

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 10: Basics of Finite Volume Method

Hello everyone, welcome back once again with another lecture on CFD applications in chemical processes. Today we will briefly discuss on the basics of one of the major computational techniques to solve these set of governing equations we have seen so far. The necessity of it also we have discussed because we understood by now, that the conventional Navier-Stokes equation in its full form without any approximation or even say any other governing equations that may arise in a complex flow scenario without any simplification it is very difficult to solve analytically because in the analytical solution what happens in the analytical method. It is tried to solve those, we try to derive those solutions by neglecting say the unimportant parameters and also considering several simplifications or assuming several simplifications for the problem.

that may dilute the solution accuracy and for example in the Navier-Stokes equation we have seen we have discussed that when it boils down to Euler's form or even the creeping flow equations. Now analytical equations of Euler equations and its forms several analytical equations are available but you can understand that several simplifications or assumptions have been done in such cases. But a complete momentum equation if we consider along with the continuity equation cannot be solved analytically. And also it is very difficult to experimentally gather those insightful information for a particular flow scenario. So, we require computational method the computational flow dynamics the utility of it we discussed in comprehensive method in the previous earlier classes.

So, here I will introduce because you have heard by now several times this term called the finite volume method and you may be interested in understanding what is this finite volume method. So, I will give you an overview of these several methods that are available, but at first today I will take you through the sketch the over the very basics of finite volume method in this class. So, what happens when you are given any problem We discussed that we have to at first consider our solution domain and say the simplest form I can consider a rectangular form of it. So, this is our computational domain say for example, this is the wall or this top wall bottom wall my flow is happening from this side and it is going out from the domain on this side.

I have to say check the temperature profile if my temperatures are different at the different locations or say the boundary conditions are different than the flowing fluid. So how the

temperature is varying? How the say my enthalpy is changing? So this kind of information when we try to solve the first thing that we do you have seen earlier when you have solved such problem in heat conduction is one method you have seen is called the finite difference method. in short we call that as the FDM. So, in that case what you have already done is that you started by drawing several small cells and you name those say this is the i a direction, this is the j th direction.

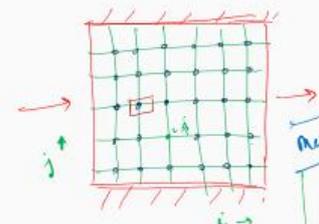
So, you have considered say one point your point of interest is ij and by marching it you have solved it. Marching it in different direction you have solved for that I and J point. You have found out that what is the temperature or what is the other flow variables that are there. The similar thing we start for the case of finite volume method. So in finite volume method we also draw such grids or the cells or meshes.

So these are we call mesh, computational mesh or grid or cells. We will come to the details that how those are drawn later. But at first you should understand that why do we do that. because we have to find out say the temperature or pressure in the domain. We have to find the profile that how the temperature is varying along the flow direction.

If we have to find out that thing that means, we have to find those at a finite location and those locations are identified by the junction of these I and J lines. if we find out at these circled locations all those variables the flow variables be it scalar or the velocities. So, in these circled positions if we find we can easily find out or plot how the what is the variation of it that is happening. Okay, so how the what is the variation if we find out at each and every location of these points that I have drawn this circled location the junction of I and J point. As I told you that we can easily then analyze that what is my profile in X direction, what is my profile in Z directions or what is its contour, how it looks like etc.

So, which means at these locations we are solving our governing equations. Now, if I again summarize the governing equations that we have learned or we have seen what we see is that for continuity Let me write it for a generic form which is say the compressible fluid in three dimension. So, compressible Newtonian fluid in three dimension. and in divergence form or the conservative form. So, if we do that the equation that will have





Finite Difference Method (FDM)
 $i = \text{specific enthalpy}$

Energy

Finite volume Method (FVM)

Continuity (Compressible Newtonian fluid in 3D)

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0$$

x-momentum

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \mathbf{u}) = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{grad } \mathbf{u}) + S_{m_x}$$

y-momentum

$$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v \mathbf{u}) = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{grad } \mathbf{v}) + S_{m_y}$$

z-momentum

$$\frac{\partial(\rho w)}{\partial t} + \text{div}(\rho w \mathbf{u}) = -\frac{\partial p}{\partial z} + \text{div}(\mu \text{grad } \mathbf{w}) + S_{m_z}$$

Energy

$$\frac{\partial(\rho i)}{\partial t} + \text{div}(\rho i \mathbf{u}) = -p \text{div } \mathbf{u} + \text{div}(k \text{grad } T) + \Phi + S_i$$

$p = p(\rho, T)$ & $i = i(\rho, T)$
 perfect gas $p = \rho R T$ & $i = C_v T$

So, basically you have to look into that So, the $P = f(\rho, t)$ for perfect gas this for perfect gas is $P = \rho R T$ and $I = C_v T$. And, for the ϕ what we have? It has quite a complicated expression this is called the distribution function. that has a form like this:



Distribution function

$$\phi = \mu \left\{ 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 \right\} + \lambda (\text{div } \mathbf{u})^2$$

Rate of increase of ϕ if fluid element

$$\frac{\partial(\rho \phi)}{\partial t} + \text{div}(\rho \phi \mathbf{u}) = \text{div}(\Gamma \text{grad } \phi) + S_\phi$$

Rate of increase of ϕ due to sources.

Net rate of flow of ϕ out of fluid element

Rate of increase of ϕ due to diffusion

Transport Equation for property ϕ

$\phi = T, u, v, w, i(T, \rho)$

So basically the distribution function has an expression which can be estimated, but this is here, this comes here. and rest of the cases that you have seen. So, this energy or the temperature have to be solved if we have the temperature inward in the case of the problem or else we have

this continuity and the momentum equations that you have to solve for only hydrodynamics. So, these equations are solved inside this computational domain.

at each and every location to find out the flow variables that is of our interest. Now, what we can see that there is a commonality in the form of the equations, the equations that we have starting from the continuity. What is that? What compactly we can write this thing as . So, compactly what we have written here this is the case of the diffusivity in upper case that we have written here instead of all the variables.

So, compactly it can be written like this. So, the first term for any variable ϕ that we can write this is the rate of increase of ϕ of a fluid element. The second term is the net rate of flow of ϕ out of the fluid element. So, we consider a fluid particle or fluid element the elemental analysis that you have seen in the fluid mechanics or in other classes. So, if we consider that so, this is this first term is considered that the rate of increase of this variable ϕ in the fluid of the fluid element.

The net rate of flow of ϕ that goes out of the fluid element, this is the rate of increase of ϕ due to diffusion and this is the source term the rate of increase of due to sources any sources that we have. So, this in short what we call as the transport equation for property ϕ . So, it actually highlights or it actually indicates various transport processes that is the rate of change, convective part that is flowing out of the fluid element, this is the convective part, the diffusive part and the source term.

So, the point is this generic expression from here to these expressions we can go if we consider $\phi = (1, u, v, w)$ and internal energy or the specific internal energy I or say that can be T or H whatever for the energy equation. And the diffusion coefficient we have to choose appropriately in those cases what would be my diffusion coefficient and the source terms. and if we do that then you will see that we eventually land up with the continuity equations for ϕ is 1, for ϕ is u we have the x momentum, for v we have the y momentum, this is w for the z momentum, i for the energy equation.

So, this helps us in having a compact form or the generic expression of the transport equation that is the cornerstone or the fundamentals from where we will begin our understanding of the different methods and particularly the finite volume method. So, in finite volume method let me tell you what is done first of all. Like here in the finite difference method you look into this IJ cross section and find out the T_{ij} or P_{ij} at these locations by having it discretized either by central differencing backward or forward. The first thing in this finite volume method that differentiates it from the other computational techniques in CFD is that we this governing equation this transport equation we do the control volume integration at first.

Which means we consider a control volume around each and every such nodal points. We consider a imaginary control volume and in this control volume we integrate this transport equation or the governing equations. So, in finite volume method the first step the first step is that the control volume or we will say Cv the control volume integration. So, this is the first step and that results I mean the whatever that comes is that conservation relevant property for each finite cell.

The image shows handwritten notes on a white background. At the top left, 'FVM' is circled in red. Below it, '1st step:' is written in red, followed by 'Control volume (Cv) integration' and 'conservation of relevant property for each finite cell.' in red. In the top right corner, there are two logos: the Indian Institute of Technology (IIT) logo and the NPTEL logo. The main part of the notes contains mathematical equations in blue ink. The first equation is
$$\int_{Cv} \frac{\partial(\rho\phi)}{\partial t} dV + \int_{Cv} \text{div}(\rho\phi\mathbf{u}) dV = \int_{Cv} \text{div}(\Gamma \text{grad}\phi) + \int_{Cv} S_p dV$$
 with arrows pointing to the terms. Below this is 'Gauss's Divergence Theorem' underlined. The second equation is
$$\int_{Cv} \text{div}(\mathbf{a}) dV = \int_A \mathbf{n} \cdot \mathbf{a}$$
 with a note: ' $\mathbf{n} \cdot \mathbf{a}$ = component of vector \mathbf{a} in the direction of vector normal to the surface element dA '. A dark blue rounded rectangle is partially visible on the right side of the page.

Whatever we get from here by having this control volume integration of the governing equations, the resulting statement gives us the conservation of relevant property for each finite cell. So, we will have a integrate in I mean integration form or the say if we do that the previous expression if we integrate it over the control volume this thing what it forms a three-dimensional form is that what we do in this case is that over the control volume. So, the divergence of grand phi control volume and the source term the control volume over the control volume.

So, the integration of this governing equation over a three-dimensional control volume is the first step or the key step that differentiates this finite volume method from the other technique that is the finite difference method or the finite element method that I will briefly discuss in the next class from this technique. Now, the point is that we have these are all the volume integration. So, this volume integration particularly of this convective term and say this diffusive term, we actually write those in terms of the entire bounding surface of the control volume by considering Gaussian I mean Gauss divergence theorem. So, Gauss divergence theorem what it tells?

It helps us that if I have a vector A then it can be interpreted $A \cdot n$. So, basically this term is the component vector is a component of a vector A in the direction of vector the normal to the surface element dA . So, this is basically the component of say vector A in the direction of normal vector which is the vector normal to the surface element dA . So, what we do?

We convert with the help of Gauss divergence theorem a volume integral to surface integral and then this is summed up over the entire domain ok. So, then what happens? This volume integral is converted to area integral and through each area, then this term is approximated by the proper discretization scheme. So, we will go into these intricate details of all the things that what is discretization, how that happens and what is the utility of that discretization, etc., in the forthcoming classes. So, the basic thing that I wanted to tell you with the finite volume method here is that we consider a control volume an imaginary control volume around a grid point, grid point means now you understand these junctions of the cells

and we integrate our governing equations in that control volume. And then the next big step is that the conversion of volume integral to surface integral to and that with the help of Gauss divergence theorem and then the area integrals are further approximated with the proper discretization scheme and further simplified. That helps us in achieving this partial differential equation to a set of algebraic equation. So with this overview I stop here today and I hope to see you in the next class. Thank you.