

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 15: Numerical Methods for CFD

Hello everyone welcome back with another lecture on CFD applications in chemical processes we were discussing numerical methods for CFD we discussed finite difference method and method and we are in finite element method a brief overview of the finite element method where we started the understanding of its basic by looking at an example where I cited an example from J N Reddy's book Introduction to Finite Element Method that to estimate the perimeter of a circle. Now, three steps, three basic steps that are involved in finite element method. The first step is the discretization of the domain, then approximation of the governing equation

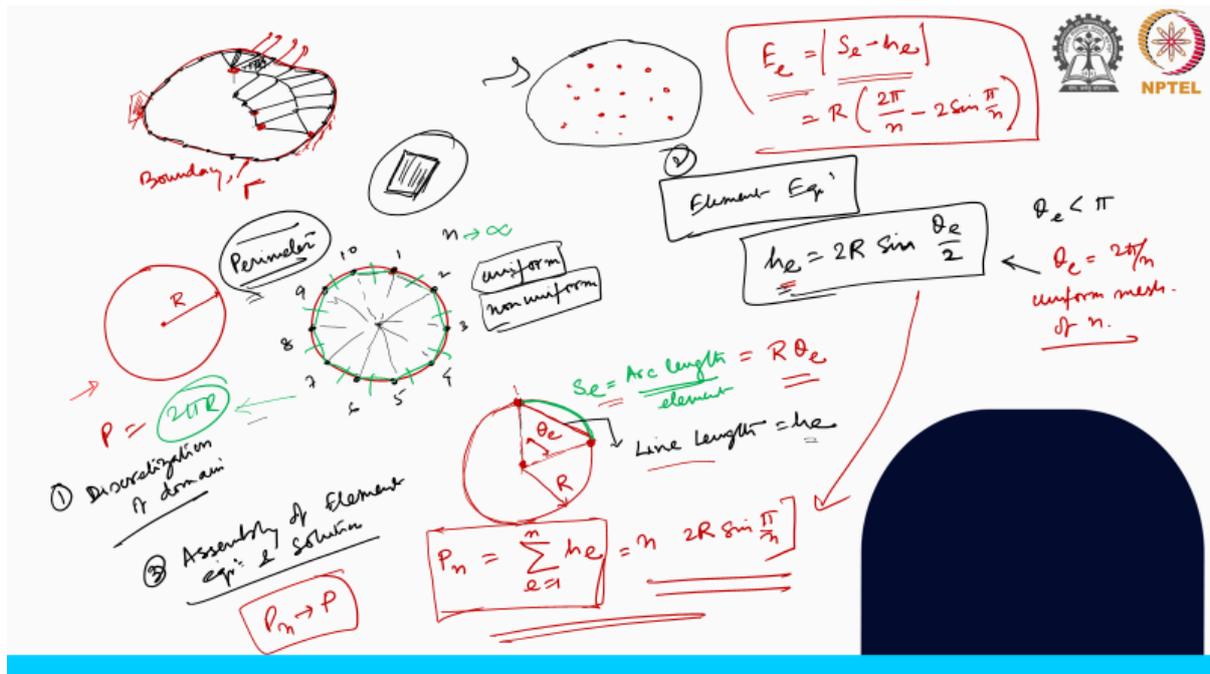
for each and every element the finite element that we created by discretization and the third step is the assembly of those expressions and then its solution. So, in the first step when we considered this example that to estimate the perimeter of this circle say So here we have considered 10 segments. So we considered that these black dots are essentially the segments that we have discretized in the first step. Then in the second step is that we had to approximate and here this is the very simple problem.

So, there we will actually have the exact solution of the estimate that is our perimeter and here the distance between the two line segment two points here because this results in a straight line. So, for this straight line we know the distance and then as I told you that we will have the of all the 10 segments in order to estimate the total perimeter of this circle. Now, here I have deliberately shown one thing is that say the points or this nodes specifically that I have considered here are equidistant. if that is the case then we have this uniform meshing ok.

If it is not then we have non-uniform mesh because this terminologies will be applied throughout now uniform mesh non-uniform mesh how it is created. So, here we have 10 starting from here 1, 2, 3, 4, 5, 6, 7, 8, 9, 10. So, 10 line so, 10 segments and 10 resulting in 10 line segments. If these are of the different length then we have non uniform mesh, if those are of equal length then we have the uniform mesh.

So, once this is done then the thing is that we have to in the second step we have to find out what is the element equation in the second step. So, the first step is the discretization of the domain. The second stage is that we have to write the governing equation or the element equation. Now, here the governing or the required parameter is the perimeter ok. So, how we estimate that between these two points?

So, here what we have say this circle that I have and say I have divided it. So, this is considered say the one segment this is taken just for the illustration purpose that how this distance is estimated. So, here what means this angle if I consider for one element is theta E this is the arc. This is actually the arc length which we are estimating. So, this Se is essentially the arc length for one element.



this is the line length which we are approximating for this arc length. Let us say this is h_e . So, this S_e is being approximated by the value h_e . So, we have to find out for this element equation what is the expression of h_e . So, for this typical element one element that is here this is the element. So, h_e is the length of this element that we are considering in the mesh. So, h_e expression from this geometry that we can see is the $2r \sin \theta_e$ by 2.

Here R is the radius of the circle. θ_e is less than π , the angle which is subtended by the line segment. So this here for our desired value, we call this as the element equation. Clear? So now we have the third part, which is the assembly.

assembly of element equations and then subsequent solution. So, the approximate value of this perimeter of this circle that we are considering is that by putting all these line segments together that I showed here last time in this figure it is clear that all these line segments that we have. So, all these green line segments once we club it we make a summation of it we basically get the total perimeter. So, which means if I consider

the perimeter by doing so is say p_n because we have say n number of such elements. So, it is essentially element number 1 to n summation of h_e for each element what we have calculated summation of all these elements gives me the perimeter that is predicted by this finite element

method, which is essentially if we consider this mesh to be uniform for the sake of simplicity, then what happens? θ_e is basically 2π by N for uniform mesh. uniform mesh of n number which means P_n is essentially we have $2r \sin \pi/n$.

So, what we have P_n is n times $2r \sin \pi/n$. Now, we know the exact solution we started this whole objective assuming that we did not know earlier what is the value of this perimeter which is $2\pi r$. Now, we have come to this conclusion that by finite element method for n number of elements the perimeter is this value this expression you put the value of n you get the value of p . Now, the point is that means, there is an error as I told you since we have this number of finite n if n is infinite this P_n should tend to be the value of P ok. So, in the limit of n tends to infinity the P_n should be P , but presently these two are different.

Now, this error in approximating this by the line segments how much that is how do we quantify that and whether it actually gives me or shows me that when n tends to infinity whether P_n tends to P . Let us check that. So, these errors are introduced for each and every element if we consider this error for every element to be $E_{subscript e}$ small e which is essentially the difference between this S_e and H_e . S_e is should have been the exact it is the exact arc length, but we are estimating that with the line length which is H_e . if it is big enough if it is large enough we will have higher deviation from the actual value.

So, basically for each element my error is mod of SE minus HE fine where SE is essentially $R\theta_e$ the length of this particular sector. So, if I now here write those expressions. So, $r\theta_e$ essentially is $r\theta_e$. So, what we have is $r\theta_e - 2r \sin \pi/n$ ok. So what I have the error to be $r\theta_e - 2r \sin \pi/n$. The previous expression I have written once again. This is for one element. So, what is the total error the global error?

It is the summation of e_e over the entire domain or number of elements for n which means the total or the global error is n times because n is the number of mesh here we have considered n times e which is essentially so 2 if I take this 2 out of this bracket it becomes $2r\pi - n \sin \pi/n$. I am multiplying this with the n . So, what I have $2r\pi - n \sin \pi/n$ which is if you look at it this expression is essentially the actual P . In the previous slide we have shown is that P_n is essentially pn from here if you look at it from this expression is $n 2r \sin \pi/n$ here the same expression is here that $2r n \sin \pi/n$ which means this is my pn . that means, which we were telling that the total error is essentially this value.

Now, E should go to 0 if n tends to infinity is not it that is what we are talking about that if I have infinite number of elements. I should have the exact value of the perimeter. So, if I consider that say x is equals to $1/n$ then P_n becomes from this expression $2r \sin \pi/n$ which is $2r \sin \pi x$ divided by x replacing n as $1/x$. So, what I have now P_n is equals to $2r \sin \pi x$ by x . Now, in the limit of P_n , n tends to infinity what I have

$2 R \sin \pi x$ by x is equals to $2 \pi r$. So, if n tends to infinity I will have the exact solution as that of the perimeter of the circle. And this E_n or say for a particular total if I say the global error here you can consider E_n also. this global error tends to 0 if n tends to infinity. And this part is the point is that we can have a convergent solutions or say this we can also say this is the proof of convergence.

The image shows handwritten mathematical derivations and notes on a white background. At the top right, there are logos for a university and NPTEL. The main derivation starts with the formula for the error of one element: $E_e = R \left(\frac{2\pi}{n} - 2 \sin \frac{\pi}{n} \right)$. This is then multiplied by n to get the global error: $E_{\text{Global Error}} = n E_e = 2R \left(\pi - n \sin \frac{\pi}{n} \right) = P - P_n$. A boxed equation states $E_n = P - P_n$ and notes that $E \rightarrow 0$ as $n \rightarrow \infty$. The perimeter of the circle is given as $P = 2\pi R$. The perimeter of the polygon is $P_n = 2R n \sin \frac{\pi}{n} = 2R \frac{\sin \pi n}{\frac{\pi}{n}}$. A boxed equation shows $P_n = 2R \frac{\sin \pi n}{\frac{\pi}{n}}$. The limit is calculated as $\lim_{n \rightarrow \infty} P_n = \lim_{n \rightarrow \infty} \left(2R \frac{\sin \pi n}{\frac{\pi}{n}} \right) = 2\pi R$. A box labeled 'Grid Sensitivity Test' points to this limit calculation. Another box labeled 'Mesh Sensitivity' is also present. To the right, a box contains the text: 'No. of Meshes', 'Convergence Criteria', and '& Computation time/Resources'. A large blue arch is visible at the bottom right of the page.

when your n tends to infinity, but when it is not in practice when you define or divide a domain into finite number of points then it is difficult to have maximum or say as much number of meshes or elements in the domain. And that is why the numerical error remains in the prediction. And that is why it is essential that we have grid convergence test or grid sensitivity test. That how many grids or the number of mesh, mesh sensitivity also the same term. the grid or mesh sensitivity of the solution.

So, I will also again discuss this in details, but let me introduce this mesh sensitivity or the grid sensitivity because here clearly you can see that the convergence criteria that we discussed in the last class or the last lecture also. that you set a desired level of convergence criteria or the tolerance limit difference between the two consecutive iterative state of your desired variable. If that is within your tolerance limit, you consider that has converged and you stop this. That means you are considering that some amount of error is there in my solution, but still it is fine because after two consecutive simulations or maybe more than that, there is hardly any deviation which is negligible say in the order of 10^{-6} , 10^{-8} , such kind of tolerance limit that we provide.

But that is introduced due to this number of meshes at the first point because that is the first step the discretization of the domain and that introduces numerical error. So, how many number of meshes are sufficient? Now, that as many number of meshes that you take you can see that here from this example that your convergence towards the actual solution is much higher or it will be if it is infinity the number of meshes, but that cannot happen in the actual simulation you have finite number of meshes ok. So, now, this number of meshes how many number of meshes, your convergence criteria and computational time which depends on the resources, the computational resources all these are linked.

you have to have a trade off between your computational resource and the number of mesh and the convergence criteria or the accuracy level of your prediction. So, these are linked, but still mesh sensitivity or grid sensitivity analysis is essential because without that your solution accuracy would not be reliable. People would not rely on your model prediction. So, I will discuss this in detail when we will discuss now the finite volume method from the next lecture and that we will have some exhaustive discussions. We will bring up these points once again.

And we will further elaborate that how grid sensitivity or grid sensitivity test and or the mesh sensitivity test is extremely important for your model accuracy. You have to have grid sensitivity test and then this convergence criteria and the computational time resources all would be linked together. So with this note, I will stop here today. In the next lecture, we will start the details of finite volume method. Until now, we discussed a brief overview of finite difference and the finite element method.

If you are interested in those methods, look for the several CFD books or there are books dedicated to finite elements method that one of them I mentioned. And now from the next lecture, we will discuss about the finite volume method. Thank you for your attention.