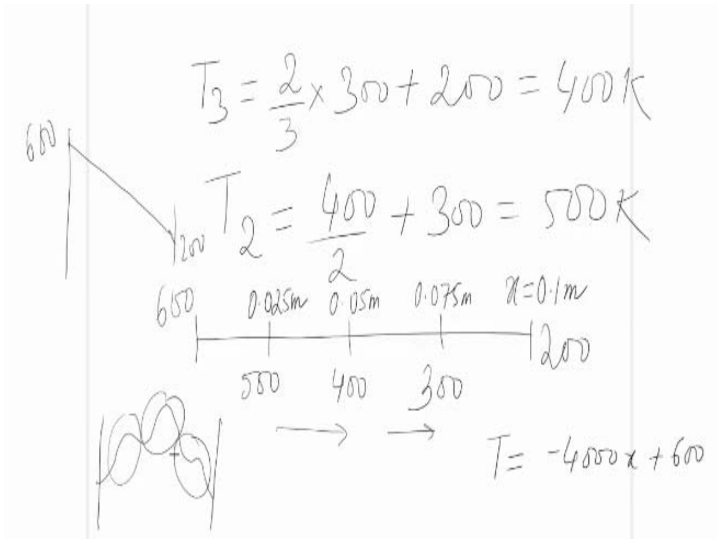
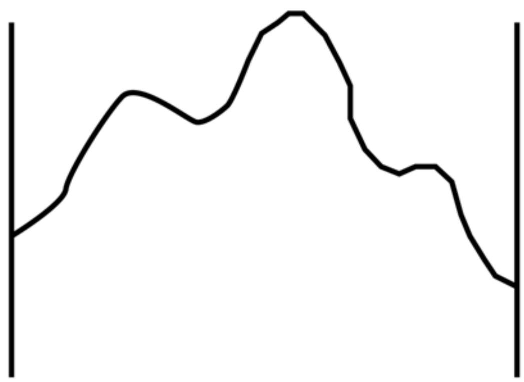


So, if you back substitute this value into the previous equations, you will get $T_3 = 400$ K and $T_2 = 500$ K. So, now, you have the solution available at all the grid points which are lying intermediately. So, if you just put in the values you have 600 here, you have 200 here and you have 4 equal intervals and you see these values are coming out to be exactly 100 K less as you move towards the right.

Now, would you like to check how good or how bad your solution was with respect to the analytical solution? For doing that, you simply need to go back and check by putting the appropriate values of x into the equation. Remember that at this point you have $x = 0.1$ meter. So, the remaining points would stand at 0.075 meter, 0.05 meters, and 0.025 meters, and if you substitute these values of x into your exact equation for T, then you will find that the finite difference values and the exact expression values exactly match. Now, this seems to be quite amazing because we just had an approximate value of derivative doing this magic, but this should not come as a surprise. It is because we have taken a linear temperature variation here. So, it does not have any contribution to higher order derivatives, which are actually figuring in the truncation error terms.

If you were having higher order derivatives coming up as nonzero values because of the typical nature of the temperature variation, then you would start seeing difference between the exact equation and the approximate values generated from the finite difference method. For example, if you had intermediate sources or sinks of heat placed in the interior domain, there would be local variations of temperature.

And there would also be a global outreach of such temperature variations through diffusion giving a very typical temperature variation, which may look more arbitrary like this.



However, ours is a very simple case, it drops straight from 600 to 200 and because of the lack of such nonlinear variations, the finite difference scheme is able to give you a solution which matches exactly with the analytical solution. We will discuss more on these issues in the next lecture. Thank you.