CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-03

Lecture 14: Numerical Methods for CFD

Hello everyone, welcome back with another lecture on CFD applications in chemical processes. We are discussing about the numerical methods that are applied for computational fluid dynamics or the CFD. Specifically, we are into the finite difference methods. so the strategy how it is applied and its different formulation and we have taken some example or one example and we have seen that for unsteady state case for the finite difference method we can have the explicit as well as the implicit formulation so what happens is that

eventually by these techniques you approximate or you convert the partial differential equation to a set or system of algebraic equations. Now, those equations you have to solve. So, that this is the same thing that will happen when we will discuss the finite volume method in detail. But before we go into that let me very briefly tell you although we will not discuss this at all in detail or the reason of the conclusions that I will show you is that this set of algebraic equations. by different process you can solve this algebraic or the linear equations which we will have and you can solve it by two different method.

One is the direct method, the other one is the iterative method. The direct one the examples are say Cramer's rule. Now, what are these if you are unaware of it or if you forgot I would suggest that you look into any CFD book or any advanced mathematics book where the solution of algebraic equation or system of algebraic equations and its algorithm would be given. So, the direct method examples are Cramer's rule, Gauss elimination method, LU decomposition, these are the examples of the direct method.

The iterative method similarly are say Jacobi method, Gauss-Siedel method, SOR. So, all these methods are there. You have to choose again as I told you our aim in this case in this course is to go into the algorithm that how are those are discretized not into these methods that how once you achieve the set of algebraic equations or a set of linear algebraic equations how you solve that. We will assume here that you are aware of these methods and can go into the details of these algorithms whenever it is needed and if you have to build your own code,

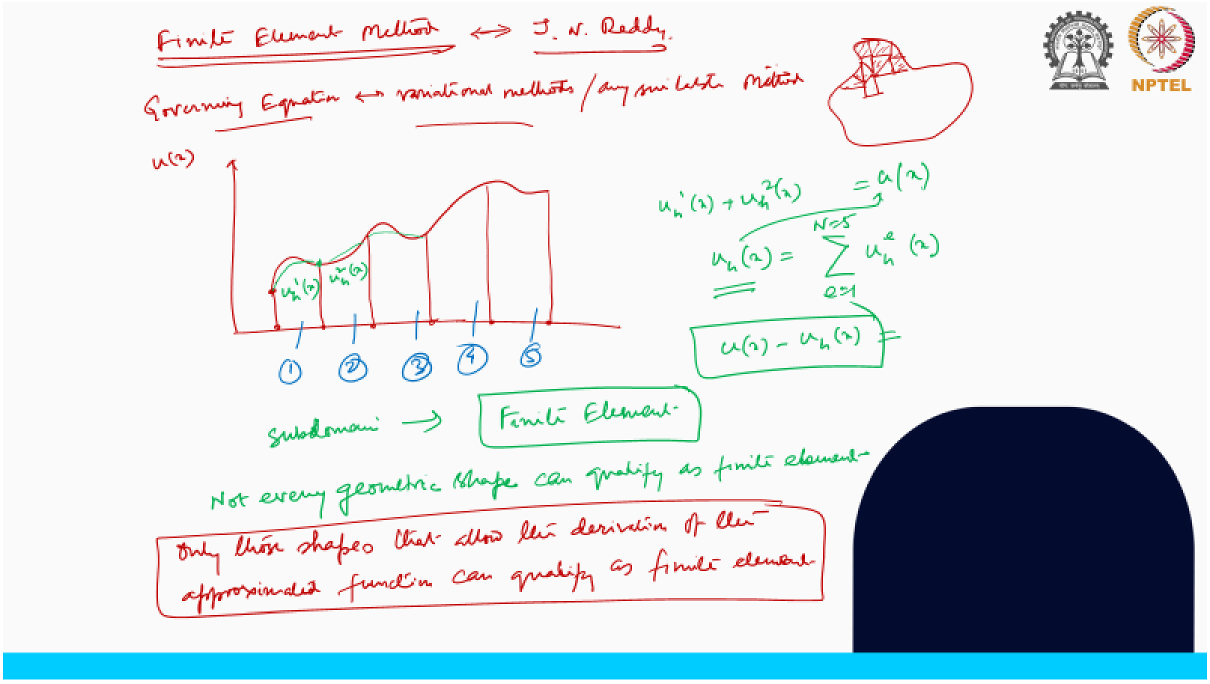
if you have to develop your own CFD code, accordingly you do that, you choose such method. But the standard or say the commercial CFD softwares takes into account of these parts as their own several different strategies. Now, usually the direct methods takes more time than the iterative method. So, the point is the iterative methods these are also sometimes are known as say the point by point method each and every point you are trying to understand get the values and for such methods you require a convergence criteria that where you will stop your simulation or where your simulation would be stopped.

This convergence criteria is usually defined by a quantitative manner where you have to set your choice when the ah values that you are calculating ok. So, the difference between the two consecutive time step whether that difference is acceptable to you or not. that with that you define your convergence criteria that if between two consecutive time step my desired value has not changed significantly or it is within my tolerance limit then I consider that it has reached the end of the simulation. So, with this brief introduction on the post discretization part.

So, let us move on to the other technique that is the finite element method before we because we will after this we will devote our most of the time on the understanding of finite volume method. So, before that briefly understand say how the finite element method works. Now, here let me be very clear that this finite element method is extremely robust is very robust method and is a very popular method. This is also The numerical method similar to this finite difference method, but it conquers several of the drawbacks of the finite difference method and it is extremely useful when we have multiphysics problem. Which means when we have not only hydrodynamics but heat transfer, mass transfer, reaction, several other physics those are coupled in a single problem.

In such cases this finite element method is extremely robust as well as very accurate method. It also starting with the that drawback that I told you earlier that the finite difference method is very difficult to implement in the say irregular shaped body or complicated geometry, complex geometry. So, in such case finite element method comes handy. And please do not expect the very details of finite element method here which is out of the scope of this current discussion of this course, because standalone finite element method is itself full length course. So, what we will have we will try to understand today the basic idea of finite element method.

If you are aware of it, it is extremely well and good. If it is not, let us see very briefly that how it is implemented with a simple example. By the way, a classical book is there. from which you those who are interested particularly in the finite element method can get acquainted with this method or can go deeper further if you do research on this is the introduction to finite element method by J N Reddy. So, I will show you one of the examples from that textbook to understand this finite element method.



So, finite element method as I told you is the similar numerical method like we have discussed the finite difference method. And here this is considered the domain or the computational domain that we consider or we have in hand. We consider that as a set of several subdomains. just like in the case of finite volume method or also in the case of finite difference method we have seen. Now, here the point is that what we try to do is that we try to consider the whole domain as a set of sub domain and the governing equation the governing equation

we try to approximate like in the finite difference we did it with the Taylor series expansion. We tried to approximate this governing equation by any of the traditional variational methods or any method that is suitable to resolve the complexity so any suitable method So, the point is say example that you can which would be easier for you to perceive is that say I have a function which is like this and I have to so, my this is say my the domain boundary the one of the domain. Now, here what we do in finite element is that we try to

So, what we try to have this? So, once we divide this into several sub domain for each sub domain we try to approximate this function by a simple polynomial which is easier to evaluate or say which we can have its derivative easily. So, for example, if if say this is a smooth polynomial we can think of that goes here for this part we approximate by the another line by the another polynomial and if it is difficult to define again the other polynomial that fits here. Such segment by such segment we approximate these

actual this domain for each and every sub domain. So, for example, if I say that or if I write here that this is my element 1. So, each and every element that these are here 1 2 this is third element fourth element and this is the fifth element. So, here then although I have this exact u x, but we are approximating this by a function which is say u h for the domain 1 as a function of x ok. So, similarly this approximated

function of the actual function is u h in domain 2 as a function of h. So, when we try to find the simpler way we naturally introduce the numerical error. So, in the first step what happens which means by now adding this all u h. we essentially get the function u x. So, basically if I have h u h x is essentially what we can write that for element 1 to element number say here 5 u h e x. So, we get u h x and we consider that this is the actual value of the function which is not the case because that is the difference is essentially our numerical error. if we can achieve or go closer to this value by taking here infinite number of domain then possibly this difference would go nearer to say the 0 value.

But the point is that these different polynomials that we are connecting here it cannot be arbitrarily it has to be continuous at the junction point and possibly its derivative also has to be continuous at the point of connection between the two segments. So, that is one of the critical criteria that we have to consider. So, what happens here that these subdomains we call these as the element. the number of subdomains. So, each subdomains also can be called as the finite element.

So, that is why the name is there is the finite element. So, each subdomain is called as the finite element. But, as I told you that not every say the geometric shape can be a finite element or an element can be considered as finite element. So, the point is not because by doing connecting these two consecutive points or again the nodal points we can call those by connecting two consecutive nodal points the element shape that we get.

So, those are having some geometric shape. The point is based on this criteria that it has to be continuous or its derivative has to be also continuous that not every or not all geometric shape can qualify as finite element. Only those shapes that allow the derivation of the approximated function can qualify as finite element.

only those shapes that allow the derivation of the approximated function or the function that we have approximated can qualify as the finite element. So, basically the discretized domain once we have this say once you will realize that this kind of several domain or sub domain as we are trying to have or approximate this complex geometry. So, each and every element these elements would only qualify as a finite element if the derivation of the approximated function this governing equations when we try to approximate by any variational method or any suitable method can happen in that element.

So, say for example, what happens is that say we have a domain that is like this. So, this is we say this is our boundary. and it has a different bound say different type of boundary conditions at various location. So, in the first step what is done is that we try to find So, for this shape, we try to find the exact its approximated value. So, considering say several points here on the boundary condition.

we try to approximate because this becomes easier as closer this becomes it is kind of a line segment and we do such kind of subdomain be it triangular, be it different kind of polygon say etcetera that can happen. So, basically what means that say this is the one of the mesh that we have here. So, that mesh this in this case are having. So, this is the one cell out from this number of sub domains.

So, first is that we tried to do the discretization of this domain, this is the original one and so, this is the original one say we had and this is the discretized version. So, what we tried to represent the domain by collection of triangles and quadrilateral elements. So, this can be further inside this thing like this. So, such kind of triangles and quadrilaterals a quadrilateral element by which we can represent the domain. So, a typical element is say this one.

ok and this junctions where this is happening. So, this essentially a domain is represented by several nodal points collection of nodes. So, the point and then we try to approximate our governing equation in this nodal point or this elements finite elements. So, say consider we are trying to the example that I told you that we will cite from this Jane Reddy is that say the perimeter of a circle calculation of perimeter of a circle.

we all know that the perimeter of the circle is the value for the 2 pi r. We clearly know this, but consider for the time being you are not aware of it. So, how to estimate that with this finite element method? So, for this the first stage is the division of this perimeter like we have done earlier by into a collection of say segment and here it is easier it is straightforward that we can have it by the line segment. So, for example, what we can have here is that we consider several say equispaced points ok.

But the point is that to represent this perimeter we actually would need infinite number of such thing of such points to exactly track this perimeter, but say we have some finite number ok. If this number of the points say n is not infinite then it is not accurate But, that is the error that is introduced when we try to approximate that and the first stage. So, the point is that once we have this then we actually have to write an equation for our interest that is here the perimeter. So, the distance between the two consecutive these points.

Now, here it is easy because these can be done simply by a straight line. So, all the connecting of these essentially is the straight line between the two points on the perimeter and we know what is the distance here. The distance between the two points we can easily estimate it and that is the approximation in the second stage that we are introducing if these were not say the straight line here it is easy straight forward.

So, that is why in this second stage we will not have any numerical error introduced further. So, and then what will happen? We will do the summation of all these line segments and expectedly this summation should give me that total perimeter of this domain. Now, since here so 1 2 3 4 5 6 7 8 9 10.

So, all these 10 line segments the summation of these line segments should give me the value of this perimeter of this circle. But expectedly, this would not be the exact value that of the thing that we have because we have approximated it by a suitable method that we discussed in the last slide. And we have taken the approximated value for this perimeter here between the two consecutive points by a straight line, we know the distance. summation of this distance gives me some value which is not exactly 2 pi r. It could have been the exact value if n is infinite that means if you had infinite number of points here. So, we will go into the details of it I will stop here we will take it for the next lecture.

Thank you for your attention and we see with the next. Thank you.